Thin Films Division
Fachverband Dünne Schichten (DS)

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Overview of Invited Talks and Sessions

(lecture rooms H 0111 and H 2032; Poster E)

Gaede Prize

DS 18.1	Tue	13:30–14:00	HE 101	**Material Design by Atomic Layer Deposition** — •Mato Knez

Invited Talks

DS 3.1	Mon	15:00–15:30	H 0111	**Focused electron beam lithography in the 1-10 nanometer range.** — •Cornelis Wouter Hagen
DS 4.1	Mon	9:30–10:00	H 2032	**The role of defects in thin film solar cells** — •Thomas Unold
DS 7.1	Mon	15:00–15:30	H 2032	**Three-dimensional hybrid organic/inorganic heterojunctions based on rolled-up nanomembranes** — •Carlos Cesar Bof Bufon, Dominic J. Thurmer, Christoph Deneke, Oliver G. Schmidt
DS 13.1	Tue	9:30–10:00	H 0111	**Free electrons for building nanodevices** — •Ivo Utke
DS 22.1	Wed	15:00–15:30	H 0111	**Trends in Atomic Layer Deposition** — •Helmut Baumgart
DS 23.1	Wed	17:30–18:00	H 0111	**Functional complex oxide materials by atomic layer deposition** — •Maarit Karppinen
DS 32.1	Thu	9:30–10:00	H 2032	**Tuning thermoelectric properties of oxides by the interplay between spin/charge/lattice** — •Sylvie Hebert
DS 32.2	Thu	10:00–10:30	H 2032	**Oxide materials for high-temperature thermoelectrics** — •Michitaka Ohtaki

Topical Talks

DS 3.2	Mon	15:30–16:00	H 0111	**Fabrication of 1 nm thick Carbon Nanomembranes using FEBIP** — •Armin Gölzhäuser
DS 3.3	Mon	16:00–16:30	H 0111	**Towards a microscopic understanding of the electron beam induced deposition of tungsten** — •Harald Jeschke, Kaliappan Muthukumar, Ingo Opahle, Juan Shen, Roser Valentí
DS 13.2	Tue	10:00–10:30	H 0111	**From electronic correlations to strain sensing: Nanongranular metals and their applications** — •Christian Schwalb, Marcel Winhold, Fabrizio Porrati, Roland Sachser, Michael Huth
DS 13.3	Tue	10:30–11:00	H 0111	**Tailored cobalt nanostructures by FEBID** — •José M. de Teresa, Rosa Córdoba, Luis Serrano-Ramón, Amalio Fernández-Pacheco, Ricardo Ibarra
DS 22.2	Wed	15:30–16:00	H 0111	**Energy conversion devices made using ALD** — •Julien Bachmann
DS 22.3	Wed	16:00–16:30	H 0111	**Role of substrate chemistry in ALD revealed by in-situ techniques** — •Massimo Tallarida, Marcel Michling, Chittaranjan Das, Daniel Friedrich, Matthias Städter, Dieter Schmeisser

DS 23.2	Wed	18:00–18:30	H 0111	**Uniform ZnMnO and ZnCoO films grown by Atomic Layer Deposition** — •Marek Godlewski, Małgorzata Łukasiewicz, Aleksandra Wójcik-Głodowska, Elzbieta Guziewicz, Bartłomiej Witkowski
DS 23.3	Wed	18:30–19:00	H 0111	**Atomic layer deposition of oxide thin films for non-volatile memory applications** — •Susanne Hoffmann-Eifert
DS 32.3	Thu	10:30–11:00	H 2032	**Investigations of the thermal conductivity of thermoelectric thin films and nanostructures** — •Friedemann Voelklein, Heiko Reith, Matthias Schmitt, Daniel Huzel
DS 33.1	Thu	11:15–11:45	H 2032	**Calculation of thermoelectric properties of nanostructured semiconductors** — •Peter Kratzer, Gregor Fiedler
DS 42.1	Fri	11:30–12:00	H 2032	**Employing laterally nanostructured ZnO-based thin-films as model systems for studying interface effects in themoelectrics** — •Peter J. Klar
DS 43.1	Fri	13:30–14:00	H 2032	**Potential Seebeck Microprobe: Considerations on Accuracy and Spatial Resolution** — •Pawel Ziolkowski, Gregor Oppitz, Gabriele Karpinski, Eckhard Müller

Invited talks of the joint symposium SYTM

See SYTM for the full program of the symposium.

SYTM 1.1	Mon	9:30–10:00	H 0105	**Thermally Assisted Magnetic Recording at 620 Gb/in^2 using Granular L1$_0$ FeCuPtAg-X Media** — •D. Weller, O. Mosendz, S. Pisana, T. Santos, G. Parker, J. Reiner, B. C. Stipe
SYTM 1.2	Mon	10:00–10:30	H 0105	**Large-area hard magnetic L1$_0$-FePt and composite L1$_0$-FePt based nanopatterns** — •Dagmar Goll, Thomas Bublat
SYTM 1.3	Mon	10:30–11:00	H 0105	**Electric field control of magnetic exchange coupling in FePt / Fe-O thin fims** — •Karin Leistner
SYTM 1.4	Mon	11:00–11:30	H 0105	**FePt-based exchange coupled composite media** — •Manfred Albrecht
SYTM 1.5	Mon	11:30–12:00	H 0105	**Optimization of FePt films for recording applications by micromagnetic modeling** — •Josef Fidler, Jehyun Lee, Barbara Dymerska, Dieter Suess

Invited talks of the joint symposium SYTI

See SYTI for the full program of the symposium.

SYTI 1.1	Tue	9:30–10:00	H 0105	**Search for Majorana fermions in topological insulators** — •Carlo Beenakker
SYTI 1.2	Tue	10:00–10:30	H 0105	**Cooper Pairs in Topological Insulator Bi$_2$Se$_3$ Thin Films Induced by Proximity Effect** — •Jinfeng Jia
SYTI 1.3	Tue	10:30–11:00	H 0105	**Gate tunable normal and superconducting transport through a 3D topological insulator** — •Alberto Morpurgo
SYTI 1.4	Tue	11:00–11:30	H 0105	**Weyl Metal States and Surface Fermi Arcs in Iridates** — •Sergey Savrasov
SYTI 1.5	Tue	11:30–12:00	H 0105	**Engineering a Room-Temperature Quantum Spin Hall State in Graphene via Adatom Deposition** — •Marcel Franz

Invited talks of the joint symposium SYRS

See SYRS for the full program of the symposium.

SYRS 1.1	Thu	15:00–15:30	H 0105	**Redox-based resistive memories - recent progress** — •Rainer Waser
SYRS 1.2	Thu	15:30–16:00	H 0105	**Electric Formation of Metal/SrTiO$_3$ Junctions and its Correlation to Multi-Dimensional Defects** — •Dirk C. Meyer, Hartmut Stöcker, Juliane Hanzig, Florian Hanzig, Matthias Zschornak, Barbara Abendroth, Sibylle Gemming
SYRS 1.3	Thu	16:00–16:30	H 0105	**The Connecting between the Properties of Memristive Material Systems and Application Requirements** — •Thomas Mikolajick, Stefan Slesazeck, Hannes Mehne

SYRS 1.4	Thu	16:30–17:00	H 0105	**Mechanism of resistive switching in bipolar transition metal oxides** — •Marcelo Rozenberg
SYRS 1.5	Thu	17:00–17:30	H 0105	**Resistive switching memories: Mechanisms, modeling and scaling** — •Daniele Ielmini

Sessions

DS 1.1–1.11	Mon	9:30–12:15	H 0111	**Layer properties: electrical, optical, and mechanical properties**
DS 2.1–2.4	Mon	12:30–13:30	H 0111	**Nanoengineered thin films**
DS 3.1–3.5	Mon	15:00–17:00	H 0111	**Focused electron beam induced processing for the fabrication of nanostructures I (focused session, jointly with O – Organizers: Huth, Marbach)**
DS 4.1–4.1	Mon	9:30–10:00	H 2032	**Thin film photovoltaics**
DS 5.1–5.4	Mon	10:00–11:00	H 2032	**Thin film photovoltaics: CIGSe + CdTe**
DS 6.1–6.6	Mon	11:15–12:45	H 2032	**Thin film photovoltaics: CIGSe + processing**
DS 7.1–7.4	Mon	15:00–16:15	H 2032	**Organic electronics and photovoltaics I (jointly with CPP, HL, O)**
DS 8.1–8.6	Mon	16:30–18:00	H 2032	**Thin film photovoltaics: oxides and nanostructures**
DS 9.1–9.11	Mon	9:30–12:45	EB 301	**Multiferroics I: Junctions and thin films / Magnetoelectric coupling (jointly with MA, DF, KR, TT)**
DS 10.1–10.12	Mon	15:00–18:30	EB 301	**Multiferroics II: Hexagonal manganites / Incommensurate multiferroics (jointly with MA, DF, KR, TT)**
DS 11.1–11.4	Mon	16:45–18:00	H 3005	**Multiferroics: Matter at low temperature (jointly with MA, DF, TT, KR)**
DS 12.1–12.5	Mon	15:00–17:45	EB 202	**FePt Nanoparticles (jointly with MA, MM – Organizer: Farle)**
DS 13.1–13.5	Tue	9:30–11:30	H 0111	**Focused electron beam induced processing for the fabrication of nanostructures II (focused session, jointly with O – Organizers: Huth, Marbach)**
DS 14.1–14.4	Tue	11:45–12:45	H 0111	**Ion irradiation effects**
DS 15.1–15.7	Tue	9:30–11:15	H 2032	**Organic electronics and photovoltaics: simulations and optics I (jointly with CPP, HL, O)**
DS 16.1–16.6	Tue	11:30–13:00	H 2032	**Organic electronics and photovoltaics: simulations and optics II (jointly with CPP, HL, O)**
DS 17.1–17.12	Tue	9:30–12:45	EB 301	**Multiferroics III: Strain / New routes towards multiferroicity (jointly with MA, DF, KR, TT)**
DS 18.1–18.1	Tue	13:30–14:00	HE 101	**Gaede Prize talk (Mato Knez)**
DS 19.1–19.90	Tue	12:15–15:15	Poster A	**Poster I: Multiferroics (jointly with MA, DF, KR, TT), Spins in organic materials (jointly with MA), FePt Nanoparticles (jointly with MA, MM)**
DS 20.1–20.8	Wed	9:30–11:30	H 0111	**Application of thin films**
DS 21.1–21.8	Wed	11:45–13:45	H 0111	**Micro- and nanopatterning (jointly with O)**
DS 22.1–22.6	Wed	15:00–17:15	H 0111	**Trends in atomic layer deposition I (Focused session – Organizer: Nielsch)**
DS 23.1–23.6	Wed	17:30–19:45	H 0111	**Trends in atomic layer deposition II (Focused session – Organizer: Nielsch)**
DS 24.1–24.7	Wed	9:30–11:15	H 2032	**Organic electronics and photovoltaics: electronic properties I (jointly with CPP, HL, O)**
DS 25.1–25.6	Wed	11:30–13:00	H 2032	**Organic electronics and photovoltaics: electronic properties II (jointly with CPP, HL, O)**
DS 26.1–26.6	Wed	15:00–16:30	H 2032	**Thin film characterization: structure analysis and composition (Ion assisted methods and analysis)**
DS 27.1–27.4	Wed	16:30–17:30	H 2032	**Thin film characterization: structure analysis and composition (post growth analysis XRD, etc..)**
DS 28.1–28.8	Wed	17:45–19:45	H 2032	**Thin film characterization: structure analysis and composition (Spectroscopy)**
DS 29.1–29.6	Wed	9:30–11:30	EB 407	**High-k and low-k dielectrics (joint session with DF)**
DS 30.1–30.6	Thu	9:30–11:00	H 0111	**Thin film characterization: structure analysis and composition (TEM, LEED, PAS)**
DS 31.1–31.7	Thu	11:15–13:00	H 0111	**Organic thin films I**
DS 32.1–32.3	Thu	9:30–11:00	H 2032	**Thermoelectric materials I (Focused session – Organizers: Meyer, Heiliger)**

DS 33.1–33.5	Thu	11:15–12:45	H 2032	**Thermoelectric materials II: Reduced dimensionality (Focused session – Organizers: Meyer, Heiliger)**
DS 34.1–34.10	Thu	15:00–17:30	H 2032	**Organic thin films II: Interface spectroscopy**
DS 35.1–35.7	Thu	17:45–19:30	H 2032	**Organic thin films III: Monolayers and crystals**
DS 36.1–36.9	Thu	16:45–19:00	H 1012	**Spins in Organic Materials (jointly with MA)**
DS 37.1–37.47	Thu	15:00–17:00	Poster E	**Poster II: Focused electron beam induced processing for the fabrication of nanostructures (focused session, jointly with O); Nanoengineered thin films; Layer properties: electrical, optical, and mechanical properties; Thin film characterization: structure analysis and composition (XRD, TEM, XPS, SIMS, RBS,..); Application of thin films**
DS 38.1–38.49	Thu	17:30–19:00	Poster E	**Poster III: Resistive switching (jointly with DF, KR, HL); Thermoelectric materials (Focused session); Micro- and nanopatterning (jointly with O); Ion irradiation effects**
DS 39.1–39.5	Fri	9:30–10:45	H 0111	**Resistive switching I (jointly with DF, KR, HL)**
DS 40.1–40.6	Fri	11:00–12:30	H 0111	**Resistive switching II (jointly with DF, KR, HL)**
DS 41.1–41.7	Fri	9:30–11:15	H 2032	**Thermoelectric materials III: Heterostructures (Focused session – Organizers: Meyer, Heiliger)**
DS 42.1–42.5	Fri	11:30–13:00	H 2032	**Thermoelectric materials IV: Glass, sintered materials (Focused session – Organizers: Meyer, Heiliger)**
DS 43.1–43.9	Fri	13:30–16:00	H 2032	**Thermoelectric materials V: Bulk materials (Focused session – Organizers: Meyer, Heiliger)**
DS 44.1–44.60	Fri	9:30–12:00	Poster E	**Poster IV: Thin film photovoltaics; Organic electronics and photovoltaics (jointly with CPP, HL, O); Organic thin films; Trends in atomic layer deposition (Focused session)**

Annual General Meeting of the Thin Films Division

Thursday 19:00–20:00 Raum MA 144

Annual General Meeting of the German Vacuum Society (DVG)

Monday 17:25–18:00 Raum H 0111

DS 1: Layer properties: electrical, optical, and mechanical properties

Time: Monday 9:30–12:15 Location: H 0111

DS 1.1 Mon 9:30 H 0111

Emission of x-rays produced by peeling adhesive tape in vacuum — •Daniel Krämer, Dirk Lützenkirchen-Hecht, and Ronald Frahm — Bergische Universität Wuppertal

Adhesive tapes can produce x-rays with energies up to about 100 keV when being peeled in a vacuum. The spectra of the emitted photons were measured with an Amptek Si-PIN-Detector and their dependence on several parameters like type of adhesive tape, gas pressure and peeling speed was investigated in detail.

The mechanism for x-ray emission is: Charge separation at the peeling vertex and build-up of an electric field with an accelerating potential up to typically 100 kV, acceleration of free electrons of the residual gas, and x-ray photon production by bremsstrahlung on the tape, thus leading to continuous spectra without characteristic emission peaks. A maximum count rate was found at $p_{Max} = 10^{-2}$ mbar. Below p_{Max} fewer photons are produced because of less molecules in the gas which could be ionized and be a source for free electrons. Above p_{Max} the separated charges are neutralized by ions, resulting in a decreasing count rate that vanishes at ∼1 mbar.

DS 1.2 Mon 9:45 H 0111

Characterizing periodic gratings and metamaterials using spectroscopic ellipsometry — •Thomas Oates[1], Babak Dastmalchi[2], Goran Isic[3], Iris Bergmair[4], Kurt Hingerl[2], and Karsten Hinrichs[1] — [1]Leibniz Institut für Analytische Wissenschaften - ISAS - e.V., 12489 Berlin — [2]Johannes Kepler University, Linz — [3]Institute of Physics Belgrade, Belgrade — [4]PROFACTOR GmbH, Steyr-Gleink, Austria

The recent availability of relatively large area Vis-NIR metamaterials (cm2) now allows accurate optical measurements by well established plane-wave reflection and transmission techniques. In this work we use spectroscopic ellipsometry (SE) to characterize subwavelength periodic gratings and fishnet metamaterials with artificial magnetic resonances. The materials are fabricated by nanoimprint lithography (NIL). Three samples are investigated, all with period of 365 nm; a single layer square silver grating on silicon; a 3 layer silver/SiO2/silver grating on silicon; and an identical 3 layer grating on glass. VASE data is measured from 245 - 1700 nm. We will show that a comparative study of the same metamaterials on different substrates assists in mode identification, but changes the effective material parameters. Any ellipsometric investigation necessarily requires consideration of the angular-dependent optical response. We will show that this aids in the identification of the physical origin of the optical modes. We will conclude by exploring the potential of standard ellipsometric analysis to identify magnetic-type resonances and negative refraction.

DS 1.3 Mon 10:00 H 0111

In Situ-Controlled Oxidation of High-Speed Surface Emitting Lasers and Single-Photon Sources — •Gunter Larisch, Werner Hofmann, and Dieter Bimberg — Institute of Solid State Physics & Center of Nanophotonics, Technische Universität Berlin

Precise control of the oxidation progress is needed for the production of the apertures of oxid-confined VCSELs and single photon sources [1]. So far, the size of the aperture was determined by ex situ measuring of the electrical resistance of oxidized test samples [2]. This method proved to be very time consuming and not reliable. Therefore, an optical in situ method was developed that will be presented here. Problems such as vibration-free mounting of the microscope (used for imaging) and high-contrast fluoroscopy of the top DBR with a suitable light source are presented and illustrated with examples. Test structures adapted to the new method are introduced and discussed. The improved process of oxidation control allows the visualization of the progress of oxidation during the oxidation. This enables a significant reduction of processing time and cost. In addition, a higher yield of precision components processed by increasing the processing accuracy is achieved.

[1] Mutig, A. et al.: ”Progress on High-Speed 980 nm VCSELs for Short-Reach Optical Interconnects,” IEEE J. Sel. Top. Quantum Electron., 2011. [2] Choquette, K. et al.: ”Advances in Selective Wet Oxidation of AlGaAs Alloys,” IEEE J. Sel. Top. Quantum Electron., 1997.

DS 1.4 Mon 10:15 H 0111

Picosecond ultrasound spectroscopy on NiTi and NiMnGa thin film shape memory alloys — •Jan Mayer, Mike Hettich, Martin Schubert, and Thomas Dekorsy — Department of Physics, University of Konstanz, D-78457 Konstanz

Shape memory alloys are characterized by a reversible and diffusionless structural transition from a high-temperature austenitic phase to a low-temperature martensitic phase, induced by stress or temperature [1]. The material systems we investigate are NiTi and Ni_2MnGa thin films of 110 nm and 150 nm thickness, respectivly. Ni_2MnGa is ferromagnetic and has a great potential for applications due to the magnetic-field-induced shape memory effect with reversible strains of up to 9 % [2]. The films are investigated using asynchronous optical sampling (ASOPS). ASOPS is a novel technique for ultrafast time domain spectroscopy [3] and enables optical pump-probe measurements with femtosecond resolution. By measuring the change in reflectivity the vibrational dynamics of the samples are studied. The obtained coherent phonon spectra allow to study the structural phase transition in alloys of various stoichiometry. Due to the strong dependence of the transition temperature on composition [4], it is possible to investigate both phases at room temperature. The vicinity of the phase transition is analyzed by heating and cooling the samples.

[1] Martynov and Kokorin, J. Phys. III France 2, 739-749 (1992)
[2] Sozinov et al., Appl. Phys. Lett, 80, 1746 (2002)
[3] Bartels et al., Rew. Sci. Instr. 78, 035107 (2007)
[4] Chernenko et al., Acta Materialia 50, 53-60 (2002)

DS 1.5 Mon 10:30 H 0111

Influence of ion beam and geometrical parameters on properties of Si thin films grown by Ar ion beam sputtering — •Carsten Bundesmann, René Feder, and Horst Neumann — Leibniz-Institut für Oberflächenmodifizierung e.V., Permoserstr. 15, 04318 Leipzig, Germany

Ion beam sputtering (IBS) offers, in contrast to other physical vapour deposition techniques, such as magnetron sputtering or electron beam evaporation, the opportunity to change the properties of the layer forming particles (sputtered and scattered particles) by varying ion beam parameters (ion species, ion energy) and geometrical parameters (ion incidence angle, emission angle). Consequently, these effects can be utilized to tailor thin film properties [1].

The goal is to study systematically the correlations between the primary and secondary parameters and, at last, the effects on the properties of Si thin films, such as optical properties, stress, surface topography and composition. First experimental results are presented for Ar-ion sputtering of Si.

Financial support by DFG within project BU2625/1-1 is gratefully acknowledged.

[1] C. Bundesmann, I.-M. Eichentopf, S. Mändl, and H. Neumann; Thin Solid Films 516, 8604-8608 (2008).

DS 1.6 Mon 10:45 H 0111

Stress induced buckling in laser deposited polymer/metal-nanocomposites — •Susanne Schlenkrich, Felix Schlenkrich, Inga Knorr, Cynthia Volkert, and Hans-Ulrich Krebs — Institut für Materialphysik, Universität Göttingen, Friedrich Hund Platz1, 37077 Göttingen

Multilayer thin films with dimensions at the nanometer scale represent a technologically important class of materials where the interface and size effects play an important role. Interestingly, when polymer/metal multilayers are deposited by pulsed laser deposition (248nm, 30ns pulse duration) one observes stress induced buckling of the metal layers in case of polymers with low young*s modulus. Compressive stress in the metal layers is induced due to the high energy of the deposited ions. The beam theory can be used to describe the relation between the wavelength of the buckles and the properties of both film components. This understanding makes it possible to use the wavelength as a measurement for the mechanical properties of the film components. Furthermore, the wavelength can be tuned by changing/adjusting the layer thicknesses of both components. In this contribution buckling effects of these periodic structures are discussed and a new measurement technique to characterize the mechanical properties of extremely soft and thin films will be presented.

DS 1.7 Mon 11:00 H 0111

Role of surfactants and defect generation in CdSe quantum dot layers for separation of photo-generated charge carriers — •Elisabeth Zillner, Steffen Fengler, and Thomas Dittrich — Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin

Thin layers of CdSe quantum dots (QDs) were prepared by dip coating of ITO substrates in QD suspension. Surface modification of QDs was done by surfactant exchange in suspensions and layers. Interparticle distances between QDs in layers were monitored by transmission electron microscopy. Absorption and photoluminescence spectra showed an increase in defect states by proceeding surfactant exchange. The charge separation in the CdSe QD layers was strongly influenced by the surface modification. Both spectral and time dependent SPV showed a high dependency on surfactant exchange. Results are discussed on basis of asymmetric trapping at defect states within the first monolayer of QDs at the interface during initial charge separation.

DS 1.8 Mon 11:15 H 0111

Temperature dependent relaxation of separated charge carriers at CdSe-QD / ITO interfaces — •Steffen Fengler, Elisabeth Zillner, and Thomas Dittrich — Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin

One and 5 monolayers of CdSe quantum dots with fixed diameter were deposited on ITO substrates by dip coating and investigated by transient surface photovoltage (SPV) at temperatures up to 250°C. The SPV transients were excited with laser pulses (duration time 5 ns) and measured in vacuum at times up to 0.2 s. SPV transients arose within the laser pulse and could be well fitted with one (one monolayer of CdSe-QDs) or two (5 monolayers of CdSe-QDs) stretched exponentials. The parameters of the stretched exponentials changed depending on defect generation during heating as well as on thermal activation processes during heating and cooling. During cooling, the mean relaxation times of both processes were thermally activated with an activation energy of 0.9 eV. Defect generation strongly affected charge separation and relaxation within the first monolayer at the CdSe-QD / ITO interface and between the first monolayer of CdSe-QDs and following CdSe-QD layers.

DS 1.9 Mon 11:30 H 0111

Electrical conductivity of CNT modified surfaces: Theoretical model — •Fedor Semeriyanov, Alexander Chervanyov, and Gert Heinrich — Leibniz Institute of Polymer Research Dresden, Dresden, Germany

We use a combination of the Monte Carlo simulations and self-consistent field theory in order to calculate electrical conductivity of non-uniform layer of carbon nanotubes (CNT) deposited onto a glass surface. As a first step, we determine density structure of this CNT layer by using the self-consistent field theory with the effect of CNT stiffness taken into account. The developed method makes it possible to study the dependence of the CNT layer density structure (including relative amounts of loops, tails and trains) on the affinity of the substrate surface for CNT's. Next, we incorporate the obtained density structure into the Monte Carlo simulations of the electrical conductivity of CNT modified surface. As a final step, we obtain the relation between the number of CNT-CNT contacts in the film with depth dependent density and its dc conductivity. This work is supported by DFG SPP1369.

DS 1.10 Mon 11:45 H 0111

Electromigration in Ag Nanowires with a Controlled Single Grain Boundary — •Simon Sindermann, Michael Horn-von Hoegen, Guenter Dumpich, and Frank-J. Meyer zu Heringdorf — Faculty of Physics and Center for Nanointegration Duisburg-Essen (CeNIDE) University Duisburg-Essen

The combination of epitaxial growth and focused ion beam (FIB) milling enables us to fabricate single- and bi-crystalline electromigration (EM) test structures. Depending on the growth parameters, epitaxial Ag islands on a Si(111) surface can consist of a composition of two areas of different lattice orientation [1]. Such islands are used to be structured into Ag nanowires. For electrical isolation, a silicon on insulator (SOI) substrate is used, the device layer of which is cut with FIB [2]. To monitor the EM process, an image sequence of the Ag nanowires during electrical stressing is captured *in-situ* with a scanning electron microscope (SEM). We are able to identify nm-sized voids and hillocks, and can follow them from nucleation up to the failure of the test structure. Amongst stationary (growing and shrinking) voids, some voids were found to propagate along the nanowire and merge with other voids. The shape of voids is strongly influenced by the crystal lattice symmetry [3], especially for voids overcoming the grain boundary. A correlation of the point of failure and the position of the grain boundary will be discussed.

[1] D. Wall et al. IBM J. Res. and Dev., **55** (2011) 9
[2] S. Sindermann et al. Rev. Sci. Instrum., (2011) in revision
[3] A. Latz et al. Phys. Rev. B, (2011) in revision

DS 1.11 Mon 12:00 H 0111

Simulation of electromigration effects on voids in monocrystalline Ag films — •Andreas Latz and Dietrich E. Wolf — Physics, University Duisburg-Essen, Duisburg, Deutschland

Due to the decreasing width and thickness of interconnects with each integrated circuit generation, electromigration phenomena in the different monocrystalline parts of the interconnects become of increasing interest. We investigate how voids penetrating a monocrystalline silver film are affected by electromigration. Based on the kinetic Monte Carlo method, we developed a three dimensional, atomistic simulation model that is fast enough to access the desired time scales to investigate electromigration phenomena on an atomistic scale. A clear dependency between the strongly facetted non-equilibrium shape of the voids and the crystallographic orientation of the film is found, which is in accordance with experimental results on bicrystalline silver wires. This work has been supported by German Science Foundation within SFB 616: Energy Dissipation at Surfaces.

DS 2: Nanoengineered thin films

Time: Monday 12:30–13:30 Location: H 0111

DS 2.1 Mon 12:30 H 0111

Growth of strained, ferroelectric NaNbO3 thin films by pulsed laser deposition — •Jan Sellmann, Jutta Schwarzkopf, Andreas Duk, Albert Kwasniewski, Martin Schmidbauer, and Roberto Fornari — IKZ, Berlin, Deutschland

Due to its promising ferro-/piezoelectric properties and high Curie temperature NaNbO3 has attracted much attention. In contrast to bulk crystals, thin epitaxial films may incorporate and maintain a certain compressive or tensile lattice strain, depending on the used substrate/film combination. This deformation of the crystal lattice is known to strongly influence the ferroelectric properties of perovskites. In the case of NaNbO3 compressive strain is achieved in films deposited on NdGaO3 and SrTiO3 substrates while deposition on DyScO3 and TbScO3 leads to tensile in-plane strain. In order to characterize and practically apply the ferroelectric films, it is necessary to embed them in a capacitor structure for which we use pseudomorphically grown SrRuO3 as bottom electrodes. We report on the deposition of SrRuO3 and NaNbO3 single layers on SrTiO3, DyScO3, TbScO3 and NbGaO3 substrates by means of pulsed laser deposition. By adjusting the substrate temperature, the oxygen partial pressure and the laser frequency we have successfully deposited smooth, strained, single phase NaNbO3 thin films. Investigations of the films by atomic force microscopy and high resolution X-ray diffraction reveal the dependence of the surface morphology and the incorporated lattice strain on the deposition parameters and the lattice mismatch, respectively. All films exhibit piezoelectric properties, as proven by piezoresponse force microscopy.

DS 2.2 Mon 12:45 H 0111

Local control of molecular glass wrinkling by designed magnetic stray fields — •Henning Huckfeldt, Holger Klein, Florian Ahrend, Thomas Fuhrmann-Lieker, and Arno Ehresmann — Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel

An IrMn/CoFe exchange bias substrate has been patterned into artificial parallel stripe magnetic domains by ion bombardment induced magnetic patterning without topographic elevations. PMMA and CoFe were subsequently deposited on top of the exchange bias layer system. Thermal treatment induced internal stress in the viscoelastic/metallic layer combination, which relaxes by wrinkling.

The interaction of the local stray fields emerging from the domain walls between the artificial domains with the CoFe layer on top of the organic PMMA layer, leads to a directional wrinkling parallel and perpendicular to the magnetic domain walls of the substrate. A qualitative model has been developed to explain the observed local alignment of the wrinkles.

DS 2.3 Mon 13:00 H 0111

Guiding block copolymers into sequenced patterns via inverted terrace formation — •Sungjune Park[1], Larisa Tsarkova[1], Stephanie Hiltl[1], Stefan Roitsch[2], Joachim Mayer[2], and Alexander Böker[1] — [1]DWI an der RWTH Aachen e. V., Lehrstuhl für Makromolekulare Materialien und Oberflächen, RWTH Aachen University, D-52056 Aachen, Germany. — [2]Gemeinschaftslabor für Elektronenmikroskopie, RWTH Aachen University, Ahornstr. 55, D-52074 Aachen, Germany.

We present a facile one-step route to achieve sequenced patterns from microphase separated structures in asymmetric polystyrene-b-polybutadiene (PS-b-PB) diblock copolymer films. For the guided block copolymer assembly we used topographically corrugated SiCN ceramic substrates which were fabricated by a facile replication process using non-lithographic PDMS masters. Homogeneous block copolymer films have been floated onto the corrugated substrate without significant changes to the corrugations topography. During thermal annealing of PS-b-PB diblock copolymer, the material transport was guided by a wrinkled substrate to form regular modulations in the film thickness. As a consequence of the thickness-dependent morphological behavior, the film surface appears as sequenced patterns of alternative microphase separated structures. The ordering process is attributed to a newly observed phenomenon of inverted terrace formation which is induced by the corrugations on substrate, so that the resulting surface patterns are free from the surface relief structures within macroscopically large areas.

DS 2.4 Mon 13:15 H 0111

Ultraschall unterstützte Deposition von kolloidalen Kristallen — •Sabine Wollmann, Hubert Krenner, and Achim Wixforth — Universität Augsburg, Universitätsstraße 1, 86159 Augsburg

Colloidal crystals are a versatile system to realize templates and masks for etching and deposition processes or to realize photonic band gap materials. We present investigations on ultrasonic assisted deposition of colloidal crystals employing surface acoustic waves. For this, droplets of an aqueous solution of polystyrene beads with diameters ranging from 0,5 μm to 3 μm are drying under surface acoustic wave agitation. The beads show a periodical arrangement after the water is evaporated. By means of optical diffraction we study in-situ the resulting colloidal films for different colloid concentrations, evaporations rate of the solvent and the pulse width and amplitude of the surface acoustic wave. We present first results on an improved formation of ordered domains and a control of the nucleation site within the droplet under acoustic agitation.

DS 3: Focused electron beam induced processing for the fabrication of nanostructures I (focused session, jointly with O – Organizers: Huth, Marbach)

Time: Monday 15:00–17:00 Location: H 0111

Invited Talk DS 3.1 Mon 15:00 H 0111

Focused electron beam lithography in the 1-10 nanometer range. — •Cornelis Wouter Hagen — Delft University of Technology, Charged particle Optics Group, Lorentzweg 1, 2628CJ Delft, The Netherlands

What if one would like to make something really small, for instance something consisting of only a few thousand atoms, then how would one do it? And what if one would also like to have control over its final shape and its composition? How could that be achieved? The answer is: with focused electron beam induced processing (FEBIP), because an electron beam can be focused down to a tiny sub-nanometer spot. When such a beam is scanned over a substrate with an adsorbed monolayer of precursor molecules, the molecules are dissociated. Only at the positions where the electron beam has been, solid fragments are left behind at the surface, forming a high-resolution pattern. I will review what we have learned about this process, focusing on the superb resolution, and the fundamentals of the dissociation process. To turn FEBIP into a user-friendly lithography technique, dedicated instruments will have to be developed. I will sketch the route that we envision towards such instrumentation.

Topical Talk DS 3.2 Mon 15:30 H 0111

Fabrication of 1 nm thick Carbon Nanomembranes using FEBIP — •Armin Gölzhäuser — Universität Bielefeld, Bielefeld, Germany

We employ a combination of molecular self-assembly and focused electron beam induced processing (FEBIP) to fabricate only 1 nm thick, but mechanically stable carbon nanomembranes (CNM). Self-Assembled Monolayers (SAMs) of amphiphilic biphenylthiols are formed on gold surfaces and then exposed to electron beams that lead to a C-H cleavage. The dehydrogenation is followed by a lateral cross-linking between neighboring molecules [1]. The resulting two-dimensional film can be released from the surface, forming a mechanically stable CNM with the thickness of the original monolayer, i.e. 1 nm [2]. We have developed procedures for the handling of CNMs, i.e. to transfer them onto arbitrary surfaces and to prepare them as free-standing films. It will be shown that free-standing CNMs can be used as supports for transmission electrons microscopy [3]. Free-standing CNMs also can act as substrates for a FEBIP fabrication of very small metal clusters [4].

[1] A. Turchanin et al. Langmuir 25, 7342 (2009).
[2] A. Turchanin et al. Adv. Mater. 21, 1233 (2009).
[3] C.T. Nottbohm et al. Ultramicroscopy 108, 885 (2008).
[4] W.F. van Dorp et al. Nanotechnology 22, 115303 (2011).

Topical Talk DS 3.3 Mon 16:00 H 0111

Towards a microscopic understanding of the electron beam induced deposition of tungsten — •Harald Jeschke, Kaliappan Muthukumar, Ingo Opahle, Juan Shen, and Roser Valentí — Institut für Theoretische Physik, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany

We present two density functional theory investigations into the electron beam induced deposition with tungsten hexacarbonyl $W(CO)_6$ as precursors. For the initial adsorption of the precursor on SiO_2 substrates, we consider two different surface models, a fully hydroxylated and a partially hydroxylated SiO_2 surface, corresponding to substrates under different experimental conditions and leading to physisorption and chemisorption, respectively. On the partially hydroxylated surface, we find a spontaneous dissociation of the precursor molecule with chemisorption of $W(CO)_5$ and removal of one of the CO ligands [1]. Other precursors like $MeCpPtMe_3$ and $Co_2(CO)_8$ are discussed. We also investigate the nature of the granular deposits with varying compositions of tungsten, carbon and oxygen that are produced in the EBID process. We employ an evolutionary algorithm to predict the crystal structures starting from a series of chemical compositions known from experiment. We approximate the amorphous structures by reasonably large unit cells that can accommodate local structural environments that resemble the true amorphous structure. Our predicted structures show an insulator to metal transition close to the experimental composition at which this transition is actually observed.

[1] K. Muthukumar *et al.*, Phys. Rev. B **84**, 205442 (2011).

DS 3.4 Mon 16:30 H 0111

Proximity Effects in Focused Electron Beam- Induced Processing on Ultra-thin Membranes — Marie-Madeleine Walz, Florian Vollnhals, Florian Rietzler, Michael Schirmer, Hans-Peter Steinrück, and •Hubertus Marbach — Lehrstuhl für Physikalische Chemie II and Interdisciplinary Center for Molecular Materials (ICMM), Friedrich-Alexander-University, Erlangen-Nuremberg, Egerlandstr. 3, 91058 Erlangen

A fundamental challenge in lithographic and microscopic techniques employing focused electron beams are so-called proximity effects due to backscattering in the sample or forward scattering in an already formed deposit. In this work, we apply a method which allows for visualizing processes on the substrate surface triggered by an electron beam. The resulting defects are decorated by iron deposits formed by decomposition of, e.g., $Fe(CO)_5$ and the corresponding technique is denoted as electron beam induced surface activation (EBISA). Applying this technique for the deposition of nanostructures has the advantage that no forward scattering in an already formed deposit occurs [1,2]. Conventional wisdom holds that by using thin membranes proximity effects can be effectively reduced. We demonstrate that, contrary to the expectation, proximity effects on a 200 nm SiN-membrane are even larger than on the respective bulk substrate. A peculiar charging effect is suggested to play a key role in this unexpected phenomenon.
This work is supported by the DFG through grant MA 4246/1-2.
[1] Walz et al., Angew.Chem.Int.Ed.49 (2010) 4669, [2] Walz et al., PCCP, 13 (2011) 17333.

DS 3.5 Mon 16:45 H 0111

Binary Pt-Si Nanostructures Prepared by Focused Electron-Beam-Induced Deposition — •Marcel Winhold[1], Christian Schwalb[1], Fabrizio Porrati[1], Roland Sachser[1], Achilleas S. Frangakis[2], Britta Kämpken[3], Andreas Terfort[3], Norbert Auner[3], and Michael Huth[1] — [1]Physikalisches Institut, Goethe-Universität, Max-von-Laue-Str.1, 60438 Frankfurt am Main — [2]Institut für Biophysik, Goethe-Universität, Max-von-Laue Str. 1, 60438 Frankfurt am Main — [3]Institut für Anorganische und Analytische Chemie, Goethe-Universität, Max-von-Laue Str. 7, 60438 Frankfurt am Main

Binary systems of Pt-Si were prepared by focused electron-beam-induced deposition (FEBID) using the two precursors trimethyl(methylcyclopentadienyl)platinum(IV) ($MeCpPt(Me)_3$) and neopentasilane ($Si(SiH_3)_4$) simultaneously. By this new approach for the preparation of binary systems with FEBID, we can vary the relative flux of the two precursors during deposition. We analyzed the binary composites of platinum and silicon by means of energy dispersive X-ray spectroscopy, atomic force microscopy, electrical transport measurements, and transmission electron microscopy. The results show strong evidence for the formation of an amorphous, metastable Pt_2Si_3 phase, leading to a maximum in the conductivity for a Si:Pt ratio of 3:2.[1] Furthermore the influence of post-treatment by electron irradiation as well as annealing on samples with Si:Pt ratios of 3:2 and 1:1 will be presented.

DS 4: Thin film photovoltaics

Time: Monday 9:30–10:00 Location: H 2032

Invited Talk DS 4.1 Mon 9:30 H 2032

The role of defects in thin film solar cells — •Thomas Unold — Helmholtz-Zentrum Berlin, Institut für Technologie

Thin film solar cells are an attractive technological option for electricitiy production, because they require only very little active material, compared to conventional crystalline silicon wafer-based solar cells, and because they can be directly deposited on large areas by a variety of vacuum-based or also non-vacuum based processing techniques. In order to achieve conversion efficiencies comparable to crystalline silicon solar cells, the reduction of defects and therefore minority carrier recombination are critical issues. We will show that zero-dimensional defects (point defects), one-dimensional defects (dislocations) and two-dimensional defects (grain boundaries) play different roles in the different adamantine thin film absorber materials silicon, CdTe and chalcopyrites. In particular the chalcopyrite-type semiconductor Cu(In,Ga)Se2 has been found to be extremely tolerant to deviation from stoichiometry, with minority carrier lifetimes up to 300ns for material compositions where structural defects in the percent range are expected. This can be explained with the formation of electronically benign secondary phases and the absence of deep levels in optimized material, leading to low recombination activities of point-defects, dislocations and grain boundaries in this material.

DS 5: Thin film photovoltaics: CIGSe + CdTe

Time: Monday 10:00–11:00 Location: H 2032

DS 5.1 Mon 10:00 H 2032

Diffusion of Zn in solar-grade $Cu(In,Ga)Se_2$ and single-crystal $CuInSe_2$ thin films — Jens Bastek[1], Roland Würz[2], Jürgen Albert[3], Sascha Sadewasser[3], and •Nico Stolwijk[1] — [1]Universität Münster, Institut für Materialphysik, 48149 Münster — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg, 70565 Stuttgart — [3]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 14109 Berlin

The diffusion behaviour of Zn in polycrystalline CIGSe is found to be very similar to that in monocrystalline CISe, which indicates that grain boundaries only play a minor role as segregation sites and fast-transport pathways. The Zn diffusion coefficient shows a slightly stronger temperature dependence than Cd in CIGSe while its values are lower by about one order of magnitude. Surprisingly, the diffusion profiles exhibit peculiar shapes with a second maximum near the CI(G)Se-substrate interface. Zn may be relevant to CIGS technology as it is a major component of the transparent oxide layer. In addition, Zn may penetrate into the active zone during solar-cell processing when the CdS buffer layer is replaced by ZnS. The present results were obtained from diffusion experiments with the radiotracer Zn-65 using lamp-oven annealing followed by ion-beam sputter-sectioning. We will discuss possible implications with regard to diffusion mechanisms and site occupancy.

DS 5.2 Mon 10:15 H 2032

Strongly Confined and Chemically Flexible Grain Boundaries in $Cu(In,Ga)Se_2$ Thin Films — Daniel Abou-Ras[1], Sebastian S. Schmidt[1], •Raquel Caballero[1,2], Thomas Unold[1], Hans-Werner Schock[1], Christoph T. Koch[3], Bernhard Schaffer[4], Miroslava Schaffer[4], Oana Cojocaru-Mirédin[5], and Pyuck-Pa Choi[5] — [1]HZB, Berlin, Germany — [2]UAM, Madrid, Spain — [3]Ulm University, Germany — [4]SuperSTEM, UK — [5]MPI for Iron Research, Düsseldorf, Germany

In the present work, we will show by means of electron holography, EFTEM and APT with spatial resolutions in the subnanometer range that substantial changes in composition with respect to the grain interiors are found at GBs in $Cu(In,Ga)Se_2$ (CIGSe) thin films within only about 1 nm wide regions. At Se-cation terminated twin boundaries, Cu depletion was measured, whereas considerable In enrichment and Cu depletion are visible in EFTEM maps of the Se/Se-terminated twins. At random GBs, Cu enrichment and In depletion as well as Cu depletion and In enrichment were found. Often, also enhanced Na, O, and K signals are detected at random GBs. Although no general compositional change at random CIGSe GBs was identified , the trends in Cu and In concentrations were always anticorrelated. These results suggest mechanisms of atomic/ionic redistribution at twin boundaries and random GBs, occurring within regions confined to only about 1 nm in width around the GBs, being also influenced by the trace elements segregated to the GBs. The apparent anticorrelation of Cu and In signals suggests a preferential site exchange of Cu and In atoms.

DS 5.3 Mon 10:30 H 2032

Investigation of the chlorine A-Center in polycrystalline CdTe layers by photoluminescence spectroscopy — •Christian

Kraft[1], Heiner Metzner[1], Mathias Hädrich[1], Pascal Schley[2], and Rüdiger Goldhahn[3] — [1]Institut für Festkörperphysik, Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Institut für Physik, Technische Universität Ilmenau, 98684 Ilmenau, Germany — [3]Institut für Experimentelle Physik, Universität Magdeburg, 39016 Magdeburg, Germany

Polycrystalline CdTe is a well known absorber material for thin film solar cells. However, the improvement of CdTe-based solar cells for industrial application is mainly based on empirical enhancements of certain process steps which are not concerning the absorber itself. Hence, the defect structure of CdTe is still not understood in detail. One of the most discussed defects in CdTe is the so called chlorine A-center. In general, the A-Center describes a defect complex of the intrinsic cadmium vacancy defect and an extrinsic impurity. By means of photoluminescence spectroscopy at temperatures of 5 K we investigated the behavior of the chlorine A-center under different CdTe activation techniques. Therefore, we were able to determine the electronic level of that defect and to analyze its influence on the crystal quality and the functionality of solar cells that were prepared of the corresponding samples.

DS 5.4 Mon 10:45 H 2032

Impedance Spectroscopy of CdTe Thin Film Solar Cells — •Charlotte Weiss, Christoph Heisler, Udo Reislöhner, Carsten Ronning, and Werner Wesch — Institute of Solid State Physics, University of Jena, Max-Wien-Platz 1, D-07743 Jena

Impedance Spectroscopy (IS) is a widely used method to analyze dielectric properties of specimen as a function of frequency. Typically this characterization method delivers an equivalent circuit diagram of the device under examination to describe its electrical properties. Traditionally IS is used in coating evaluation, corrosion monitoring and in electrochemistry. During the last years the method became more important also in the field of electrical characterization of solar cells.

In our work we use IS for the electrical characterization of thin film CdTe solar cells. The measurement is done at room temperature without illumination in a frequency domain from 20Hz to 2MHz. The samples are measured under variable forward bias. The results match insufficiently with the model of two resistor-capacitor circuits in series which is commonly used to describe the p-n junction and the blocking back contact. For better consistency, other models from the literature are used and discussed. From the results a conclusion is drawn about the properties of the solar cell such as the nature of the p-n junction or the performance of the back contact.

DS 6: Thin film photovoltaics: CIGSe + processing

Time: Monday 11:15–12:45 Location: H 2032

DS 6.1 Mon 11:15 H 2032

Properties of dislocations in Cu(In,Ga)Se2 film and their formation during growth — •Jens Dietrich[1], Daniel Abou-Ras[2], Thorsten Rissom[2], Thomas Unold[2], Tore Niermann[3], Michael Lehmann[3], Hans-Werner Schock[2], and Christian Boit[1] — [1]Technische Universität Berlin, Department of Semiconductor Devices, Einsteinufer 19, 10587 Berlin — [2]Helmholtz Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin — [3]Technische Universität Berlin, Institute of Optics and Atomic Physics, Hardenbergstrasse 36, 10623 Berlin

Transmission electron microscopy (TEM) studies were performed on Cu(In,Ga)Se2 (CIGSe) thin films for solar cells with a special focus on dislocations. A sample series of glass/Mo/CIGSe stacks with varying [Cu]/([Ga]+[In]) ratio were prepared by interrupting the growth processes at several stages. TEM imaging and elemental distribution maps by energy-dispersive X-ray spectroscopy gave structural and compositional information at certain film growth states. Furthermore, high resolution TEM imaging was used to confirm a structural model of dislocations in complete CIGSe solar cells and by means of in-line electron holography we examined changes in the mean inner potential. A decrease of the mean inner potential at the position of the dislocations was observed. This might be attributed to a change of the atomic density due to the dislocation, a local segregation or a charge at the dislocation core.

DS 6.2 Mon 11:30 H 2032

Novel Laser Structuring Method for Chalkopyrite Solar Cells — •Manuel Schüle[1], Christof Schultz[1], Heinrich Endert[2], Björn Rau[3], Rutger Schlatmann[3], Volker Quaschning[1], Bert Stegemann[1], and Frank Fink[1] — [1]University of Applied Sciences (HTW) Berlin, Wilhelminenhofstr. 75a, 12459 Berlin, Germany — [2]Newport Spectra-Physics GmbH, Ruhlsdorfer Strasse 95, 14532 Stahnsdorf, Germany — [3]PVcomB - Competence Centre Thin-Film- and Nanotechnology for Photovoltaics Berlin, Schwarzschildstr. 3, 12489 Berlin, Germany

In thin-film photovoltaics laser structuring is aimed to achieve appropriate monolithic serial interconnection. Generally, three structuring steps P1, P2, and P3 are necessary to separate the solar cells and to perform monolithic interconnection. However, manufacturing of chalcopyrite (CIGSe) thin film solar cells involves typically only one laser structuring step (P1), whereas two mechanical structuring steps (P2 and P3) are carried out.

In our approach, complete laser structuring of CIGSe solar cells is successfully demonstrated by application of short nanosecond laser pulses (<10 ns) with a single wavelength of 532 nm. The P1 and the P3 trenches are scribed by induced direct and induced indirect ablation respectively. For the P2 scribe, the thermal input of the ns laser pulses is used to transform the CIGSe absorber layer locally into a highly conductive compound that provides proper electrical interconnection between the front and back contact. These findings promise further simplification and flexibility to thin film solar cell production.

DS 6.3 Mon 11:45 H 2032

Investigation of CIGSe Solar Cell Performance Deviations in Nominally Equal Absorbers — •Robin Knecht[1], Jürgen Parisi[1], Ingo Riedel[1], Raymund Schäffler[2], and Bernhard Dimmler[2] — [1]Energy and Semiconductor Research Laboratory, University of Oldenburg, Germany — [2]Würth Solar GmbH & Co. KG, Schwäbisch-Hall, Germany

$Cu(In,Ga)Se_2$ (CIGSe) solar cells were fabricated independently by industrial scale co-evaporation in two separate production lines with the same nominal composition and thickness of the absorber film. Although the device properties were believed to be the same we observed substantial deviations of the respective values of the open circuit voltage ($\triangle V_{OC} = 40mV$) and of the fill factor ($\triangle FF = 4\%$), whereas the short circuit current was essentially the same. We performed fundamental device analysis, space charge and defect spectroscopy, transient photoluminescence as well as in-depth profiling of the chemical gradients of the absorber films. Using the results from the experiments we set up a simulation baseline which allowed us to conclude that the apparent deviations can be related to the presence of deep recombination centers with different concentration within the CIGSe absorber as well as to variations of the band gap grading.

DS 6.4 Mon 12:00 H 2032

Influence of the mechanical properties of sputtered Mo solar cell back contacts on laser scribing — Christof Schultz[1], Manuel Schüle[1], Heinrich Endert[2], •Jörn Bonse[4], Björn Rau[3], Rutger Schlatmann[3], Volker Quaschning[1], Bert Stegemann[1], and Frank Fink[1] — [1]University of Applied Science (HTW) Berlin, Wilhelminenhofstr. 75A, 12459 Berlin, Deutschland — [2]Newport Spectra-Physics GmbH, Ruhlsdorfer Strasse 95, 14532 Stahnsdorf, Deutschland — [3]PVcomB - Competence Centre Thin-Film and Nanotechnology for Photovoltaics Berlin, Schwarzschildstr. 3, 12489 Berlin, Deutschland — [4]BAM Bundesanstalt für Materialforschung und -prüfung Unter den Eichen 87 12205 Berlin, Deutschland

In thin-film photovoltaics complete laser structuring of the solar modules is aimed to perform appropriate monolithic serial interconnection. We have studied the laser ablation behavior of sputtered molybdenum back contacts for chalcopyrite solar cells. The properties of these Mo layer are sensitive to the sputter conditions. The process pressure influences the mechanical layer properties and, thus, contributes directly to the quality of the laser scribes. Precise, reliable and reproducible laser scribing requires the proper adaptation of the laser parameters to the material properties. In our study it was achieved by comprehensive analysis of the laser matter interaction and by detailed determination of the ablation thresholds as a function of the Mo layer thickness and ductility for different laser wavelengths and pulse durations, accompanied by thermal modeling.

DS 6.5 Mon 12:15 H 2032

Untersuchung der Selenisierung von Cu2ZnSnS4 mit energiedispersiver Röntgenbeugung — •Ole Zander, Roland Mainz, Alfons Weber, Justus Just, Thomas Unold und Hans-Werner Schock — Hahn-Meitner-Platz 1, 14109 Berlin

Die Selenisierung von sulfidischem Cu2ZnSnS4 (CZTS) durch schnelle thermische Prozessierung wurde mit Hilfe energiedispersiver Röntgenbeugung (EDXRD) in-situ untersucht. Dazu wurden verschiedene Präkursoren bestehend aus Binär- und Ternär- und Quarternärverbindungen des Cu-Zn-Sn-S Materialsystems durch Koverdampfung bei verschiedenen Substrattemperaturen hergestellt. Die Selenisierung der Präkursoren erfolgte durch schnelle Erhitzung unter Zugabe von elementarem Selen in einer Reaktionskammer am Bessy II Synchrotron. Durch die Beobachtung der Fluoreszenz- und Beugungssignale während der Selenisierung konnte die Bildung von CZTSe und Sekundärphasen, die Rekristallisation der Schichten, und der Verlust von Sn bei hohen Temperaturen beobachtet werden. Ein Modell welches die Kinetik der stattfindenden Teilprozesse und Substitutionsreaktionen beschreibt wird diskutiert.

DS 6.6 Mon 12:30 H 2032

Spectral variations in thin film PV module performance under real conditions — •Yvonne Boose[1], Martin Bucher[2], Christian Heller[2], Mark Lynass[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik Department, LS Funktionelle Materie, James-Franck-Str.1, 85748 Garching, Germany — [2]General Electric Global Research, Freisinger Landstraße 50, 85748 Garching, Germany

For planning and monitoring of large scale solar parks an exact as possible prediction of the energy yield is essential. In this work we investigate the solar spectrum for one location (48°15'N, 11°39'E). Spectral data of the incoming global irradiance from 300 to 1680 nm, the electrical parameters of a commercial CdTe and a CIGS solar module and weather data such as global, direct and diffuse irradiation, ambient temperature and humidity are recorded with a high temporal resolution of less than 10 seconds which allows also the investigation of short term meteorological effect such as cloud enhancement and fast moving cumulus clouds. Furthermore photographic weather records support the evaluation. Aerosol, ozone and water vapor data from the AERONET database are consulted to evaluate spectral variations. Experimental results are compared with simulations from the SMARTS2 and the SANDIA model.

DS 7: Organic electronics and photovoltaics I (jointly with CPP, HL, O)

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

Invited Talk DS 7.1 Mon 15:00 H 2032

Three-dimensional hybrid organic/inorganic heterojunctions based on rolled-up nanomembranes — •Carlos Cesar Bof Bufon[1], Dominic J. Thurmer[1], Christoph Deneke[1], and Oliver G. Schmidt[1,2] — [1]Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany — [2]Material Systems for Nanoelectronics, Chemnitz University of Technology, Reichenhainerstrasse 70, 09107 Chemnitz, Germany

In this work we present a method based on self-released strained nanomembranes (metallic and/or semiconducting) for electrically contact single molecular layers [1]. During release of the nanomembrane, the strain relaxation gives rise to a self-rolling process in which the membrane bonds back to substrate top surface where the thin organic layer was previously deposited. By this means, we are able to fabricate semiconductor-molecule-semiconductor heterojunctions. In this last case, the type of doping and its concentration can be independently and precisely set for each electrode in order to tune the device electronic properties. Such a novel hybrid devices was observed to display completely different electric characteristics which are not expected or possible to be demonstrated by using their elements separately. In addition, the strained nanomembrane based electrodes provide a soft and robust contact on top of the organic film. Furthermore, applying the self-rolling phenomenon, we achieve an approach that is fully integrative on a chip, and several components can be fabricated in parallel using well-established semiconductor processing technologies. [1] Bufon,C.C.B., Nano Lett.11,3727(2011)

DS 7.2 Mon 15:30 H 2032

Transport properties of hybrid organic/ferromagnetic metal heterojunctions based on strained nanomembranes — •Maria Esperanza Navarro Fuentes, Carlos Cesar Bof Bufon, Daniel Grimm, and Oliver G Schmidt — Institute for Integrative Nanosciences, IFW-Dresden, Helmholtz Strasse 20, 01069 Dresden, Germany

In this work we investigated the transport properties of organic/inorganic hybrid heterojunctions formed by rolled-up nanomembranes. This method allowed us to create soft metallic contacts on self-assembled monolayers (SAM) of phosphonic acids. As previously reported, the metal/SAM contact can be accomplished regardless the presence of pinholes in the thin organic layer [1]. By comparing the field-emission plots of hybrid heterojunctions formed by the combination of noble and ferromagnetic metals we were able to evaluate the influence of the interfacial oxide layer in transport properties of such heterojunctions. Moreover, the evaluation of the current-voltage curves allow us to clearly distinguish whether the tunneling behaviour is due to the native oxide of the ferromagnet or to the SAM layer behaving as an ultra-thin insulating material. In this particular case, the capability of understanding the nature of the organic/inorganic interface and their influence on the transport properties is an essential step in the creation organic spin valves.

[1] Bufon, C.C.B. et.al.; Nano Lett., 2011, 11 (9), 3727.

DS 7.3 Mon 15:45 H 2032

Contact property tailoring by SAM treatment of the Au/P3HT interface — Shahidul Alam, •Torsten Balster, and Veit Wagner — School of Engineering and Science,Jacobs University Bremen, Campus Ring 1, 28759 Bremen

The properties of the contact between the organic semiconductor and the metal not only influence the injection behaviour and limit the switching speed of an organic field effect transistor, they also determine the rectification in a Schottky diode. In this study, vertical Au/P3HT/Au structures on PET foils has been prepared and investigated by means of I-V measurements.

Due to the asymmetry in the deposition of the top and bottom metal electrode the devices showed diode, i.e. rectifying behaviour. To change the contact properties, especially the barrier heights self-assembled monolayers by 1-hexanethiol and nonafluoro-1-hexanethiol on top of the bottom electrode have been prepared prior to the P3HT and top electrode deposition.

The overall current density was reduced in comparison to the untreated sample due to the tunneling barrier introduced. However, the rectification ratio of the 1-hexanethiol has been increased by more than a factor of 2. The influence of the SAMs on the barrier height was analyzed using the Fowler-Nordheim tunneling model.

DS 7.4 Mon 16:00 H 2032

Organic Field Effect Transistor Studies on Contact Phenomena and Charge Carrier Injection in Bottom Contact Devices — •Christopher Keil, Dominik Klaus, and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392, Gießen.

Thin films of the perfluorinated phthalocyanine $F_{16}PcCu$ were prepared under high vacuum conditions. As substrate a SiO_2 insulating layer on a Si gate was chosen. Different metal contacts were evaporated as bottom contacts before the organic layer deposition. Organic thin film transistors of the molecular semiconductors were thereby achieved. The electrical contact behaviour of the organic semiconductor to electrodes of different metals (Au, Ag, Al) was investigated. The contact characteristics and the formation of an injection barrier will be discussed. Modelling of transistor characteristics and charge carrier injection are shown and their influence on the calculation of the intrinsic charge carrier mobility in the semiconductor channel is shown.

DS 8: Thin film photovoltaics: oxides and nanostructures

Time: Monday 16:30–18:00 Location: H 2032

DS 8.1 Mon 16:30 H 2032

Si-nanosponge embedded in SiO_2 as a new absorber material for photovoltaics

— •Bartosz Liedke[1], Karl-Heinz Heinig[1], Bernd Schmidt[1], David Friedrich[1], Arndt Mücklich[1], Jeffrey Kelling[1], and Dirk Hauschild[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf , 01314 Dresden, Germany — [2]LIMO Lissotschenko Mikrooptik GmbH, 44319 Dortmund, Germany

Silicon based nanostructures became within the last years most promising material for the PV market. Quantum confinement effect of nanostructured silicon allows for band gap engineering just by size manipulation to absorb the light in more efficient way.

Here, we consider SiO_x layers fabricated by magnetron co-sputter deposition, which after thermal treatment decompose into a network of Si nanowires embedded in SiO_2. The thermally activated spinodal decomposition is performed by rapid thermal processing within a few seconds and by very rapid thermal processing within several ms using diode laser. The morphology and crystallinity of the Si-nanosponge was measured by energy filtered TEM and Raman, respectively. The details of decomposition are studied using the atomistic kinetic Monte-Carlo (KMC) simulations at different concentrations defined by the x parameter. The spatiotemporal temperature profiles $T(x, t)$ of the scanned laser has been calculated as a function of thickness and time by the heat transport equation. The obtained profiles are used in the KMC. The combined theoretical and experimental investigations support the band gap engineering of the Si-nanosponge absorber via a control of the quantum confinement.

DS 8.2 Mon 16:45 H 2032

Combination of Zinc Phthalocyanines and Zinc Oxide for Hybrid Solar Cells

— •Michael Kozlik, Steffen Milz, Roman Forker, Alina Donat, Sören Paulke, Carsten Ronning, and Torsten Fritz — University of Jena, Institute of Solid State Physics, Max-Wien-Platz 1, 07743 Jena, Germany

Zinc phthalocyanine (ZnPc) is an organic molecule with high absorbance [1]. In combination with zinc oxide (ZnO) the interface forms a p-n-junction [2]. Therefore, the materials can be used in hybrid solar cells, i.e., photovoltaic devices made of organic and inorganic materials in order to utilize the advantages of the two material classes: high absorbance and good conductivity, respectively [3]. In our work, we investigate the planar sandwich setup and nanostructured devices, the latter consisting of ZnO nanowires covered with ZnPc. The interface between the two materials is analyzed by scanning electron microscopy (SEM), together with energy dispersive X-ray spectroscopy (EDX) and photo electron spectroscopy (PES) to characterize the electronic properties. The results of UV-Vis spectroscopy and external quantum efficiency (EQE) measurements highlight the generation of excitons in ZnPc and link these with the photo current in the visible range.

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[1] N. Papageorgiou et al., Prog. Surf. Sci. 77 (2004) 139.
[2] C. Ingrosso et al., Electrochim. Acta 51 (2006) 5120.
[3] S. Günes et al., Inorg. Chim. Acta 361 (2008) 581.

DS 8.3 Mon 17:00 H 2032

Sol-Gel Templated Zinc oxide Films for Solar Cell Application

— •Kuhu Sarkar, Monika Rawolle, Eva M. Herzig, Weijia Wang, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany

Zinc oxide (ZnO) nanostructures are synthesized on silicon substrates forming different morphologies comprising of foam-like structures, worm-like aggregates, circular vesicles and spherical granules. The synthesis is using a sol-gel mechanism coupled with an amphiphilic diblock copolymer polystyrene-block-polyethyleneoxide, P(S-b-EO), acting as a template. The different morphologies are designed by adjusting the weight fractions of the good-poor solvent pair and the ZnO precursor, zinc acetate dihydrate (ZAD). To visualize the compositional boundaries of various morphologies, a ternary phase diagram is mapped. The surface morphologies of the ZnO nanostructure are studied with scanning electron microscopy (SEM). The inner structures of the samples are probed using grazing incidence small angle X-ray scattering, complementing the SEM investigations. X-ray diffraction measurements are performed to confirm the crystallization of the ZnO to the wurtzite polymorph phase upon calcination of the nanocomposite film in air.

DS 8.4 Mon 17:15 H 2032

DC magnetron sputtering of ZnO:Al from metallic and reduced ceramic targets: comparison of ion energy distributions

— •Christian Wilde and Mykola Vinnichenko — Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden, Germany

Magnetron sputtering is a common technique for deposition of transparent conductive oxides (TCO) such as Al-doped ZnO (AZO). The film growth using either metallic (reactively) or reduced ceramic targets often show different properties and morphology even in case of optimized processes. Therefore it is crucial to understand differences in magnetron plasma leading to such variations of properties.

The energy of ions emitted from the target in these processes is important, because it influences nucleation and the quality of the TCO. The negative ions with energies high enough to damage the growing film are of special interest.

In this contribution we report results of comparative analysis of ion energy distributions in a broad energy range for DC magnetron sputtering using metallic and ceramic targets. The energy distributions of low-energy ions show a similar behaviour for both processes, while in case of high-energy negative ions and fragments of them, they are substantially different . Moreover, magnetron plasma in case of metallic target sputtering shows substantially lower fraction of negatively charged ions with high energy. The observed differences indicate the potential of reactive magnetron sputtering to produce AZO films with less damage, and as a result, with improved properties.

DS 8.5 Mon 17:30 H 2032

Tantalum incorporation in TiO2 based transparent conductive thin films

— •Marcel Neubert, Mykola Vinnichenko, Steffen Cornelius, and Andreas Kolitsch — HZDR

The growing number of applications of transparent electrodes in optoelectronic devices drives the need for novel cost-efficient transparent conductive materials. The epitaxial films of TiO2 doped with Nb or Ta show electrical resistivity values comparable to those of the best In2O3:Sn and ZnO:Al films. However, it is still challenging to achieve low electrical resistivity in polycrystalline TiO2-based films. In order to address this problem, we studied the films formed on glass substrates without heating by DC magnetron sputtering of reduced TiO2:Ta ceramic targets followed by vacuum annealing. It was crucial to use a plasma feedback system in order to enable a fine tuning of the oxygen supply into Ar and O2 gas mixture during the deposition. This approach yielded the 400 nm thick films with optical transmittance above 80%, electrical resistivity in the range of 10-3 *cm and free electron mobility of 8 cm*/Vs. The electrical activation of Ta dopant was above 60% that is substantially higher than that of Al in ZnO.

DS 8.6 Mon 17:45 H 2032

Ultra-short laser pulse structuring of thin zinc oxide layers on 30 cm x 30 cm CIS solar cell modules

— •Christian Miller, Daniel Harangozo, Juergen Sotrop, Gerhard Heise, and Heinz Huber — Hochschule München, Laserzentrum, Lothstr. 34, 80335 München, Deutschland

In order to avoid resistive losses and for voltage transformation thin film solar cells must be separated into serially connected sub cells. In the case of CIS thin film solar cells the interconnection is performed in industry by ns-laser structuring and mechanical scribing, to separate the Molybdenum p-contact as well as the CIS-absorber and the Zink oxide n-contact, respectively. In contrast, ps-laser enables selective structuring of a specific layer, reducing the damage of the subjacent layer. For this purpose, we demonstrate an all-pico-second-laser process on 30 cm x 30 cm samples. Module efficiencies of 11.8 % where achieved reducing the width of the interconnection down to about 150 um.

DS 9: Multiferroics I: Junctions and thin films / Magnetoelectric coupling (jointly with MA, DF, KR, TT)

Time: Monday 9:30–12:45 Location: EB 301

Topical Talk DS 9.1 Mon 9:30 EB 301

Reversible electrical switching of spin polarization in multiferroic tunnel junctions — •Marin Alexe, Daniel Pantel, Silvana Götze, and Dietrich Hesse — Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle

Spin polarized transport in ferromagnetic tunnel junctions, characterized by tunnel magnetoresistance, has already proven a high application potential in the field of spintronics and in magnetic random access memories (MRAM). Until recently, in such a junction the insulating barrier played only a passive role keeping apart the ferromagnetic electrodes in order to allow electron tunneling. However, a new dimension was added to these devices by replacing the insulator with a ferroelectric material, which possesses permanent dielectric polarization switchable between two stable states. The obtained multiferroic tunnel junction (MFTJ) is a non-volatile memory device with four states, given by two possible ferroelectric polarization directions in the barrier and two different magnetization alignments of the electrodes. Here, we will show that due to the coupling between magnetization and ferroelectric polarization at the interface between a magnetic electrode and the ferroelectric barrier of a MFTJ, the spin polarization of the tunneling electrons can be reversibly and remanently inverted by switching the ferroelectric polarization of the barrier. Selecting the spin direction of the tunneling electrons by short electric pulses in the nanosecond range rather than by an applied magnetic field is highly relevant for spintronics, especially for spin-based information technology.

DS 9.2 Mon 10:00 EB 301

First Principles Modelling of Spin Transport in Functional Oxide Tunnel Junctions — •Nuala M. Caffrey, Thomas Archer, Ivan Rungger, and Stefano Sanvito — School of Physics and CRANN, Trinity College Dublin, Ireland

Spin-dependent tunnelling between ferromagnetic electrodes separated by insulating oxide barriers has long attracted scientific and commercial interest. In the last decade it became evident that the insulating layer was more than just a simple barrier through which electrons tunnel. It is wave-function symmetry selective, making the tunnelling process sensitive to its electronic structure. The understanding of such a concept suggests that one can engineer the transport properties of a tunnel junction by carefully selecting the insulating barrier and the metallic electrodes. Ferroelectric materials are of particular interest as barriers due to additional functionality offered by the electric polarisation.

We investigate, from first-principles, the properties of a multifunctional tunnel junction combining two materials with different ferroic states (ferromagnetic and ferroelectric). We demonstrate massive tunnelling magnetoresistance (TMR) in a SrRuO3 / BaTiO3 / SrRuO3 junction. We also consider the implications of introducing structural asymmetry into this junction by using a thin layer of dielectric material at one interface. In such a junction we demonstrate a sizable tunnelling electroresistance (TER) that increases with the thickness of the dielectric layer.

DS 9.3 Mon 10:15 EB 301

FeO at Iron/Oxide interfaces — •Andrea Neroni, Daniel Wortmann, Ersoy Sasioglu, Stefan Blügel, and Marjana Ležaić — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We present density-functional theory (DFT) based first-principles calculations of tunneling and magnetoconductance properties of nanoferronic devices consisting of oxide barriers between iron contacts. Several experimental works have indicated the presence of an iron-oxide layer at the contacts of this barrier, that can significantly alter the tunneling properties of the junction. The effect of this layer is still unclear. From the theoretical point of view, one unexplored point are the electron correlations in the single FeO layer at the interface. We account for these correlations with a Hubbard U parameter determined by the constrained random phase approximation (cRPA) [1] and calculate the change of the tunneling magnetoresistance ratio under this condition, using the full-potential linearized augmented plane wave (FLAPW) method `FLEUR` [2]. The electronic transport properties of nanoferronic junctions have been investigated using an embedded Green-function approach [3].

Work is supported by Helmholtz Young Investigators Group Program VH-NG-409 .

[1] E. Şaşıoğlu, C. Friedrich, and S. Blügel, PRB **83**, 121101(R) (2011)
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DS 9.4 Mon 10:30 EB 301

Thermally stimulated currents in $BiFeO_3$ — •Akash Bhatnagar, Ayan Roy Chaudhuri, Dietrich Hesse, and Marin Alexe — Max Planck Institute of Microstructure Physics, Weinberg 2, Halle(Saale), Germany

Bismuth ferrite($BiFeO_3$)-BFO is a well known multiferroic material, with high ferroelectric Curie temperature (1103 K) and a saturated ferroelectric hysteresis with a remnant polarization of 100 C/cm^2. However, it has been found that pure BFO usually exhibits a high leakage current that could limit wide applications of this material. The thermally stimulated current (TSC) technique was used to get insights into the electronic origin of the leakage, which includes the study of energy levels that might be present in the band gap. These levels can act as trapping centers for charge carriers, thus affecting conductivity. Three systems of BFO, namely, single crystals, thin films and ceramics were studied. Measurements for ceramics and single crystals were performed in capacitor mode, whereas for thin films in-plane electrodes were made using a normal lift-off process. The effect of orientation of the electrodes with respect to domain patterns in thin films, have been investigated. Consequently, trap activation energies and density calculations were performed to fully characterize different levels. Photoconductive and photovoltaic properties were also investigated which corroborate the TSC data.

DS 9.5 Mon 10:45 EB 301

Preparation and characterization of multiferroic thin films grown with an Oxid-MBE — •Paul Zakalek, Markus Waschk, Alexander Weber, and Thomas Brückel — Jülich Centre for Neutron Science JCNS und Peter Grünberg Institut PGI, Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany

An oxygen-assisted Molecular Beam Epitaxy (MBE) gives the possibility to engine artificial materials on a nanoscale with promising effects. With our machine it is possible to grow complex materials like $La_xSr_{1-x}MnO_3$ (LSMO) or $La_xBi_{1-x}MnO_3$ (LBMO) with remarkably good crystalline quality.

The materials show a variety of interesting effects. For example the La concentration affects the magnetic and electric properties of this systems. The LSMO and LBMO layers can either be antiferromagnetic, ferromagnetic or multiferroic, depending of the La concentration.

Different LSMO/LBMO systems were grown with oxygen-assisted MBE on a $SrTiO_3$ (STO) substrate with different La concentrations. We will present the preparation process and the structural in-house characterization of this systems. First results show good structural quality, like surface roughnesses of not more then one unit cell. Additionally magnetic and electric measurements of the samples will be shown.

15 min. break

DS 9.6 Mon 11:15 EB 301

Guest molecules in ABX3 metal-organic frameworks: multiferroicity and magnetoelectricity — •Alessandro Stroppa[1], Prashant Jain[2], Paolo Barone[1], Martijn Marsman[3], Juan Manuel Perez-Mato[4], Anthony K. Cheetham[5], Harold W. Kroto[2], and Silvia Picozzi[1] — [1]CNR-SPIN, L'Aquila, Italy — [2]Department of Chemistry and Biochemistry, Florida State University Tallahassee, FL 32306 (USA) — [3]University of Vienna, Faculty of Physics and Center for Computational Materials Science (Austria) — [4]Departamento de Fisica de la Materia Condensada Facultad de Ciencia y Tecnologia, UPV/EHU, Bilbao (Spain) — [5]Department of Materials Science and Metallurgy University of Cambridge (UK)

Metal-organic frameworks (MOFs) are increasingly regarded as promising materials. MOFs with perovskite architecture have recently branched out into the field of multiferroics, materials which have both magnetic and ferroelectric orders. Here, we focus on a MOF compound and theoretically show that it is ferroelectric and this ferroelectricity is the cause of a weak ferromagnetic coupling. In inorganic perovskite-like compounds, octahedral tilting and Jahn-Teller distortions are usually non-polar modes. In this MOF, however, their cooperative link to A-groups via hydrogen bondings finally breaks inversion symmetry, and induces a ferroelectric polarization. We show that the switching of polarization direction implies the reversal of the weak ferromagnetic component, therefore allowing the long-sought electrical control of the magnetization.

DS 9.7 Mon 11:30 EB 301

magnetoelectric effects in the cubic ferrimagnet Cu_2OSeO_3 — •Maria Eleni Belesi[1,2], Mohamed Abid[1], Helmuth Berger[1], and Jean-Philippe Ansermet[1] — [1]Institute of Condensed Matter Physics, EPFL, Station 3, CH-1015 Lausanne, Switzerland — [2]Leibniz Institute for Solid State and Materials Research, Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany

We present magnetic and dielectric measurements in single crystals of the cubic magnetoelectric compound Cu_2OSeO_3. The magnetic measurements show a transition to a ferrimagnetic state at 60 K. This state shows a finite magnetocapacitance which is temperature dependent and varies significantly upon changing the direction of the magnetic field with respect to the crystallographic axes. The magnetocapacitance is also shown to vary with the relative orientation of the magnetic and electric fields. In addition, we found that the magnetically ordered state shows a magnetic field induced electric polarization, whose temperature dependence and anisotropic properties will be discussed.

DS 9.8 Mon 11:45 EB 301

Microscopic Mechanisms for Magnetoelectric Effect in $LiMPO_4$ (M=Mn,Fe,Co,Ni) — •Andrea Scaramucci, Eric Bousquet, and Nicola Spaldin — Materials Theory, Department of Materials, ETH Zurich, Zurich, Switzerland

We theoretically investigate the microscopic mechanisms leading to the linear magnetoelectric effect in the $LiMPO_4$ series. This is of particular interest since some of its constituents possess toroidal moments and shows large magnetoelectric effect.

By using symmetry analysis we obtain the microscopic couplings between spins and electric polarization responsible for each component of the magnetoelectric tensor. Furthermore, we identify couplings with exchange-strictive and relativistic origin. By using *ab initio* calculation and by enforcing numerous non collinear spin configurations we extract the strength of these couplings together with the exchange coupling constants. We use mean field approximation and Monte Carlo simulation to calculate the temperature evolution of magnetoelectric tensor. Our calculations explain the features of the temperature dependence found in experiments.

DS 9.9 Mon 12:00 EB 301

Manipulation of the antiferromagnetic structure in $LiNi_{(1-x)}Fe_xPO_4$ (x = 0.03, 0.2) by iron substitution — •Anne Zimmermann[1] and Manfred Fiebig[1,2] — [1]HISKP, University of Bonn, Germany — [2]Materials Department, ETH Zurich, Switzerland

The $LiMPO_4$ system (M = Fe, Ni, Co, Mn) includes crystallographically isostructural compounds with antiferromagnetic (AFM) order differing in the spin direction only. Thus, the system offers the opportunity to study fundamental mechanisms of AFM 180° domain formation in a range of similar but not identical compounds.

In order to investigate the interplay between the different types of spin order $LiNi_{(1-x)}Fe_xPO_4$ samples with different mixing ratios of nickel and iron were studied using optical second harmonic generation (SHG). SHG coupling linearly to the AFM order parameter was identified in spectroscopy measurements and used for domain imaging. A small iron substitution of $x = 0.03$ yields no change in the domain pattern as well as in the magnetic structure in contrast to pure $LiNiPO_4$. However, for an iron substitution of $x = 0.2$ the spin structure changes significantly: the spin direction lies in the yz-plane and thus between the two spin directions for $LiNiPO_4$ and $LiFePO_4$. The change in magnetic structure is revealed in a different domain pattern as well. Furthermore the order parameter exhibits an unsual, photosensitive temperature dependence which is discussed in detail.

- Work supported by the SFB 608 of the DFG.

DS 9.10 Mon 12:15 EB 301

Multiferroicity and magnetoelectricity in a doped topological ferroelectric — Marco Scarrozza, Maria Barbara Maccioni, Giorgia M. Lopez, Alessio Filippetti, and •Vincenzo Fiorentini — Dept of Physics, U of Cagliari and CNR-IOM, Cagliari, Italy

$La_2Ti_2O_7$ is a “topological” ferroelectric where dipoles are produced by antiferrodistortive rotations failing to compensate due to the layered structure. To turn on multiferroicity, we investigated magnetic doping from first-principles within density-functional theory. The isovalent substitution of Mn for Ti produces antiferromagnetism at all dopings as expected due to superexchange between Mn d^3 ions. In the fully-substituted compound $La_2Mn_2O_7$, many ordering patterns compete, the lowest being a variant of G-type antiferromagnetism. The same system is also magnetoelectric, because the rotations are involved in both magnetic and ferroelectric order: as a coercive field undoes the rotations and depolarizes ferroelectricity, magnetic coupling doubles in intensity. However, the ferromagnetic phase of $La_2Mn_2O_7$ is always much higher in energy. On the other hand, we find that heterovalent substitution of Ti with Cr, Sc, and V always yields robust ferromagnetism. In particular, V orders in rows orthogonal to the P direction, with a covalency gap of 0.2 eV: $La_2Ti_{2-x}V_xO_7$ is therefore properly multiferroic. We are currently investigating the magnetoelectric tensors.

DS 9.11 Mon 12:30 EB 301

***Ab initio* study of the properties of $BaTiO_3$/Co-Pt alloy interface** — •Konstantin Z. Rushchanskii, Stefan Blügel, and Marjana Ležaić — Peter Grünberg Institut, Forschungszentrum Jülich and JARA,52425 Jülich, Germany

Multiferroics are materials which exhibit more that one ferroic order parameter. They can be made of a single phase, where multiple ferroic order parameters co-exist simultaneously, or of composites, where different ferroic order parameters are combined in separate phases. Due to the limited number of known single phase multiferroics, most of which present multiple ordering only at low temperatures, engineering of composite junctions based on interfaces of magnetic and ferroelectric compounds are therefore of great scientific interest but are also promising due to their potential applications.

Cobalt-platinum alloys are known as compounds with a strong potential for applications in magnetic data storage, due to the strong exchange interactions and strong spin-orbit coupling (and, as a consequence, a large magnetocrystalline anisotropy energy). We present results of *ab initio* calculations based on density functional theory (DFT) of the magneto-electric coupling in cobalt-platinum alloys interfaced with $BaTiO_3$ ferroelectric.

We acknowledge the support by Helmholtz Young Investigators Group Program VH-NG-409.

DS 10: Multiferroics II: Hexagonal manganites / Incommensurate multiferroics (jointly with MA, DF, KR, TT)

Time: Monday 15:00–18:30 Location: EB 301

Invited Talk DS 10.1 Mon 15:00 EB 301

Anisotropic conductance of ferroelectric domain walls — •Dennis Meier — Dept. of Physics, University of California, Berkeley, USA

Domain walls are natural interfaces that can exhibit structural, physical, and chemical properties which drastically differ from the surrounding bulk material. This applies to a large variety of phenomena including chemical/electrical transport, multiferroicity, or superconductivity. In addition to the fascinating physical properties domain walls are small in size and their position can be controlled rendering them interesting for future device design. In my talk I report on the exotic nature of trimerization-polarization domain walls in hexagonal ErMnO$_3$. Using piezoforce-response microscopy and conductive atomic force microscopy we revealed that the domain walls represent a structural discontinuity being electrically dressed. While the structural component basically guarantees stability, the electrical dressing generates interesting and new nanoscale physics that I will discuss. The ferroelectric domain walls in ErMnO$_3$ for instance exhibit highly anisotropic electrical properties resulting in directional domain wall conductance. Remarkably, the local electrical conductance is a continuous function of the domain wall orientation which can be explained as a combined consequence of electrostatic and band-structure changes at the walls.

DS 10.2 Mon 15:30 EB 301

Structures and energetics of domain walls in polar hexagonal manganites — •Yu Kumagai and Nicola Spaldin — Department of Materials, ETH Zurich

We use first-principles density functional calculations to study the domain walls in the multiferroic hexagonal manganites, h-RMnO$_3$ (R=Sc, Y, Dy–Lu). These materials show an improper ferroelectricity induced by structural trimerization, resulting in $2 \times 3 = 6$ domains (2 for ferroelectricity and 3 for trimerization origin) below the Curie temperature with an intriguing cloverleaf pattern of domains [1,2]. Our calculations explain the observation that ferroelectric (FE) domain walls exist only in combination with antiphase DWs. We find that interlocked ferroelectric and antiphase domain walls have lower energies than typical FE domain walls in conventional ferroelectrics, as well as a much narrower wall width; both factors result from the layered geometry of the h-RMnO$_3$ structure.

[1] T. Choi *et al.*, Nature Mater. 9, 253 (2010).

[2] T. Jungk *et al.*, Appl. Phys. Lett. 97, 012904 (2010).

DS 10.3 Mon 15:45 EB 301

Hexagonal InMnO$_3$ - An Outsider Among The Family Of Multiferroic Hexagonal Manganites — •Martin Lilienblum[1], Yu Kumagai[1], Alexei A. Belik[2], Naemi Leo[1], Nicola A. Spaldin[1], and Manfred Fiebig[1] — [1]Department of Materials, ETH Zurich — [2]International Center for Materials Nanoarchitectonics, NIMS

So far, it was believed that hexagonal (h-) InMnO$_3$ exhibit the same type of multiferroic order as the other compounds from the h-RMnO$_3$ family (R = Sc, Y, Dy - Lu), including, in particular, a unit-cell-tripling improper ferroelectric order. Here we present experimental evidence for the *absence* of ferroelectricity in hexagonal InMnO$_3$ based on three different techniques: x-ray diffraction (XRD), piezoresponse force microscopy (PFM) and optical second harmonic generation (SHG). XRD data are ambiguous because they can be described likewise by the non-ferroelectric $P\overline{3}c$ structure and by the ferroelectric $P6_3cm$ structure present in the other h-RMnO$_3$ compounds. However, PFM at room temperature and SHG measurements at low temperature uniquely reveal the absence of ferroelectric order in InMnO$_3$. We therefore propose that InMnO$_3$ exhibits antiferrodistortive, but non-ferroelectric order according to the $P\overline{3}c$ symmetry. Density functional calculations show that the relative energy between the $P\overline{3}c$ and $P6_3cm$ structures is determined by a competition between electrostatic and covalency effects, with an *absence* of covalency favoring the ferroelectric structure. We gratefully acknowledge the support by DFG through SFB 608.

DS 10.4 Mon 16:00 EB 301

Direct observation of multiferroicity in TbMnO$_3$ thinfilms — •Artur Glavic[1], Jörg Voigt[1], Enrico Schierle[2], Eugen Weschke[2], and Thomas Brückel[1] — [1]Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT, Forschungszeutrum Jülich GmbH, Jülich, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, BESSY II, Albert-Einsteinstr. 15, Berlin, Germany

Multiferroic rare earth manganites as TbMnO$_3$ have been studied a lot in the past ten years because of their complex magnetic structure, which leads to a ferroelectric polarization. So far investigations on TbMnO$_3$ thin films grown on LaAlO$_3$ or SrTiO$_3$ showed an emergent ferromagnetism, destroying the multiferroic properties.

We have investigated TbMnO$_3$ films grown with sputter deposition on YAlO$_3$ substrates using soft x-ray resonant magnetic scattering with linear and circular polarized light. By measuring the circular dichroism originating from the chirality of the magnetic structure we could directly observe multiferroic domains in the thin films. Although the transition temperatures found were comparable to bulk, an additional influence of the Tb magnetic order on the ferroelectricity was observed.

DS 10.5 Mon 16:15 EB 301

Sinusoidal electromagnon in RMnO$_3$: Indication of anomalous magnetoelectric coupling — •Markku Stenberg[1] and Rogério de Sousa[2] — [1]Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany — [2]Department of Physics and Astronomy, University of Victoria, Victoria, B.C., V8W 3P6, Canada

The optical spectra in the family of multiferroic manganites RMnO$_3$ is a great puzzle. Current models can not explain the fact that two strong electromagnons are present in the non-collinear spin cycloidal phase, with only one electromagnon surviving the transition into the collinear spin sinusoidal phase. We show that this is a signature of the presence of anomalous magnetoelectric coupling that breaks rotational invariance in spin space and generates oscillatory polarization in the ground state.

DS 10.6 Mon 16:30 EB 301

Neutron scattering studies on chiral multiferroics: magnetic structure and excitations — •Max Baum[1], Thomas Finger[1], Jeannis Leist[2], Karin Schmalzl[3], Paul Steffens[3], Petra Becker[4], Ladislav Bohatý[4], Götz Eckold[2], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Physikalische Chemie, Georg-August-Universität Göttingen — [3]Institut Laue Langevin (ILL), Grenoble — [4]Institut für Kristallographie, Universität zu Köln

Multiferroic materials or compounds with a strong magnetoelectric effect posses a large application potential in data storage techniques. Quite recently, systems with a peculiar spiral magnetic order were shown to directly induce a spontaneous electric polarisation and to exhibit giant magnetoelectric effect. Neutron scattering with spherical polarisation analysis gives access to the chiral component of the magnetic structure which is directly linked to the electric polarisation. Therefore, it is possible to control the chiral components by an external electric field. We present neutron scattering experiments on IN14 and IN20 using spherical polarisation analysis documenting the poling of the elastic magnetic chiral terms for MnWO4, TbMnO3 and Ni3V2O8 by cooling in an electric field. In addition, it is possible to switch the chiral components by varying the electric field at constant temperature; thereby measuring multiferroic hysteresis curves. For MnWO4, this experiment was performed with time resolution detecting the typical relaxation times. Tor TbMnO3 we discuss a newly discovered excitation which exhibits a chirality opposite to the static one.

DS 10.7 Mon 16:45 EB 301

Theoretical study of Magnetoelectric effects in Multiferroic RMn2O5 — •Safa Golrokh Bahoosh[1], Julia Wesselinowa[2], and Steffen Trimper[3] — [1]Max Planck Institute of Microstructure Physics, 06099 Halle, Germany — [2]Department of Physics, University of Sofia, 1164 Sofia, Bulgaria — [3]Institute of Physics, Martin-Luther-University, 06120 Halle, Germany

The magnetoelectric behavior of the rare-earth RMn2O5 perovskites is studied theoretically using a quantum model. Whereas the magnetic subsystem is described by nearest-neighbor ferromagnetic coupling and next nearest neighbor antiferromagnetic order, the ferroelectric subsystem is characterized by an Ising model in a transverse field.

Due to frustration, the magnetic system offers spiral structures. The coupling between both systems is a symmetry-allowed linear coupling.

Using Green*s functions we find analytically the temperature and wave vector dependent elementary excitation of the Magnetoelectric system, the polarization and the magnetization for different magnetoelectric coupling strengths.

Lowering the temperature, the system undergoes a magnetic transition at TN and a further reduction of the temperature leads to a ferroelectric transition at TC < TN. The magnetoelectric coupling is manifested as a kink in both the magnetization and the elementary excitation at TC. The polarization is enhanced under the presence of a finite external magnetic field. In the same manner the magnetization is slightly changed by an applied electric field near to TC.

15 min. break

DS 10.8 Mon 17:15 EB 301

Origin of spin canting in multiferroic perovskites — •Carlo Weingart, Eric Bousquet, and Nicola Spaldin — Materials Department, ETH Zurich, Switzerland

In magnetic perovskites with oxygen octahedral distortions, it is usually admitted that the Dzyaloshinsky-Moriya interaction (DM) is responsible for the spin canting. This statement is however partially true since the single-ion anisotropy (SIA) can also allow for similar spin canting. By decomposing the different magnetic interactions (exchange, DM and SIA) from first-principles calculations, we show that depending on the magnetic cation, the DM and the SIA can be of similar amplitude. This allow us to reconsider the origin of the weak ferromagnetism in multiferroics.

DS 10.9 Mon 17:30 EB 301

A further step of understanding the complex magnetic order in magnetoelectric Co_3TeO_6 — •Vera Carolus[1], Thomas Lottermoser[2], Matthias Hudl[3], Pierre Tolédano[4], and Manfred Fiebig[2] — [1]HISKP, University of Bonn, Germany — [2]Department of materials, ETH Zurich, Switzerland — [3]Department of Engineering Sciences, Uppsala University, Box 534, SE-751 21 Uppsala, Sweden — [4]Laboratory of Physics of Complex Systems, University of Picardie, 33 rue Saint-Leu, 80000 Amiens, France

Like most of the known magnetoelectric multiferroics, Co_3TeO_6 exhibits a complex spin structure with a series of consecutive phase transitions. Contrary to common compounds, Co_3TeO_6 possesses two independent commensurate k-vectors in the multiferroic low-temperature phase. In addition, magnetic-field dependent measurements of the ferroelectric polarization show a strongly anisotropic behaviour.

Here we show our results using spatially resolved optical second harmonic generation (SHG) under external magnetic and electric fields in the multiferroic low-temperature phase. However, the SHG gives only access to the magnetic subsystem. Like the ferroelectric polarization, the magnetic structure shows strongly anisotropic behaviour. In crossed magnetic and electric fields we were able to reach a single-domain state, while a magnetic field solely always leads to distinctively different multi-domain states. Most remarkably, for a certain direction of magnetic field, we were able to invert the multi-domain state. Furthermore, this behaviour indicates the existence of a pronounced memory effect.

DS 10.10 Mon 17:45 EB 301

The multiferroic, geometric frustrated $CuCrO_2$ compound: a case of the $p-d$ hybridization spin-charge coupling? — •Matthias Frontzek, Georg Ehlers, and Andrey Podlesnyak — Neutron Scattering Science Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

Multiferroic materials have become of interest for their unusual low-temperature properties in general, and in particular for the observation that one can affect their magnetic structure through an electric field and their electric polarization through a magnetic field. The delafossite $CuCrO_2$, which crystallizes in the rhombohedral $R\overline{3}m$ space group, is a multiferroic compound with an apparent strong coupling of spin and charge. In contrast to other multiferroic compounds $CuCrO_2$ shows a spontaneous electric polarization upon antiferromagnetic ordering without an accompanying structural phase transition, although a slight in-plane lattice distortion has been measured.

In our contribution, we present a detailed study on $CuCrO_2$ single crystals using neutron diffraction and spectroscopy as well as pulsed magnetic field measurements up to 60 T of the electric polarization. Based on our study we will show a revised magnetic structure model and present a model Hamiltonian including in-plane next-next nearest neighbor and inter-layer exchange interaction. We will stress the importance of the latter for the multiferroic properties and will show evidence based on the high field polarization measurements that the proposed $p-d$ hybridization spin-charge coupling mechanism needs to be modified.

DS 10.11 Mon 18:00 EB 301

Theory of High-Temperature Multiferroicity in CuO — •Naëmi Leo[1,2], Pierre Tolédano[3], Dmitry D. Khalyavin[4], and Manfred Fiebig[1,2] — [1]ETH Zurich, Switzerland — [2]HISKP, Universität Bonn, Germany — [3]University of Picardie, France — [4]ISIS, United Kingdom

Spin-spiral multiferroics offer strong magnetoelectric coupling, although most of them have low transition temperatures which make them undesirable for technical applications. Cupric oxide is a remarkable exception with its high Curie temperature of 230 K. Understanding the interactions leading to such a high-T_C magnetically induced ferroelectricity is very desirable for future room-temperature magnetoelectric multiferroics devices.

Here we present a Landau theory analysis of the multiferroic properties of CuO [1]. Using a multi-dimensional order parameter expansion of the free energy we examine the sequence of phase transitions: The unusual direct transition to the multiferroic phase is induced by the simultaneous onset of two order parameters, enabled by the strong Cu-O superexchange. Expressing the order parameter in terms of spins we determine theoretically the magnetic structure in the spin-spiral phases. Furthermore we identify the microscopic interactions responsible for the magnetically induced spontaneous polarization.

The work in Bonn was supported by the DFG through the SFB 608.

[1] P. Toledano, N. Leo, D.D. Khalyavin, L.C. Chapon, T. Hoffmann, D. Meier, and M. Fiebig, Phys. Rev. Lett. **106**, 257601 (2011).

DS 10.12 Mon 18:15 EB 301

Resonant Elastic X-ray Scattering Studies of Multiferroic $NdFe_3(BO_3)_4$ — •Sven Partzsch[1], Jorge Enrique Hamann-Borrero[1], Claudio Mazzoli[2], A. Vasiliev[3], L. Bezmaternikh[4], Bernd Büchner[1], and Jochen Geck[1] — [1]IFW, Dresden, Germany — [2]ESRF, Grenoble, France — [3]Moscow State University, Moscow, Russia — [4]L. V. Kirensky Institute of Physics, Russian Academy of Sciences, Krasnoyarsk, Russia

Multiferroic $NdFe_3(BO_3)_4$ exhibits a strong magnetoelectric coupling, since at 2K the electric polarization raises rapidly to $400\,\mu C/m^2$ upon increasing the applied magnetic field to 2T [1]. We study this coupling by resonant x-ray scattering at the Nd L- and Fe K edges as a function of temperature and applied magnetic field. Employing full polarization control, the field dependence of the different magnetic phases has been characterized at the Nd L_2 edge. We find that the commensurate phase at 20K and no magnetic field is different from the commensurate phase induced by the magnetic field at 2K [2].

[1] A. Zvezdin et al., JMMM, 300, 224 (2006)

[2] J. E. Hamann-Borrero et al., Phys. Rev. B, 82, 094411 (2010)

DS 11: Multiferroics: Matter at low temperature (jointly with MA, DF, TT, KR)

Time: Monday 16:45–18:00 Location: H 3005

Invited Talk DS 11.1 Mon 16:45 H 3005

Multiferroicity in an organic charge-transfer salt: Electric-dipole-driven magnetism — •Peter Lunkenheimer[1], Jens Müller[2], Stephan Krohns[1], Florian Schrettle[1], Alois Loidl[1], and Michael Lang[2] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]Institute of Physics, Goethe-University Frankfurt, Germany

Multiferroics, showing simultaneous electrical and magnetic ordering, are remarkable materials from both an academic and technological point of view. A prominent mechanism is the spin-driven ferroelectricity, often found in materials with helical spin order. However, recently a different mechanism, namely purely electronic ferroelectricity, where charge order breaks inversion symmetry, has attracted considerable interest. In the present talk, I will treat examples for both types of multiferroics like perovskite manganites and magnetite, concentrating on their dielectric properties, which often are only poorly characterized. An especially interesting case is a two-dimensional organic charge-transfer salt, which shows ferroelectricity, accompanied by antiferromagnetic spin order and belongs to a new class of multiferroics [1]. In this material, the ferroelectric ordering leads to a breaking of spin frustration, which triggers simultaneous dipolar and spin order. Hence, here the spin order is driven by the ferroelectricity, in marked contrast to the spin-driven ferroelectricity in helical magnets.

[1] P. Lunkenheimer, J. Müller, S. Krohns, F. Schrettle, A. Loidl, B. Hartmann, R. Rommel, M. de Souza, C. Hotta, J.A. Schlueter, M. Lang, preprint (arXiv:1111.2752).

DS 11.2 Mon 17:15 H 3005

Critical dynamics in $LiCuVO_4$ — •Christoph Grams[1], Maximilian Schalenbach[1], Daniel Niermann[1], Sandra Niesen[1], Petra Becker[2], and Joachim Hemberger[1] — [1]II. Physikalisches Institut,

Universität zu Köln, Germany — [2]Institut für Kristallographie, Universität zu Köln, Germany

Without an external magnetic field $LiCuVO_4$ has a phase transition into a cycloidal spin ordered phase below 2.3 K where it simultaneously is antiferromagnetic and ferroelectric. The transition temperature of this phase transition can be lowered with increasing magnetic field.

Ferroelectric phase transitions are of continuous fashion and are accompanied with a symmetry lowering that yields soft modes. Near the critical point the dynamics of the ionic polarization mechanisms are slowed down and therefore denoted as critical ("critical slowing down").

We observe the critical dynamics of the low temperature multiferroic phase transition of $LiCuVO_4$ with broadband dielectric spectroscopy. Therefore the compound's dielectric response to an external electric AC field of frequencies from 10 mHz to several GHz in the temperature range 20 mK to 300 K was measured in dependence of magnetic fields up to 14 T.

Work supported by the DFG through SFB 608.

DS 11.3 Mon 17:30 H 3005

Vortex domain walls in helical magnets — •Thomas Nattermann[1], Fuxian Li[2], and Valery L. Pokrovsky[2,3] — [1]Institut für Theoretische Physik, Universität zu Köln, D-50937 Köln, Germany — [2]Department of Physics, Texas A&M University, College Station, Texas 77843-4242 — [3]Landau Institute for Theoretical Physics, Chernogolovka, Moscow District, 142432, Russia

The theory of domain walls in both centrosymmetric and non-centrosymmetric helical magnets is presented. With the exception of discrete orientations domain walls consist of an array of parallel vortex lines, their width is only weakly depending anisotropy, in contrast to ferromagnets and antiferromagnets. In conical phases vortex walls carry Berry phase flux which gives rise to an anomalous Hall effect. In multi-ferroics vortices are electrically charged.

DS 11.4 Mon 17:45 H 3005

Infrared and THz spectroscopy in multiferroic $Eu_{1-x}Ho_xMnO_3$ — •Zhenyu Chen[1], Michael Schmidt[1], Franz Mayr[1], Zhe Wang[1], A.A. Mukhin[2], Joachim Deisenhofer[1], and Alois Loidl[1] — [1]Experimentalphysik V, EKM, University of Augsburg, 86135 Augsburg, Germany — [2]General Physics Institute of the Russian Academy of Sciences, 119991 Moscow, Russia

We investigated $Eu_{1-x}Ho_xMnO_3$ with the concentration varying from 0.1 to 0.5. On cooling, $Eu_{0.9}Ho_{0.1}MnO_3$ enters an incommensurate antiferromagnetic phase, which turns into an commensurate antiferromagnetic one at lower temperatures. Doping leads to ferroelectricity with polarization parallel to the a-axis, which flips to P//c by further doping. In order to detect the coupling between low energy phonons and electromagnons [1-4], we performed systematic polarization dependent IR and THz studies. The data will be compared to $TbMnO_3$ and the related system $Eu_{1-x}Y_xMnO_3$.

[1] A.Pimenov et al., Nature Phys., 2, 97(2006).
[2] A.Pimenov et al., Phys. Rev. B, 77, 014438(2008).
[3] N.Kida et al., Phys. Rev. B, 78, 104414(2008).
[4] R.Valdés Aguilar et al., Phys. Rev. Lett., 102, 047203(2009).

DS 12: FePt Nanoparticles (jointly with MA, MM – Organizer: Farle)

Time: Monday 15:00–17:45 Location: EB 202

Topical Talk DS 12.1 Mon 15:00 EB 202

Prediction of morphology-, composition- and size-related trends in FePt nanoparticles from first principles — •Markus Ernst Gruner — Faculty of Physics and Center for Nanointegration CeNiDE, University of Duisburg-Essen, 47048 Duisburg

Owed to the large magneto-crystalline anisotropy (MCA) of bulk FePt alloys, nanostructures with effective diameters as small as 4 nm are considered for ultra-high density recording applications. Structural defects as multiple twinning, segregation and partial ordering effectively reduce the MCA and thus severely limit the integration density. First principles calculations in the framework of density functional theory permit independent insight into the size-dependent interrelation between composition, structural stability and magnetism granting access to the electronic level. Site-resolved orbital moments and MCA are obtained a fully relativistic treatment including spin-orbit interaction.

Large scale calculations with up to 1415 atoms demonstrate that for diameters around 4 nm a close competition between multiply twinned and single crystalline morphologies is present, while the low energy of Pt surfaces enhances segregation. The systematic variation of 3*d* and 5*d* components reveals that especially addition of Mn can reduce twinning, while complicating the magnetic configuration. Structural and electronic changes which may degrade the magnetic properties must also be expected from a protective encapsulation with main group elements.

Topical Talk DS 12.2 Mon 15:30 EB 202

Coulomb Blockade effects in FePt nanoparticles — •Artur Erbe[1], Ulrich Wiesenhütter[1], Darius Pohl[2], Bernd Rellinghaus[2], and Jürgen Fassbender[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf — [2]IFW Dresden

In order to correlate the size and crystallinity of FePt nanoparticles with their respective electrical and mangeto-electrical properties individual nanoparticles are contacted using electron beam lithography. The particles are prepared from gas phase on electron transparent SiN membranes which allows the transmission electron microscopy of the same nanoparticle which is characterized electrically. The fabrication results in junctions, in which single FePt nanoparticles are connected to external leads. These junctions are tested electronically by measuring the current-voltage characteristics at various gate voltages, temperatures and magnetic fields. We observe Coulomb Blockade effects which are in agreement with the dimensions obtained from the TEM studies. The results of the magnetic nanoparticles are compared to measurements taken on Au nanoparticles of similar sizes.

Topical Talk DS 12.3 Mon 16:00 EB 202

Pt surface segregation and its impact on magnetism in FePt nanoparticles — •Ulf Wiedwald — Institut für Festkörperphysik, Universität Ulm, Albert-Einstein-Allee 11, 89069 Ulm, Germany

The appealing magnetic properties of chemically ordered FePt alloys strongly depend on composition. In nanoparticles with diameters below 10 nm the relative number of surface-near atoms strongly increases, thus any tendency of segregation will significantly change the stoichiometry of the interior. As a result, magnetic moments as well as magnetic anisotropy may vary compared to the bulk. In the frame of the collaborative research center SFB 569 we prepared size-selected, hexagonally arranged metallic particles by precursor loaded reverse micelles and plasma etching [1]. Pt segregation [2] and its impact on magnetism were examined in-situ for naked, non-interacting FePt particles on Si/SiO_2 as function of size (2-10nm) by photoelectron spectroscopy and x-ray magnetic circular dichroism. For partially $L1_0$-ordered particles we observe reduced spin moments with decreasing diameter while the orbital moment is found rather independent of size. As connected to the orbital magnetism, the effective magnetic anisotropy is also conserved for decreasing diameters, though reduced relative to the bulk [3]. Reasons for these astonishing observations are discussed.

[1] A. Ethirajan, U. Wiedwald, et al., Adv. Mater. 19, 406 (2007).
[2] L. Han, U. Wiedwald, B. Kuerbanjiang, P. Ziemann, Nanotechnology 20, 285706 (2009).
[3] U. Wiedwald, L. Han, J. Biskupek, U. Kaiser, P. Ziemann, Beilstein J. Nanotechnol. 1, 24 (2010).

Topical Talk DS 12.4 Mon 16:30 EB 202

Understanding the Metal-Carbon Interface in FePt terminated carbon nanotubes — •Darius Pohl[1], Franziska Schäffel[1], Christine Täschner[1], Marc H. Rümmeli[1], Christian Kisielowski[2], Ludwig Schultz[1], and Bernd Rellinghaus[1] — [1]IFW Dresden, P.O. Box 270116, Dresden, D-01171, Germany — [2]Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

Plasma-enhanced chemical vapour deposition (PE-CVD) onto FePt catalyst films is used to synthesize carbon nanotubes (CNT) which are teminated with L10-ordered FePt nanomagnets with high magnetic anisotropy [1]. The CNT are characterized by means of low voltage aberration-corrected HRTEM. To gain a deeper insight into the growth mechanism and in order to understand the relative crystallographic orientation of the particles with respect to the CNT axes structural investigations are conducted with a strong focus on the atomically resolved characterisation of the FePt-CNT interface. An interface-near expansion of the metal lattice is observed and attributed to a segregation of Pt towards the surface of the catalyst particle. Detailed statistical HRTEM analyses of these interfaces reveal that the CNT preferentially emanate from {111} facets of the catalyst particle. Molecular dynamic simulations were conducted to estimate the desorption energy of carbon atoms for various surfaces. Our results indicate that the physical principle based upon which the interfacial metal facet is chosen is a reduction of the desorption energy for carbon [2].

[1] F. Schäffel et al., Appl. Phys. Lett. 94 (2009) 193197.
[2] D. Pohl et al., Phys. Rev. Lett. 107 (2011) 185501.

Topical Talk DS 12.5 Mon 17:00 EB 202

Atomistic characterisation of ultrahard nanomagnets — •Carolin Antoniak — Experimentalphysik/AG Wende and Center for Nanointegration Duisburg-Essen (CeNIDE), Universität Duisburg-Essen, Lotharstr. 1, 47057 Duisburg

A combination of x-ray absorption spectroscopy (XAS) and density functional theory (DFT) has been used to study the magnetic properties like spin and orbital magnetic moments and effective magnetocrystalline anisotropy of chemically ordered FePt nanoparticles on an atomistic lengthscale. By choosing the appropriate capping material, these properties can be tuned between hard and soft magnetic with either high or low magnetic moments [1]. Focus of this talk will be the results of XAS allowing for an element-specific analysis of magnetic properties. Complemented with DFT calculations, it helps to gain more insight to the mutual influence of nanoparticles and capping material allowing to state design guidelines for improved materials which will be presented in this contribution.

This work was done in collaboration with M.E. Gruner, M. Spasova, A. Rogalev, F. Wilhelm, A.V. Trunova, F.M. Römer, A. Warland, B. Krumme, K. Fauth, S. Sun, P. Entel, M. Farle, and H. Wende. We thank the HZB-BESSYII and ESRF staff as well as the staff of the Jülich Supercomputing Center, and P. Vezolle of IBM for their kind support. Funded by BMBF (05 ES3XBA/5), EU and DFG (SFB445, SPP1239)

[1] C. Antoniak, M.E. Gruner et al., Nature Comm. 2, 528 (2011)

15 min. break

DS 13: Focused electron beam induced processing for the fabrication of nanostructures II (focused session, jointly with O – Organizers: Huth, Marbach)

Time: Tuesday 9:30–11:30 Location: H 0111

Invited Talk DS 13.1 Tue 9:30 H 0111

Free electrons for building nanodevices — •Ivo Utke — Empa, Swiss Federal Laboratories for Materials Science and Technology, Thun, Switzerland

Finely focused electron beams in scanning electron microscopes are routinely used to visualize small nanometer-sized objects. But add chemistry and they give you materials and structures for exciting physics to do at the nanometer scale! When functional gas molecules (metal-carbonyls, siloxanes, biphenyls, etc.) are injected into an electron microscope chamber held at a pressure of 1e-6 mbar or lower, they form adsorbed layers on many substrates. Focused electron beams can interact with these molecular layers, triggering surface reactions that can be used to locally etch or deposit, or to induce intermolecular reactions between the adsorbed molecules. All of these focused electron beam induced processes (FEBIP) can be performed on almost any kind of substrate [1]. This presentation will cover the fundamentals of FEBIP and give a state of the art overview on exciting nanodevices realized in the fields nanoelectronics, nanomechanics, nanophotonics, and nano(bio)sensors. Special attention will be given to FEBIP with two molecules involved, which led to the development of high performance magnetic sensors [2] having applications in bead detection.

[1] I. Utke, A. Gölzhäuser, Angew. Chem. Int. Ed. 2010, 49, 9328.
[2] L. Bernau et al., Angew. Chem. Int. Ed. 2010, 49, 8880.

Topical Talk DS 13.2 Tue 10:00 H 0111

From electronic correlations to strain sensing: Nanongranular metals and their applications — •Christian Schwalb, Marcel Winhold, Fabrizio Porrati, Roland Sachser, and Michael Huth — Physikalisches Institut, Goethe-Universität, Max-von-Laue-Str.1, 60438 Frankfurt am Main

Granular metals are artificial materials that consist of a conducting phase of metallic nanoparticles embedded in a carbon-rich dielectric matrix. The charge transport in such systems is dominated by tunneling between neighboring metallic nanoparticles, a process that is strongly influenced by correlation effects, such as the Coulomb blockade in the limit of weak inter-grain coupling. Additionally the tunneling coupling in these materials has an intrinsically exponential dependence on the inter-grain distance.

In this work, we present a practical application for these fundamental processes. Using focused electron-beam-induced deposition (FEBID) we can create strain-sensing elements based on nanogranular metals. The gauge factor for these sensing elements depends on their conductivity that can be altered by electron-beam irradiation leading to a change in the sensitivity that can be attributed to a persistent change of the dielectric carbon matrix. Due to the high resolution of the FEBID process strain-sensing elements with dimensions below 20 nm are feasible, therefore enabling, e.g., the fabrication of nano-cantilevers for ultra-fast AFM applications.

Topical Talk DS 13.3 Tue 10:30 H 0111

Tailored cobalt nanostructures by FEBID — •José M. de Teresa[1,2], Rosa Córdoba[2], Luis Serrano-Ramón[1,2], Amalio Fernández-Pacheco[1,2], and Ricardo Ibarra[1,2] — [1]Instituto de Ciencia de Materiales de Aragón, Universidad de Zaragoza-CSIC, Spain — [2]Laboratorio de Microscopías Avanzadas, Instituto de Nanociencia de Aragón, Universidad de Zaragoza, Spain

Focused-electron-beam-induced-deposition (FEBID) using Co2(CO)8 gas precursor allows the direct writing of cobalt-based magnetic structures [1]. We first grew high-purity cobalt structures with FEBID using high beam currents [2, 3]. The coercive field of these structures can be controlled via the shape anisotropy [4], and single-domain behavior can be observed [5]. Interestingly, the domain-wall propagation field can be lower than the domain-wall nucleation field, with potential magnetic applications [6]. The spin polarization of these cobalt deposits is large enough for its use in Spin Electronics [7]. We have recently achieved the growth of narrow high-cobalt-content nanowires (30 nm) and Hall sensors (100 nm), opening the route for the growth of cobalt structures tailored at the nanoscale [8].

[1] I. Utke et al., J. Vac. Sci. Technol. B 26 (2008) 1197 [2] A. Fernández-Pacheco et al, J.Phys. D: Appl. Phys. 42 (2009) 055005 [3] R. Córdoba et al., Nanoscale Res. Lett. 6 (2011) 592 [4] A. Fernández-Pacheco et al, Nanotechnology 20 (2009) 475704 [5] M. Jafaar et al., Nanoscale Res. Lett. 6 (2011) 407 [6] A. Fernández-Pacheco et al, Appl. Phys. Lett. 94 (2009) 192509 [7] S. Sangiao et al., Solid State Commun. 151 (2011) 37 [8] L. Serrano-Ramón et al., ACSnano 5 (2011) 7781

DS 13.4 Tue 11:00 H 0111

Structural, electrical and magnetic properties of CoPt-C alloys prepared by focused electron-beam induced deposition — •Fabrizio Porrati[1], Evgenyia Begun[1], Marcel Winhold[1], Roland Sachser[1], Achilleas Frangakis[2], and Michael Huth[1] — [1]Physikalisches Institut, Goethe Universität, Frankfurt am Main — [2]Institut für Biophysik, Goethe Universität, Frankfurt am Main

CoPt-C binary alloys have been fabricated by focused electron beam-induced deposition with the simultaneous use of the $Co_2(CO)_8$ and $(CH_3)_3CH_3C_5H_4Pt$ precursor gases. The alloys are made of CoPt nanoparticles embedded in a carbonaceous matrix. TEM investigations show that as-grown samples are in an amorphous phase. By means of a post-growth low-energy electron irradiation treatment the CoPt nanoparticles transform into face-centred tetragonal $L1_0$ CoPt nanocrystallites. In pararrel, the system undergoes a transition from a superparamagnetic to a ferromagnetic state at room temperature. By variation of the post-growth electron irradiation time the electrical-and magneto-transport properties of the alloy can be continuously tuned.

DS 13.5 Tue 11:15 H 0111

Electron Beam Induced Surface Activation of Oxide Surfaces for Nanofabrication — •Florian Vollnhals[1], Tom Woolcot[2], Steffen Seiler[1], Marie-Madeleine Walz[1], Hans-Peter Steinrück[1], Geoff Thornton[2], and Hubertus Marbach[1] — [1]Lehrstuhl für Physikalische Chemie II and Interdisciplinary Center for Molecular Materials (ICMM), Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen — [2]London Centre for Nanotechnology and Department of Chemistry, University College London, 17-19 Gordon Street, London WC1H 0AH, UK

The controlled fabrication of structures on the nanoscale is a major challenge in science and engineering. Direct-write techniques like Electron Beam Induced Deposition (EBID) were shown to be suitable tools in this context. Recently, Electron Beam Induced Surface Activation (EBISA) has been introduced as a new focused electron beam technique. In EBISA, a surface, e.g. SiO_2, is irradiated by a focused electron beam, resulting in an activation of the exposed area. The activated area can then react and decompose precursor gases like iron pentacarbonyl, $Fe(CO)_5$. This leads to a primary deposit, which continues to grow autocatalytically as long as $Fe(CO)_5$ is supplied, resulting in pure (>90%at.), crystalline iron nanostructures.[1] We expand the use of this concept by exploring EBISA to produce metallic nanostructures on $TiO_2(110)$ in UHV; atomistic insight into the process is obtained via Scanning Tunneling Microscopy (STM) and chemical insight via Auger Electron Specroscopy (AES). Supported by the DFG (MA4246/1-2).

[1] M.-M. Walz et al., Angew. Chem. Int. Ed. 49 (2010), 4669

DS 14: Ion irradiation effects

Time: Tuesday 11:45–12:45 Location: H 0111

DS 14.1 Tue 11:45 H 0111

In-Situ Investigation of Swift Heavy Ion Induced Dewetting in Edge- and Hole-Symmetry — •Knut Dautel, Redi Ferhati, Daniel Garmatter, Susanne Weidenfeld, and Wolfgang Bolse — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart

Previous experiments have shown that swift heavy ion (SHI) irradiation of thin oxide films on Si-substrates results in dewetting patterns even at temperatures far below the coatings melting point [1]. It was found that an initially coherent and smooth film under SHI bombardment breaks up into circular holes which then grow in diameter until they coalesce and form a meander- or dot-like structure of the film material. In our present study we have extended the materials range by the metallic glass $Fe_{40}Ni_{40}B_{20}$, in addition to NiO and Fe_2O_3, and furthermore changed the initial geometry by coating only half of the substrate, with a sharp edge between the uncovered and the covered side. In this case different dewetting kinetics are expected because of the infinite lateral curvature radius of the backward moving edge as compared to the circular rim around holes (which also form in the coherent part of the film). The experiments were carried out with our in-situ SEM/EDX-setup at the UNILAC accelerator of the Helmholtz Center for Heavy Ion Research (GSI) as decribed in [2]. We will compare the dewetting rates for the above mentioned different symmetries and materials in order to shed light on the dewetting mechanisms and the driving forces. [1] T. Bolse, et al., Nucl. Instr. Meth. 245 (2006), [2] S. Amirthapandian et al., Rev. Sci. Instr. 81 (2010)

DS 14.2 Tue 12:00 H 0111

Ion implantation-induced defects in Oxide Dispersion Strengthened (ODS) steel probed by positron annihilation spectroscopy — •Wolfgang Anwand[1], Maik Butterling[1], Gerhard Brauer[1], Andreas Wagner[1], Astrid Richter[2], Reinhard Koegler[3], and C.-L. Chen[4] — [1]HZDR, Institut für Strahlenphysik — [2]Technische Hochschule Wildau — [3]HZDR, Institut für Ionenstrahlphysik und Materialforschung — [4]I-Shou University, Kaohsiung, Taiwan

ODS steel is a promising candidate for an application in fission and fusion power plants of a new generation because of its advantageous properties as stability and temperature resistance. A microscopic understanding of the physical reasons of the mechanical and thermal properties as well as the behaviour of the material under irradiation is an important pre-condition for such applications. The investigated ODS FeCrAl alloy *PM2000* has been produced in a powder metallurgical way. Neutron-induced damage at ODS steel was simulated by He+ and Fe2+ co-implantation with energies of 2.5 MeV and 400 keV, respectively, and different fluences. The implantation has been carried out with a dual ion beam which enables a simultaneous implantation of both ion types. Thereby the Fe2+ implantation was used for the creation of radiation defects, and He+ was implanted in order to reproduce He bubbles as they are expected to appear by neutron irradiation. The implantation-induced damage was investigated by depth dependent Doppler broadening measurements using a variable energy slow positron beam.

DS 14.3 Tue 12:15 H 0111

Ion beam induced stress formation and relaxation in semiconductors — Tobias Steinbach, •Aaron Reupert, and Werner Wesch — Institute of Solid State Physics, Friedrich Schiller University Jena

The irradiation of crystalline semiconductors leads to the formation of defects, which accumulate with increasing ion fluence until in many materials a continuous amorphous surface layer is formed. In general, this phase transition causes expansion of the materials due to density change, which consequently leads to the formation of stress. However only a few studies on ion beam induced stress phenomena have been made, even though stresses in microelectronic structures cause substrate bending, delamination and cracking as well as anomalous diffusion of dopands. To investigate the ion beam induced formation and relaxation of stress due to density change and plastic phenomena in semiconductors a new modified scanning laser reflection technique based on the concepts of Volkert[1]. was established at the FSU Jena. By means of this technique the bending of a freestanding sample away from the irradiated surface is defined by the compensation of forces and moments between the underlying substrate and the irradiated regions. We present a brief overview of the configuration and the general principle of this technique. Furthermore, first results from wafer curvature measurements made during amorphization are shown for the irradiation of germanium and silicon. The results will be discussed based on the effects of density change, radiation-enhanced plastic flow and plastic deformation. [1]C. Volkert, J. Appl. Phys. 70, 3521 (1991)

DS 14.4 Tue 12:30 H 0111

In-Situ Analysis of Nanostructures Induced by Slow Highly Charged Ions — •Richard A. Wilhelm, René Heller, and Stefan Facsko — Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

The sum of the binding energies of all missing electrons (potential energy) of highly charged ions can induce surface modifications on the nanometer scale. We present results of a set-up for slow highly charged ion irradiations and scanning probe microscopy studies under in-situ conditions. A Dresden-EBIT is used to provide ions of different species with charge states up to $q = 40$ (e.g. for Xe). An electrostatic deceleration lens system allows to vary the kinetic energies of the ions in the range of $10\text{eV}\cdot q$ up to $5\text{keV}\cdot q$. Furthermore, we studied surface nanostructures on various substrates by an Omicron ultra high vacuum (UHV) scanning probe microscope, which is directly connected to the ion source. The size and the shape of nanostructures created by the deposition of potential energy and analyzed in-situ under UHV conditions are discussed and compared to those observed by recent studies under ex-situ conditions.

DS 15: Organic electronics and photovoltaics: simulations and optics I (jointly with CPP, HL, O)

Time: Tuesday 9:30–11:15 Location: H 2032

DS 15.1 Tue 9:30 H 2032

Excited states of terminally dicyanovinyl-substituted oligothiophenes and C_{60}: Frenkel vs. charge-transfer excitons — •Björn Baumeier[1], Denis Andrienko[1], and Michael Rohlfing[2] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Department of Physics, University of Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany

Excited states of terminally dicyanovinyl-substituted oligothiophenes (DCVnT) and C_{60}, a donor-acceptor combination used in state-of-the-art small-molecule-based organic photovoltaic devices, are studied using *ab initio* many-body Green's functions theory within the *GW* approximation and the Bethe-Salpeter equation. Calculations including resonant-antiresonant transition coupling and dynamical screening for DCVnT monomers yield excitation energies in excellent agreement with spectroscopic data. More importantly, it is possible with this approach to explicitly treat excited states in model dimers of DCVnT and C_{60}. This in particular allows to gain nanoscale insight into the relative energies of local (Frenkel) and charge-transfer excitations, which influence the charge generation in devices.

We will present results for model systems of DCV4T:C_{60} and DCV5T:C_{60} and will analyze the dependence of the relative excitations on, e.g., the arrangement of donor and acceptor molecules in the dimer and the length of the donor, as well as discuss the consequences for performance in organic photovoltaic devices.

DS 15.2 Tue 9:45 H 2032

Microscopic simulations of charge transport in disordered organic semiconductors — •Denis Andrienko, Bjoern Baumeier, Falk May, Manuel Schrader, and Victor Ruehle — Max Planck Institute for Polymer Research, Mainz, Germany

Charge carrier dynamics in an organic semiconductor can often be described in terms of charge hopping between localized states. The hopping rates depend on electronic coupling elements, reorganization energies, and driving forces, which vary as a function of position and orientation of the molecules. The exact evaluation of these contributions in a molecular assembly is computationally prohibitive. Various, often semi-empirical, approximations are employed instead. In this work, we review some of these approaches and introduce a software toolkit which implements them.[1] The purpose of the toolkit is to simplify the workflow for charge transport simulations, provide a uniform error-control for the methods, flexible platform for their development, and eventually allow in silico pre-screening of organic semiconductors for specific applications. All implemented methods are illustrated by studying charge transport in amorphous films of tris(8-hydroxyquine)aluminium, a common organic semiconductor.

[1] V. Rühle, A. Lukyanov, F. May, M. Schrader, T. Vehoff, J. Kirkpatrick, B. Baumeier, D. Andrienko, J. Chem. Theory Comput., 7, 3335 (2011)

DS 15.3 Tue 10:00 H 2032

Migration of singlet excitons in thin films of oligothiophene molecules — •Jens Ludwig, Susanne Hintschich, Hannah Ziehlke, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, Technische Universität Dresden, 01069 Dresden, Germany

In organic materials, such as thin amorphous films of oligothiophenes, localized singlet excitons constitute the primary photoexcitations. Via Förster Resonant Energy Transfer (FRET) they migrate between different molecular sites, represented by an inhomogeneously broadened density of states (DOS).

Dispersive exciton migration in thin films of dicyano-substituted terthiophenes is probed by time resolved spectroscopy using a streak camera and simulated with a Monte-Carlo program based on thermally activated hopping of excitons. The time-resolved spectral relaxation and its temperature dependence, as well as the energy dependent decay curves are consistently described within this picture. Side chains appended to the backbone of the oligothiophenes impact the morphology and average intermolecular distance and hence significantly influence the efficiency of exciton migration. In this presentation, oligothiophene derivates with different side chains are compared regarding their exciton dynamics in thin films. We also consider energy transfer to C_{60} in blend layers with the terthiophene derivatives, leading to a very fast quenching of luminescence from the terthiophene molecules.

DS 15.4 Tue 10:15 H 2032

Vibrational Davydov-splittings in oriented organic semiconductor crystals: polarization-dependent measurements versus theoretical calculations — •Tobias Breuer[1], Mali Celik[2], Peter Jakob[3], Ralf Tonner[2], and Gregor Witte[1] — [1]AG Molekulare Festkörperphysik — [2]AG Theoretische Oberflächenchemie — [3]AG Oberflächenphysik, Philipps-Universität Marburg, D-35032 Marburg

Vibrational properties of highly ordered crystalline perfluoropentacene (PFP) films epitaxially grown on KCl(100) and NaF(100) substrates have been studied by means of transmission infrared spectroscopy and density functional theory. The different molecular orientations adopted by PFP on both substrates (standing vs. lying) and their epitaxial ordering [1] enable precise polarization-resolved measurements along individual crystallographic directions and thus allow an unambiguous experimental determination of the polarizations of the IR modes. Computations of the vibrational spectra beyond the single-molecule approximation were employed at the periodic dispersion-corrected density functional level (PBE-D2PBC) and compared to non-periodic calculations (PBE/def2-TZVPP). Thereby, a comparison between experiment and different theoretical models was enabled. A microscopic explanation for the experimentally observed Davydov splitting of some modes and the IR-inactivity of others was derived, based on the mutual coupling of the dynamical dipole moments of the two molecules within the unit cell.

[1] T. Breuer et al., Phys. Rev. B 83, 155428 (2011).

DS 15.5 Tue 10:30 H 2032

XPS investigation of charge transfer complexes with strong donor / acceptor molecules: composites and interfaces — •Sebastian Stolz, Eric Mankel, Julia Maibach, Thomas Mayer, and Wolfram Jaegermann — Technische Universität Darmstadt, Materials Science Institute, Surface Science Division, Petersenstraße 32, 64287 Darmstadt, Germany

Organic charge transfer complexes like TTF-TCNQ have raised interest due to their electronic and optical properties being highly sensitive to small variations of the molecular constituents. In this manner, the electrical properties of TTF-TCNQ and its derivates vary significantly, and hence different applications for organic electronic devices are imaginable. Thin film layers of DBTTF-TCNQ were prepared in UHV and inert atmospheres respectively to avoid contamination. Preparation methods used were (1) evaporation of solution grown crystals, (2) drop casting under Ar atmosphere, and (3) co-evaporation of the individual molecules with varying donor / acceptor ratios. Additionally, DBTTF was deposited stepwise onto a clean TCNQ substrate in order to investigate the reaction mechanism. The resulting thin films were analyzed by in-situ photoemission spectroscopy, partially carried out at the U49/2 beamline at Bessy II. The stoichiometric ratio of donor and acceptor molecules was determined and the formation of the CT-complex was confirmed for all samples. In case of a stoichiometric ratio unequal to 1:1, the spectra show a mixture of the CT-complex and neutral excess molecules. Finally, the experimentally determined spectra were compared to DFT-calculations.

DS 15.6 Tue 10:45 H 2032

A new differential reflectance spectroscopy method with enhanced sensitivity — •Harald Zaglmayr, Lidong Sun, and Peter Zeppenfeld — Institute of Experimental Physics, Johannes Kepler Univeristät, Linz, Austria

Differential reflectance spectroscopy (DRS), measures the normalized difference of the reflectance of the bare and adsorbate covered surface, respectively. The technique possesses enhanced surface sensitivity and is thus widely used for the in-situ study of organic thin film growth [1,2]. The signal to noise ratio of the obtained spectra, which determines the sensitivity of the method, strongly depends on the stability of the light source. Here, we introduce a new method to overcome the influence of the instability of the light source by normalizing the spectrum of the reflected beam with that of the incident beam, which are measured simultaneously. Our approach shows a drastic improvement of the signal to noise ratio of the DR spectra. The new instrument has been successfully applied to monitor the in-situ growth of alpha-sexithiophene (α-6T) and cobalt-tetramethoxyphenylporphyrin (Co-TMPP) on the Cu(110)-(2x1)O reconstructed surface. The details of the technical realization and the scientific results concerning the organic thin film growth will be reported in this contribution.

[1] R.Forker, T.Fritz; Phys. Chem. Chem. Phys., 2009, 11, 2142-2155
[2] U.Heinemeyer *et al.*; Phys. Rev. Lett., 2001, 104, 257401

DS 15.7 Tue 11:00 H 2032

Interface Effects on the Glass Transition in Thin Polystyrene Films studied with High Temperature Single Molecule Fluorescence Microscopy — •Dominik Wöll[1], Bente Flier[2], Moritz Baier[2], Klaus Müllen[3], Stefan Mecking[2], and Andreas Zumbusch[2] — [1]Zukunftskolleg, Universität Konstanz, Germany — [2]Fachbereich Chemie, Universität Konstanz, Germany — [3]Max-Planck-Institut für Polymerforschung Mainz, Germany

The glass transition is a ubiquitous phenomenon in many materials. Despite its high importance and considerable research efforts, a full understanding of this property is still lacking. In thin polymer films, interfaces complicate things as they alter the glass transition in their vicinity. Experimental approaches to study the influence of interfaces on dynamics in polymers are thus very challenging. In our contribution, we present single molecule fluorescence spectroscopy as a new method to investigate such interfacial effects on the glass transition of polymers. We measured the translational diffusion coefficients of single perylene diimide molecules in thin polystyrene films up to temperatures of 150 °C and analyzed their distributions. These distributions and the number of mobile molecules depend strongly on film thickness. They can be modeled with Monte Carlo random walk simulations assuming a reduced glass transition temperature and an increased residence probability of dye molecules at the polymer surface.

DS 16: Organic electronics and photovoltaics: simulations and optics II (jointly with CPP, HL, O)

Time: Tuesday 11:30–13:00 Location: H 2032

DS 16.1 Tue 11:30 H 2032

Fast, stable and high-brightness light-emitting electrochemical cells — •Sebastian B. Meier[1,2], Daniel Tordera[3], Henk J. Bolink[3], Wiebke Sarfert[2], and Albrecht Winnacker[1] — [1]University of Erlangen-Nuremberg, Department of Materials Science, Chair VI: Materials for Electronics and Energy Technology, Erlangen, Germany — [2]Siemens AG, Corporate Technology, GTF Organic Electronics, Erlangen, Germany — [3]Instituto de Ciencia Molecular, Universitat de València, Paterna, Spain

Light-emitting electrochemical cells (LECs) are among one of the simplest class of light-emitting devices based on organic semiconducting materials. In its most facile form they just comprise a single solution-processed layer of an ionic transition metal complex (iTMC) sandwiched between two air-stable electrodes, which supports all the three events of charge injection, charge transport and radiative recombination. The ordinary architecture and the possibility to use stable electrode materials is a direct consequence of the ionic nature of the active layer enabling efficient charge injection with concomitant in-situ electrochemical doping resulting in the formation of a light-emitting p-i-n junction. There has been a longstanding issue in iTMC device operation between fast response and high stability when standard constant DC voltage is used, which is due to the dynamic nature of the junction. We will show how to stabilize the dynamic junction to achieve long-living (> 1000 h) high-brightness (> 1200 cd/m^2) iridium(III) iTMC-based LECs possessing simultaneous fast turn-on times (< 20s) at considerable light intensity (> 200 cd/m^2).

DS 16.2 Tue 11:45 H 2032

Charge Carrier Storage on Emitter Molecules in Organic Light-Emitting Diodes — •Caroline Weichsel[1], Sebastian Reineke[1,2], Björn Lüssem[1], and Karl Leo[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Str. 1, D-01069 Dresden, Germany — [2]Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA 02139, USA

In this contribution, we study trapping of charge carriers in phosphorescent organic light-emitting diodes (OLED) using the red emitter iridium(III)bis(2-methyldibenzo[f,h]quinoxaline) (acetylacetonate) [Ir(MDQ)2(acac)] by transient electroluminescence. We observe a transient overshoot exceeding regular light emission after voltage turn-off, which can be explained by delayed charge carrier recombination of charges stored in the emission layer. We study this mechanism by variation of the off-voltage and by adding thin quenching layers, which allow to determine the position of the emission zone during regular light emission and after voltage turn-off. Additionally, we show that the signal intensity is linearly proportional to the doping concentration. Investigations on the applied current and the pulse length show a saturation of the overshoot intensity, which we ascribe to the limited ability of emitter molecules to store electrons. We propose that this storage process negatively affects the external quantum efficiency of the OLED. We assume that the effect can also take place in other OLED structures and suggest that the methods presented here can help identifying charge carrier storage on emitter molecules.

DS 16.3 Tue 12:00 H 2032

Surface Modification Effect on Optical Anisotropy and Molecular Orientation of CuPc Thin Films — •L. Ding, M. Friedrich, O. Gordan, and D. R. T. Zahn — Semiconductor Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany

Copper phthalocyanine (CuPc), as an organic semiconductor, attracts much attention currently due to its potential application in organic electronic and photovoltaic devices. Molecular orientation plays a significant role to improve the device performance. In situ spectroscopic ellipsometry (SE) and reflection anisotropy spectroscopy (RAS) are employed simultaneously to investigate the out-of-plane and in-plane anisotropy as well as molecular orientation of CuPc thin films, respectively.

Chemically prepared octadecyltrichlorosilane (OTS) monolayer with upright standing molecules shows a significant influence on the out-of-plane anisotropy with an average out-of-plane tilt angle of 69.3° +/- 4.1° but little impact on the in-plane anisotropy. Nearly flat lying CuPc molecules are observed on thermally evaporated Perylene-3,4,9,10-tetracarboxylic-3,4,9,10-dianhydride (PTCDA) layers thicker than 3.4 nm, giving an average tilt angle of 19.7° +/- 8.0° due to the flat lying PTCDA molecules on Si. Meanwhile, the in-plane anisotropy of CuPc is much lower than that without PTCDA. The influence of the PTCDA layer thickness on molecular orientation can be explained by the island growth mode of PTCDA.

DS 16.4 Tue 12:15 H 2032

Stability of perfluroro-pentacene thin films on coinage metals — •Christian Schmidt[1], Tobias Breuer[1], Stefan Wippermann[2], Wolf Gero Schmidt[2], and Gregor Witte[1] — [1]Molekulare Festkörperphysik, Philipps-Universität Marburg, Germany — [2]Theoretische Physik, Universität Paderborn, Germany

The development of organic electronics greatly benefits from the systematic improvement of molecular properties by chemical functionalization. One example constitutes pentacene that can be prevented from oxidization by perfluorination. Topical investigations of the interface properties of perfluoropentacene (PFP) are frequently conducted only from an electronic point of view, measuring either macroscopic device properties or valence band spectra. In these studies possible chemical interactions have not been addressed since PFP is especially designed to be more stable than PEN. It was therefore unexpected that PFP monolayers on Cu(111) undergo degradation upon heating and that decomposition also occurs on Ag(111). This means that PFP is less stable than PEN, which desorbs intact from Ag(111). This behaviour is especially remarkable when considering that PFP is farther above metal surfaces than PEN. This unclear situation is very problematic, as the PFP-metal interface itself serves as a model system for electronic effects and is of vital interest in this field. Therefore, we systematically studied the thermal behaviour of PFP on the coinage metals by means of temperature NEXAFS and XPS. In order to understand underlying mechanisms we accompany our experimental data with density functional theory (DFT) calculations including chemical reactions.

DS 16.5 Tue 12:30 H 2032

Two dimensional band structure mapping of organic single crystals using the new generation electron energy analyzer ARTOF — •A. Vollmer[1], R. Ovsyannikov[1], M. Gorgoi[1], S. Krause[1], M. Oehzelt[1], N. Martensson[2], S. Svensson[2], P. Karlsson[3], M. Lundquist[3], J. Pflaum[4], T. Schmeiler[4], and N. Koch[1,5] — [1]Helmholtz Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [2]Uppsala University, Uppsala, Sweden — [3]VG Scienta, Uppsala, Sweden — [4]Universität Würzburg, Würzburg, Germany — [5]Humboldt-Universität zu Berlin, Berlin, Germany

We report on a novel type of photoemission instrument, the Angle Resolved Time Of Flight analyzer (ARTOF 10k)electron energy analyser. The instrument facilitates the simultaneous recording of kinetic energy and angular pattern of photoelectrons in a cone of up to 30° opening angle with very high energy resolution (100 μeV). Its transmission (250 times higher than in hemispherical analysers)allows for very mild conditions during the experiment turning the ARTOF into the predestined instrument to investigate sensitive specimens such as organic single crystals, as extremely low photon fluxes can be used. Even though organic single crystals are of increasing fundamental and applied scientific interest, knowledge of their electronic properties is still mainly based on theoretical calculations due to major experimental challenges in measuring photoemission. Here we present the band structures of rubrene and tetracene single crystals obtained with unprecedented quality using the ARTOF instrument within only a few hours of measurement time.

DS 16.6 Tue 12:45 H 2032

Electronic structure of prototypical organic-organic heterojunctions for photovoltaic applications — •Andreas Wilke[1], Raphael Schlesinger[1], Ullrich Hörmann[2], Jens Niederhausen[1], Johannes Frisch[1], Antje Vollmer[3], Julia Wagner[2], Mark Gruber[2], Andreas Opitz[1], Wolfgang Brütting[2], and Norbert Koch[1,3] — [1]Humboldt-Universität zu Berlin — [2]Universität Augsburg — [3]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH

In organic photovoltaic cells (OPVCs) typically two organic materials with electron acceptor and donor character are sandwiched between anode and cathode, forming either layered planar (PHJ) or bulk heterojunctions, where charge separation occurs. We report ultraviolet photoelectron spectroscopy (UPS) measurements done for three different organic-organic PHJs, comprising the donors sexithiophene (6T) and poly(3-hexylthiophene) (P3HT), and the acceptors diindenoperylene (DIP) and C60. The respective heterojunctions were formed on poly(ethylenedioxythiophene) : poly(styrenessulfonate) (PEDT:PSS) electrodes. The energy level alignment found experimentally for these heterojunctions are discussed in relationship to the open circuit voltages achieved in corresponding PHJ OPVCs. The offset between the highest occupied molecular orbital of the donor and the lowest unoccupied molecular orbital of the acceptor, an estimate for the maximum achievable open circuit voltage, peaked at 1.75 eV for the 6T/DIP PHJ. In actual OPVCs based on 6T/DIP, an open circuit voltage of up to 1.38 V was observed.

DS 17: Multiferroics III: Strain / New routes towards multiferroicity (jointly with MA, DF, KR, TT)

Time: Tuesday 9:30–12:45 Location: EB 301

DS 17.1 Tue 9:30 EB 301

Substrate influence on the strain in epitaxially grown $BiCrO_3$ thin films investigated using Raman spectroscopy and X-ray diffraction — •Andreas Talkenberger[1], Cameliu Himcinschi[1], Kannan Vijayanandhini[2], David Rafaja[3], Ionela Vrejoiu[2], Torsten Weissbach[1], Christian Röder[1], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute of Theoretical Physics, D-09596 Freiberg — [2]Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle — [3]TU Bergakademie Freiberg, Institute of Materials Science, D-09596 Freiberg

$BiCrO_3$ (BCO) is an interesting candidate for multiferroic applications. Therefore a deep understanding of the material properties and the fabrication of high quality epitaxial thin films is necessary. In this work we investigated epitaxially grown BCO thin films fabricated by pulsed laser deposition on $SrTiO_3$, LSAT, $NdGaO_3$ and $DyScO_3$ by means of Raman spectroscopy and X-ray diffraction (XRD). The shift of phonon modes at room temperature indicates different strains in the BCO films grown on the different substrates. Primarily, the XRD experiments helped to quantify the elastic lattice strains caused by the lattice misfit between the substrate and the thin films. The reciprocal space mapping was employed to follow the relaxation of the lattice strain through the formation of microstructure defects. This data was correlated to the observed Raman shifts. Using density functional theory the shifts of the Raman peaks were calculated for different strain states, and compared to the experimentally observed ones. This work is supported by the German Research Foundation DFG HI 1534/1-1.

DS 17.2 Tue 9:45 EB 301

Directly probing the effect of strain on magnetic exchange interactions — •Kathrin Dörr[1,2], Andreas Herklotz[2], Hans-Martin Christen[3], and Michael Biegalski[3] — [1]MLU Halle Wittenberg, Von-Danckelmann-Platz 3, 06120 Halle — [2]IFW Dresden, Postfach 270116, 01171 Dresden — [3]CNMS, Oak Ridge National Laboratory, Oak Ridge, TN 37830, USA

Thin films of transition metal oxides of the perovskite type ABO_3 (B = 3d or 4d metal) have revealed abundant examples for strain-driven changes of magnetic ordering. In spite of strong efforts, the theoretical treatment of magnetic exchange in complex oxides has remained a challenge, and experiments continue to show unpredicted large effects of the epitaxial strains in films. In order to provide meaningful experimental data on strain dependences, epitaxial thin films should be grown in various coherent strain states on different substrates without changing anything but the strain. This is inherently difficult: possible problems arise from a strain-dependent oxidation level or microstructure. As a complementary approach, the in-plane strain of epitaxial oxide films can be controlled reversibly by 0.1-0.2 percent using a piezoelectric substrate. I will address reversible-strain studies on $La_{0.7}Sr_{0.3}MnO_3$, $La_{1-x}Sr_xCoO_3$ (x = 0, 0.2, 0.3) und $SrRuO_3$ films, showing the strain response of the magnetic Curie temperature and the magnetization and discussing the current understanding of the strain effects on magnetic ordering.

DS 17.3 Tue 10:00 EB 301

Induced magnetoelectric response in Pnma perovskites — •Eric Bousquet and Nicola Spaldin — Materials Department, ETH Zurich, Switzerland

We use symmetry analysis to show that the *G*, *C* and *A*-type antiferromagnetic *Pnma* perovskites can exhibit magnetoelectric (ME) responses when a ferroelectric instability is induced with epitaxial strain. Using first-principles calculations we compute the values of the allowed ME response in strained $CaMnO_3$ as a model system. Our results show that large linear and non-linear ME responses are present and can diverge when close to the ferroelectric phase transition. By decomposing the electronic and ionic contributions, we explore the detailed mechanism of the ME response.

DS 17.4 Tue 10:15 EB 301

Search for strain-induced ferroelectricity in EuO films — •Carsten Becher[1], Masakazu Matsubara[1], Andreas Schmehl[2], Jochen Mannhart[3], Darrell G. Schlom[4], and Manfred Fiebig[1] — [1]Department of Materials, ETH Zürich, Switzerland — [2]Institut für Physik, Universität Augsburg, Germany — [3]Max Planck Institute for Solid State Research, Germany — [4]Department of Materials Science and Engineering, Cornell University, USA

Ferromagnetic EuO arouses a lot of interest due to a multitude of extreme properties, such as an insulator-metal transition, a colossal-exceptional magnetoresistance effect, and nearly 100 % spin polarization of the conduction electrons in the ferromagnetic state. In addition, recent theories predict that EuO becomes ferroelectric under epitaxial strains ≥ 4.2 %, suggesting a route to novel multiferroics combining ferromagnetic and ferroelectric order. Here, we use optical second harmonic generation (SHG) to detect changes of the electric as well as magnetic order of EuO thin films. In search of a strain-induced spontaneous polarization, we vary the sample temperature, apply electric and magnetic fields in various configurations, and use different photon energies of the incident laser pulses. So far, we verified that samples strained below 4 % do not display ferroelectricity. However, a new sample batch allows us to present results from EuO films with tensile strains up to 7 %.

DS 17.5 Tue 10:30 EB 301

On the lattice engineering of magnetoelectric couplin — •Michael Fechner and Nicola Spaldin — ETH Zurich, Department for Material Theory,CH-8093 Zurich, Switzerland

We present results of first-principles calculations of the microscopic origin of the linear magnetoelectric (ME) effect in Cr_2O_3. In general such magnetoelectric responses – that is the electric polarization created by an applied magnetic field – are small. Since they are composed of both electronic- and lattice-mediated contributions, however, an increase in the response can in principle be achieved by phonon engineering. Here we investigate this possibility by first calculating how the magnetic interaction parameters are affected by phonon modes of different symmetry, focussing particularly on those that are active in the ME coupling. We find that the exchange interactions are most strongly modified in the non-IR active rotational phonon modes which do not contribute to the ME response. We then calculate the effect on the ME response if these phonons are disabled. Based on our results we suggest new routes for engineering materials with enhanced ME couplings.

DS 17.6 Tue 10:45 EB 301

First principles study of Mn_2O_3 under pressure: Competition between Jahn-Teller distortion and charge disproportionation — •Carmen Quiroga and Rossitza Pentcheva — Dept. of Earth and Environmental Sciences, University of Munich

Contrary to most sesquioxides, which naturally occur in the corundum structure, Mn_2O_3 has a complex crystal structure corresponding to an orthorhombically distorted bixbyite [1], associated with the presence of the Jahn-Teller active Mn^{3+} cation. It has been suggested that the Jahn-Teller effect is inhibited under pressure, which could induce a phase transition to the corundum structure [2], from where the general transformation sequence of sesquioxides to perovskite and post-perovskite should follow. So far, however, only the post-perovskite has been reported experimentally above 27 GPa [3].

Using density functional theory calculations including an on-site Coulomb repulsion term, we explore the stability of the ambient phase α-Mn_2O_3 ($Pbca$) and candidate high-pressure polymorphs: corundum ($R\bar{3}c$), perovskite phases of Rh_2O_3 II ($Pbcn$) and $GdFeO_3$ ($Pbnm$) type and post-perovskite ($Cmcm$). In particular we focus on the effect of pressure on the charge, spin and structural degrees of freedom. Parallels to the pressure induced phase transitions in $MnTiO_3$ are discussed.

Funding by DFG SPP1236 (PE883/8-1) is acknowledged.

[1] S. Geller. Acta Crystallogr. **B27**, 821 (1971).
[2] C.T. Prewitt et al. Inorg. Chem. **8**, 1985 (1969).
[3] J. Santillán et al. Geophys. Res. Lett. **33**, L15307 (2006).

DS 17.7 Tue 11:00 EB 301

Investigation of Magnetoelectric Coupling in Self Assembled Ferromagnetic/Ferroelectric Heterostructures — •Fikret Yildiz[1], Chan-Ho Yang[2], Sinan Kazan[1], Yoon-He Jeong[2], and Bekir Aktas[1] — [1]Gebze Institute of Technology, Department of Physics, 41400 Gebze-Kocaeli, Turkey — [2]Pohang University of Science and Technology, Department of Physics, Pohang, 790-784 S. Korea

Creating ferromagnetic/ferroelectric heterostructures is a way for developing multifunctional materials which is called multiferroics. Exchange bias may be used to couple a normal ferromagnet to a ferroelectric antiferromagnet and thus create a multiferroic system with nonzero magnetization. In implementing this idea we developed a synthesis method for composite films of MnFe2O4 embedded in BiFeO3 [1]. The method utilizes the Bi volatility to obtain the composite films via thermal annealing of multilayer composed of BiFeO3 and BiMnO3. SEM measurements showed that the cluster size varies depending on the film thickness. The composite films possess both ferroelectric and ferromagnetic properties [1]. Magnetoelectric coupling (MEC) was investigated by Ferromagnetic resonance (FMR) technique. Analysis of FMR data showed that resonance field can be controlled by GHz range electric fields.

[1] C.H. Yang, F. Yildiz, S.H. Lee, Y.H. Jeong, U. Chon, T.Y. Koo, Apply Phys. Lett. 90, 163116 (2007).

DS 17.8 Tue 11:15 EB 301

Strain Determination in Magnetoelectric Composite Systems by X-ray Diffraction Methods — •Christian Koops[1], Madjid Abes[1], Stjepan Hrkac[1], Bridget Murphy[1], Olaf Magnussen[1], Eric Woltermann[2], Henry Greve[2], and Eckhard Quandt[2] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Germany — [2]Institut für Materialwissenschaft, Christian-Albrechts-Universität zu Kiel, Germany

Understanding the coupling at the interface between magnetostrictive and piezoelectric components in magnetoelectric composites (ME) is essential for the optimization of these composites for sensor applications. A large ME response is only possible if the lattice deformation induced by an external magnetic field in the magnetostrictive material can be transferred efficiently to the piezoelectric material. To study this coupling at the burried interface of ME composites we measured the lattice deformation in ZnO as the piezoelectric component by grazing incidence X-ray diffraction in an external magnetic field, using the high-resolution and high intensity X-ray beam provided by the Diamond Light Source (I16) and PETRA III (P08). We employ samples with thin layers of different magnetostrictive materials, $(Fe_{90}Co_{10})_{78}Si_{12}B_{10}$ and Terfenol-D, on the (001) surface of high quality, single crystalline ZnO substrates. From the Bragg peak positions we determined the interplanar spacings in the ZnO substrates close to the interface and the corresponding strain as a function of the applied magnetic field.

15 min. break

DS 17.9 Tue 11:45 EB 301

Relaxor ferroelectricity in pure and doped magnetite — •Eugen Ruff[1], Florian Schrettle[1], Stephan Krohns[1], Peter Lunkenheimer[1], Victor A. M. Brabers[2], and Alois Loidl[1] — [1]Experimental Physics V, University of Augsburg, 86135 Augsburg, Germany — [2]Department of Physics, Eindhoven University of Technology, 5600 MB Eindhoven, Netherlands

A possible example for a multiferroic material is the extensively studied magnetite Fe_3O_4, which shows charge-order (CO) below the Verwey transition at $T_V \approx 120\,K$ and is ferrimagnetically ordered below $500\,K$[1]. As shown in the present contribution, dielectric spectroscopy reveals a relaxation below T_V, indicating relaxorlike polar order in Fe_3O_4[2]. We find long-range ferroelectric order to be impeded by the continuous freezing of polar degrees of freedom and the formation of a tunneling-dominated glasslike state of electrons at low temperatures. To reveal the origin of the ferroelectric state, whose dielectric signature is partly superimposed by a so called Maxwell-Wagner (MW) relaxation, we have investigated doped samples with Al, Ga, and Mg. The dielectric spectra of these doped samples ($< 2\%$) provide further evidence for the relaxor ferroelectric state of Fe_3O_4 and demonstrate the influence of the MW relaxation.

[1] D. I. Khomskii, J. Magn. Magn. Mater. **306**, 1 (2006).

[2] F. Schrettle *et al.*, Phys. Rev. B **83**, 195109 (2011).

DS 17.10 Tue 12:00 EB 301

Full-potential DFT+U study of orbitally ordered systems: the importance of non-spherical contributions and double counting — •Adam Jakobsson[1,2], Biplab Sanyal[1], Ivetta Slipukhina[2], Marjana Ležaic[2], Ersoy Sasioglu[2], Gustav Bihlmayer[2], and Stefan Blügel[2] — [1]Department of Physics and Astronomy, Uppsala University, 75120 Uppsala, Sweden — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

DFT+U has for many years been a standard method to calculate properties of strongly correlated systems. Initially the method [1] was implemented in DFT-codes using the atomic sphere approximation (ASA) but was later also implemented into full potential DFT-codes. Various flavours of the double counting corrections used in the DFT+U method further add to the variety of different DFT+U functionals. The double counting corrections originally derived in the context of ASA are now routinely applied in full potential codes. Using the FLEUR

code [2], we have investigated the importance of the non-spherical potential and the issue of double counting for orbital ordering and magnetism, i.e. properties that play a crucial role in many multiferroic materials. A recent implementation [3] of the constrained-RPA method was used to obtain parameters for the DFT+U calculations. This work was supported by the Young Investigators Group Program of the Helmholtz Association, Germany, contract VH-NG-409.
[1] V. I. Anisimov et al. PRB **44**, 943-954 (1991) [2] www.flapw.de [3] E. Şaşıoğlu et al. PRB **83**, 121101(R) (2011).

DS 17.11 Tue 12:15 EB 301

***Ab initio* calculations of the magnetic properties of ordered perovskites** — •Igor Maznichenko[1], Alberto Marmodoro[2], Martin Lüders[3], Zdzislawa Szotek[3], Walter Temmerman[3], Ingrid Mertig[1,2], and Arthur Ernst[2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle (Saale), Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle (Saale), Germany — [3]Daresbury Laboratory, Daresbury, Warrington WA4 4AD, Cheshire, United Kingdom

Perovskites are of particular interest in condensed matter physics due to their remarkable electronic and magnetic properties. Colossal magnetoresistance, ferroelectricity, multiferroicity, superconductivity, charge ordering, orbital ordering, metal-insulator transition, Jahn-Teller, and other effects are observed in perovskites. All these properties are strongly depending on the type of cations. Here we present a first-principles study of electronic and magnetic properties of $La_{2/3}Sr_{1/3}MnO_3$ (LSMO), which is a strongly correlated $3d$ transition metal oxide with a Curie temperature of 370 K. For varying La/Sr ratios different types of antiferromagnetism are observed. Using a self-consistent KKR Green function method, we show how the electronic and magnetic properties of LSMO depend on the valency of Mn, ordering of different cations in the lattice, and their relative orientation to each other. The influence of the Mn–O–Mn angle on the double-exchange coupling was examined.

DS 17.12 Tue 12:30 EB 301

Crystal growth and scattering investigations of $YFe_2O_{4-\delta}$ — •Thomas Müller[1], Joost de Groot[1], Jörg Strempfer[2], and Manuel Angst[1] — [1]Peter Grünberg Institut PGI and Jülich Centre for Neutron Science JCNS, JARA-FIT, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Deutsches Elektronen-Synchrotron DESY, D-22607 Hamburg, Germany

$LuFe_2O_4$ is attracting attention as proposed multiferroic compound, but there is much less known about other isostructural rare-earth ferrites. We have grown single-crystals of $YFe_2O_{4-\delta}$ in a CO/CO_2-atmosphere to tune δ. Optimized crystals exhibit a magnetic behaviour identical to highly stoichiometric powder samples, i.e. two hysteretic phase transitions at 228 K and 180 K upon cooling.

Corresponding to these phases single-crystal x-ray-diffraction shows 3D-charge-ordered states, partially not compatible with the phases observed by electron diffraction [1]. At least one additional transition below 160 K, not present in magnetisation, is found in x-ray-diffraction. On one sample we found reflections at ($\frac{1}{3}$, $\frac{1}{3}$,half-integer) at 10 K , identical to the superstructure reflections of $LuFe_2O_4$. Nevertheless sample differences, due to different δ, have to be reviewed.

We further searched for anisotropy by resonant x-ray diffraction and full polarization analysis on superstructure reflections at PETRA III-P09. As for $LuFe_2O_4$ no anisotropy is observed. Although YFe_2O_4 has the same structure as $LuFe_2O_4$, the phases between 100 K and 230 K are totally different, showing much more complex incommensurate ordering. [1] N. Ikeda et al. Ferroelectrics **272**, 309 (2002)

DS 18: Gaede Prize talk (Mato Knez)

Time: Tuesday 13:30–14:00 Location: HE 101

Prize Talk DS 18.1 Tue 13:30 HE 101

Material Design by Atomic Layer Deposition — •Mato Knez — Max Planck Institute MSP, Halle, Germany — CIC nanoGUNE Consolider, San Sebastian, Spain

Atomic layer deposition (ALD) is a thin film deposition technique which was developed in the 1970s. In contrast to chemical vapor deposition (CVD), ALD incorporates the separation of the chemical reaction into two half-reactions with a growth control in a cycle by cycle manner, allowing good coating conformality even on structures with high aspect ratios. A combination of diffusion effects and ALD coating can largely extend the variation parameters of the materials design. For example, using the deposited films as platform for further chemical or physical manipulation by means of interfacial diffusion or as sacrificial spacers enables the synthesis of nanovoids or nanoparticle assemblies in a very elegant way. A further side-effect of the ALD process was investigated in more detail: If polymers are used as substrates, the highly reactive precursors can diffuse into the bulk of the polymer and chemically interact with it. As a result, physical properties of the substrates in many cases significantly alter during the process. Our focus is primarily on the mechanical properties of (bio)polymers which in many cases are most seriously changed. In summary, ALD is a method-of-choice for many applications in materials design and functionalization. Instead of being just an instrument for coating, it opens possibilities for research and development in various fields. Especially the infiltration of metals into soft materials shows a distinct, but important difference between ALD and CVD and thus its uniqueness.

DS 19: Poster I: Multiferroics (jointly with MA, DF, KR, TT), Spins in organic materials (jointly with MA), FePt Nanoparticles (jointly with MA, MM)

Time: Tuesday 12:15–15:15 Location: Poster A

DS 19.1 Tue 12:15 Poster A

Spin-resolved photoemission spectroscopy of $[\mathbf{Mn_6^{III}Cr^{III}}]^{3+}$ single-molecule magnets (SMM) deposited on surfaces and of Mn compounds as reference substances, cross comparison with XMCD — •Andreas Helmstedt[1], Aaron Gryzia[1], Niklas Dohmeier[1], Norbert Müller[1], Armin Brechling[1], Marc Sacher[1], Ulrich Heinzmann[1], Veronika Hoeke[2], Erich Krickemeyer[2], Thorsten Glaser[2], Mikhail Fonin[3], Samuel Bouvron[3], Philipp Leicht[3], Thomas Tietze[4], and Manfred Neumann[5] — [1]Faculty of Physics, Bielefeld University — [2]Faculty of Chemistry, Bielefeld University — [3]Department of Physics, University of Konstanz — [4]Max-Planck-Institut für Intelligente Systeme, Stuttgart — [5]Department of Physics, University of Osnabrueck

The properties of the Mn-based single-molecule magnet $[\mathbf{Mn_6^{III}Cr^{III}}]^{3+}$ deposited on surfaces are studied. This molecule exhibits a large spin ground state of S_T=21/2 and contains six Mn centres in two bowl-shaped Mn_3-triplesalen units linked by a hexacyanochromate. A preparation method for large-scale homogeneous samples needed for sample scanning to avoid radiation damage will be presented. The spin polarization of Auger electrons emitted from the manganese centres in $[\mathbf{Mn_6^{III}Cr^{III}}]^{3+}$ SMM after excitation with circularly polarized synchrotron radiation has been measured in the paramagnetic phase at selected excitation energies in the Mn-$L_{2,3}$ region. These results will be compared to XMCD data obtained at approx. 2K and 7T. Spin polarization data from Mn_2O_3 and Mn(II)acetate references after excitation at the Mn-$L_{2,3}$ edge are presented as well.

DS 19.2 Tue 12:15 Poster A

High-field ESR and magnetization of a Mn(III)-based single chain magnet — •Y. Krupskaya[1], Z. Tomkowicz[2], M. Rams[2], M. Balanda[3], S. Foro[4], Y. Skourski[5], J. Wosnitza[5], S.K. Nayak[6], J.V. Yakhmi[7], W. Haase[6], V. Kataev[1], and B. Büchner[1] — [1]IFW Dresden, Dresden, Germany — [2]Institute of Physics, Jagiellonian University, Kraków, Poland — [3]H. Niewodniczański Institute of Nuclear

Physics PAN, Kraków, Poland — [4]Clemens-Schöpf-Institut für Organische Chemie und Biochemie, Technische Universität Darmstadt, Darmstadt, Germany — [5]Dresden High Magnetic Field Laboratory, Rossendorf, Germany — [6]Eduard-Zintl Institut für Anorganische und Physikalische Chemie, Technische Universität Darmstadt, Darmstadt, Germany — [7]Technical Physics and Prototype Engineering Division, Bhabha Atomic Research Centre, Mumbai, India

We present high-field magnetic study of a Mn(III)-based molecular chain. The compound shows a ferromagnetic hysteretic behavior of the magnetization at relatively high temperatures (up to 3 K). High-field/high-frequency ESR measurements were performed at the excitation frequencies between 332 and 528 GHz in magnetic fields up to 15 T. The frequency dependence of the ESR spectrum yields a g-factor of 1.8 and a negative effective magnetic anisotropy D of around -6.37 K. In addition, pulsed field (up to 60 T) magnetization measurements enabled determination of the effective spin value corresponding to the ground state of the chain. In conclusion, our experimental results indicate the single molecular chain magnet behavior of the studied compound.

DS 19.3 Tue 12:15 Poster A

EPR study of hyperfine interactions in Cu(II)- bis(oxamato) complexes — •A. Aliabadi[1], A. Petr[1], M. A. Abdulmalic[2], T. Rüffer[2], V. Kataev[1], and B. Büchner[1] — [1]IFW Dresden, Dresden, Germany — [2]Institute of Chemistry, Chemnitz University of Technology, Chemnitz, Germany

The hyperfine (HF) coupling of two Cu(II)-bis(oxamato) complexes containing four nitrogen ligands has been investigated using EPR spectroscopy at 10 GHz. The EPR spectra were modeled in order to determine the g-factor and the HF coupling values. First, measurements were performed on a liquid solution at room temperature to obtain isotropic g-factor and HF coupling constants for Cu and N. From the EPR measurements on powder samples we were able to extract the g-tensor and the Cu HF coupling tensor. In addition, the angular dependence of the EPR spectra was studied by rotation of a single crystal in three mutually perpendicular planes. From that the Cu HF coupling tensor was further refined and the N HF coupling tensor was determined. The results indicate that the difference between the determined parameters for two complexes is not significant. However, these parameters are smaller compared to a previous study of Cu(II)-bis(oxamato) complex containing two nitrogen ligands [1]. The results of this work should enable the determination of the spin density distribution between the central metal ion and the ligands in the studied molecules.

[1] B. Bräuer, T. Rüffer, R. Kirmse, J. Griebel, F. Weigend, G. Salvan, Polyhedron. 26 (2007) 1773.

DS 19.4 Tue 12:15 Poster A

Magnetic properties of a mixed valence Ni(II)-Ni(III)-complex as probed by the ESR spectroscopy and static magnetization measurements — •Jaena Park[1,3], Yulia Krupskaya[1], Vladislav Kataev[1], Bernd Büchner[1], Frederik Schleife[2], Berthold Kersting[2], and Rüdiger Klingeler[3] — [1]Leibniz Institute for Solid State and Materials Research IFW Dresden, Dresden, Germany — [2]Institute of Inorganic Chemistry, University of Leipzig, Leipzig, Germany — [3]Kirchhoff Institute for Physics, University of Heidelberg, Heidelberg, Germany

We investigated magnetic properties of a mixed valence Ni(II)-Ni(III)-complex by means of high-field electron spin resonance spectroscopy and static magnetization measurements. The metal core of the complex contains one Ni^{2+} ion ($S = 1$) and one Ni^{3+} ion ($S = 1/2$) coupled by three sulphur bridges. The magnetic field dependence of the magnetization at low temperatures and the temperature dependence of the static magnetic susceptibility reveal a ferromagnetic coupling between the Ni-spins. The high-field frequency tunable electron spin resonance measurements enable determination of the g-factor and magnetic anisotropy values for the studied complex. In addition, we compare the magnetic properties of the Ni(II)-N(III)-complex with those of the similar structure Ni(II)-N(II)-complex having both Ni ions in the 2+ oxidation state.

DS 19.5 Tue 12:15 Poster A

Electrical characterization of intermetallic FePt nanoparticles — •Ulrich Wiesenhütter[1], Darius Pohl[2], Bernd Rellinghaus[2], Jürgen Fassbender[1], and Artur Erbe[1] — [1]Helmholtz-Zentrum Dresden Rossendorf, D-01328 — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung, D-01069

Magnetic nanoparticles have a large potential for applications such as medical diagnosis and therapy, (bio-)sensors or magnetic recording. Conventional techniques, e.g., MFM, electron holography or Lorentz microscopy are only suited to determine magnetical properties of macroscopic particle ensembles. In order to investigate the electrical and magnetic properties of a single, free-standing FePt nanoparticle two nano-sized Au electrodes that are fabricated by electron beam lithography, are used.The full characterization of the particle is carried out by electron microscopy and by recording current-voltage characteristics. As a result Coulomb-blockade effects have been observed at low temperatures. The capacitance of the nanoparticles is derived from the I/V characteristics.

DS 19.6 Tue 12:15 Poster A

Cobalt-Gold Core-Shell Nanoparticles as Probes for Quantitative MFM — •Tino Uhlig[1], Ulf Wiedwald[2], Denny Köhler[1], Paul Ziemann[2], and Lukas Eng[1] — [1]Institut für Angewandte Photophysik, TU Dresden — [2]Institut für Festkörperphysik, Universität Ulm

We present an easy, fast and reliable method for the preparation of magnetic force microscopy (MFM) probes based on single magnetic nanoparticles. Due to their dipole like characteristics, these kind of magnetic probes open up possibilities for quantitative measurements of magnetizations on the nano-scale. Our fabrication method is based on the deposition of cobalt nanoparticles (diameter 30 nm) on a Si substrate and subsequent photochemical deposition of a gold layer on the particle surface. Single particles were attached to standard silicon AFM tips with the aid of a linker molecule (APTMS). The applicability of the fabricated probes was tested by imaging the magnetic domains of a hard disk drive sample. Furthermore a calibration method, using the deflection of the AFM cantilever in an external magnetic field, is presented.

DS 19.7 Tue 12:15 Poster A

Shift of the blocking temperature of Co nanoparticles by Cr capping — •Melanie Ewerlin[1], Derya Demirbas[1], Leonardo Agudo[2], Gunther Eggeler[2], and Oleg Petracic[1] — [1]Institut für Experimentalphysik / Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany — [2]Institute for Materials, Department of Material Science, Ruhr-Universität Bochum, 44780 Bochum, Germany

We have prepared Co nanoparticles (NPs) on Al_2O_3 buffer layers and studied the effect of capping with various amounts of Cr onto the magnetic properties. Structural and magnetometric characterization was performed using TEM and SQUID magnetometry, respectively. The uncapped Co NPs show superparamagnetic behavior with a blocking temperature of T_B=14K. The magnetic properties are strongly influenced by the Cr capping resulting in a decrease of T_B for nominal thicknesses of Cr up to 0.15nm. However, for larger values the blocking temperature increases again. XMCD measurements at the Cr edge indicate an anti-parallel alignment of the magnetic moments in the Cr layer with respect to the moments in the Co particle, which leads to a decrease of the effective magnetic volume and hence to a decrease of T_B. The second regime is governed by inter-particle coupling via Cr-bridges.

DS 19.8 Tue 12:15 Poster A

Interaction effects between self-assembled Co nanoparticles — •Astrid Ebbing[1], Leonardo Agudo[2], Gunther Eggeler[2], and Oleg Petracic[1] — [1]Institut für Experimentalphysik/Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum — [2]Institut für Werkstoffe, Ruhr-Universität Bochum, 44780 Bochum

In this work we present the influence of Pt on self-assembled Co nanoparticles (NPs). We show that capping the Co NPs with Pt results in strong changes in the magnetic properties. With increasing Pt capping we observe a transition from 'demagnetizing' (viz. dipolar) toward 'magnetizing' (e.g. polarization type) interactions between the NPs. We performed magnetization hysteresis, ZFC/FC vs. temperature and delta(M)-measurements using a superconducting quantum interference device magnetometer to investigate the nature of coupling between the NPs. The measurements show negative delta(M)-values for small amounts of Pt capping material and positive values for 0.53 nm Pt or more, which indicates a magnetizing interaction between the NPs via the Pt-bridges.

DS 19.9 Tue 12:15 Poster A

Characterization of superparamagnetic nanoparticles for bone tissue engineering — •M. Uhlarz[1], T.

Herrmannsdörfer[1], R. De Santis[2], M. Sandri[3], A. Tampieri[3], E. Figallo[4], T. D'Alessandro[4], S. Keshari-Samal[5], G. Rischitor[6], and the MAGISTER collaboration[7] — [1]Hochfeld-Magnetlabor Dresden, HZ Dresden-Rossendorf — [2]IMCB-CNR, Napoli, Italia — [3]ISTEC-CNR, Faenza, Italia — [4]Fin-Ceramica SpA, Faenza, Italia — [5]ISMN-CNR, Bologna, Italia — [6]Western General Hospital, University of Edinburgh, UK — [7]Europäische Kommission, Bruxelles, Belgique

Currently, large bone or cartilage defects are stabilized by massively-invasive surgery. The permanent implants used for this purpose are either metallic prostheses, or body tissue taken elsewhere from the patient. In a novel tissue-engineering approach, autologous tissue regeneration is guided by implanted magnetic scaffolds under external magnetic field. These scaffolds attract superparamagnetic Fe_3O_4 (magnetite) nanoparticles tagged with Vascular Endothelial Growth Factor (VEGF) molecules. Release of the growth-factor molecules at the scaffold (optionally triggered by ac-field induced hyperthermia) attracts autologous chondrocytes and osteoblasts, which build up fresh bone and cartilage tissue. We report on the magnetic characterization of several biocompatible and biodegradable materials that might serve as scaffold materials.

This project is supported by the European Union's FP7-Cooperation Programme through the MAGISTER project (Magnetic Scaffolds for in-vivo Tissue Engineering), Large Collaborative Project FP7 - 21468.

DS 19.10 Tue 12:15 Poster A

Hall effect in nanodimensional multilayers based on island films of Pd and Fe — •Sergej A. Nepijko[1], Dmytro Kutnyakhov[1], Olena Tkach[2], Larysa Odnodvorets[2], Ivan Protsenko[2], and Gerd Schönhense[1] — [1]Institute of Physics, University of Mainz, 55099, Mainz, Germany — [2]Sumy State University, 40007, Sumy, Ukraine

Nanodimensional *n*-layers systems of $[Pd/Fe]_n/SiO_2/Si$, where $3 \leq n \leq 10$, were used to examine the Hall effect. Effective thickness of separate layers of Pd and Fe changed in the range from 0.4 to 1.4 nm (Pd) and from 0.6 to 0.9 nm (Fe). Electron microscopic studies indicate that the layers have island structure and their composition corresponds to fcc-Pd and bcc-Fe. Solid solutions of Pd-Fe with fct-lattice are formed only when the thickness of layers $\geq$ 3 nm and after annealing at $\geq$ 790 K. Measurement of Hall coefficient R_H indicate that its value monotonically decreases with increasing number of layers n. For example, for multilayer Pd(1.1 nm)/Fe(0.9 nm) R_H decreases from 5.5×10^{-9} m^3/C (n=2) to 3.97×10^{-9} m^3/C (n=10). A size dependence of R_H is observed also at fixed Fe layer thickness and variable thickness of Pd. For multilayer $[Pd(x)/Fe(0.6)]_{10}$ the Hall coefficient decreases from 4.80×10^{-9} m^3/C to 3.69×10^{-9} m^3/C while increasing the effective thickness of Pd from x= 0.4 to 1.4 nm.

DS 19.11 Tue 12:15 Poster A

Spin-fluctuation energies in $3d$ transition-metal clusters deposited on Pt (111) — •Sergej Riemer[1], Gustavo Pastor[2], Jesus Dorantes-Dávila[3], and Raul Garibay-Alonso[4] — [1]Universität Kassel, Germany — [2]Universität Kassel, Germany — [3]UASLP, San Luis Potosí, Mexico — [4]Universidad Autónoma de Coahuila, Mexico

A functional-integral theory of itinerant magnetism is applied to transition-metal clusters deposited on Pt (111). The low temperature limit of the local spin-fluctuation energies $\Delta F_l(\xi)$ at different atoms l is determined as a function of the exchange field ξ by using a real-space recursive expansion of the local Green's functions. The size, structural, and local-environment dependence of $\Delta F_l(\xi)$ is calculated for representative examples of Fe_N, Co_N and Ni_N with $N \leq 13$ atoms. The interplay between fluctuations of the module and of the relative orientation of the local magnetic moments is analyzed. Comparison between free and deposited clusters having the same structure and interatomic distances reveals remarkable changes in the spin-excitation spectrum of the clusters as a result of the hybridizations with the metallic support. For instance, in the case of small Fe clusters on Pt (111) one observes that the spin-flip energies are reduced by more than an order of magnitude as a consequence of deposition. A similar important reduction of the Curie temperature is expected. This contrasts with the results for the ground-state magnetic moments and magnetic order, which are essentially the same in the free and deposited configurations.

DS 19.12 Tue 12:15 Poster A

Coupling behavior in iron-oxide nanoparticle/Py thin film composite systems — •Caroline Fink[1], Philipp Szary[1], Giovanni Badini Confalonieri[1], Durgamadhab Mishra[1], Maria Benitez[1,2], Mathias Feyen[2], An-Hui Lu[2], Leonardo Agudo[3], Gunther Eggeler[3], and Oleg Petracic[1] — [1]Institut für Experimentalphysik/Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]Max-Planck-Institut für Kohlenforschung, D-45470 Mülheim an der Ruhr, Germany — [3]Institut für Werkstoffe, Ruhr-Universität Bochum, D-44780 Bochum, Germany

We have investigated the magnetic and electrical transport properties of iron-oxide nanoparticle/Py thin film composite systems. Ultrathin films of Permalloy (Py) have been prepared by means of UHV ion beam sputtering and subsequently covered by one monolayer of iron-oxide nanoparticles. Post-annealing of the samples under controlled atmospheric conditions allows us to transform the particles into a mixed wüstite/magnetite (FexO/Fe3O4) phase showing intra-particle exchange bias. A slight variation of the NP type yields systems of different coupling behavior. Performing magnetometry and transport measurements we observe either a strong or weak coupling between the Py film and the NPs depending on the NP type. Moreover, a strongly decoupled behavior can be observed when adding a sapphire (Al2O3) layer separating the particles from the Py. Results have been compared with reference systems consisting of only NPs or only Py.

DS 19.13 Tue 12:15 Poster A

Magnetoresistance properties of Fe_3O_4 nanoparticles in a Cu matrix — •Sergej A. Nepijko[1], Dmytro Kutnyakhov[1], Maxym Demydenko[2], Serhiy Protsenko[2], Dmytro Kostyuk[2], and Gerd Schönhense[1] — [1]Institute of Physics, University of Mainz, 55099, Mainz, Germany — [2]Sumy State University, 40007, Sumy, Ukraine

The aim of the work was the manufacturing of ordered arrays of magnetic Fe_3O_4 nanoparticles, the investigation of their structural and phase state and magneto-resistance in a wide range of annealing temperatures. Nanoparticles were prepared by chemical synthesis and drop deposited onto a Si substrate. After deposition the ordered nanoparticle array was observed by TEM. Nanoparticle sizes changed from 6.0 nm (as deposited) to 11.6 nm (after annealing at 1200 K). The phase state of the nanoparticles was cubic (spinel type) with lattice parameter varying from 0.811 nm (as-deposited) to 0.840 nm (1200 K). The magnetoresistance was measured using nanostructured systems of $Au(2nm)/Cu(20nm)/Fe_3O_4(nanoparticles)/SiO_2/Si$ with varying the angle between magnetic field direction and substrate plane from 0° to 90°. The resulted maximum value of magnetoresistance was about 2 %.

DS 19.14 Tue 12:15 Poster A

^{57}Fe Mössbauer spectroscopy on ferrite nanoparticles — •Mathias Kraken[1], Jochen Litterst[1], Ilka-Marina Grabs[2], Ingke-Christine Masthoff[2], Isabel Christina Souza Dinóla[3], Julian Andres Munevar Cagigas[3], Wiliam Trujillo Herrera[3], and Elisa Maria Baggio Saitovitch[3] — [1]Institut für Physik der kondensierten Materie | TU Braunschweig | Germany — [2]Institut für Partikeltechnik | TU Braunschweig | Germany — [3]Centro Brasileiro de Pesquisas Físicas | Rio de Janeiro | Brazil

Due to its specific timescale, Mössbauer spectroscopy is highly suitable to investigate the dynamic properties of magnetic nanoparticles. The hyperfine magnetic spectra between the blocking temperature and very low temperatures may exhibit a broad variety of different shapes. Accordingly, to describe this rich behaviour a whole range of different, controversially discussed models can be found in literature (1-3).

We performed ^{57}Fe Mössbauer measurements on $ZnFe_2O_4$ nanoparticles, prepared by a non-aqueous sol gel method and characterized by different techniques. The spectra were taken on strongly and weakly interacting particles and the fits to the spectra with the different models are compared in order to gain information about their suitability.

(1) D.H. Jones et al., J. Magn. Magn. Mater. 78, 320 (1989).

(2) S. Mørup et al., J. Magn. Magn. Mater. 40, 163 (1983).

(3) S. Bocquet et al., J. Magn. Magn. Mater. 109, 260 (1992).

DS 19.15 Tue 12:15 Poster A

Preparing of $La_{1/3}Sr_{2/3}FeO_3$ targets for sputtering of thin films — •Thomas Breuer, Thomas Brueckel, Joerg Voigt, and Joerg Persson — Peter Gruenberg Institut PGI and Juelich Centre for Neutron Science JCNS, JARA-FIT, Forschungszentrum Juelich GmbH, 52425 Juelich, Germany

$La_{1/3}Sr_{2/3}FeO_3$ is a transition metal oxide (TMO) with a perovskite structure. It exhibits strong electronic correlations, visible e.g. in a

Verwey metal-insulator transition accompanying the antiferromagnetic phase transition at about $T_C = 200\,K$.
While the material has been investigated extensively in bulk form, the aim of the present study is to clarify its properties as thin epitaxial films. We have prepared ceramic sputter targets of $La_{1/3}Sr_{2/3}FeO_3$ in a solid state reaction and characterized them by means of chemical analysis, powder x-ray diffraction and magnetic measurements by a Vibrating Sample Magnetometer on PPMS. The material tends to lose oxygen during calcination and sintering at temperatures above 600 K which was detected by thermogravimetric analysis. Significant changes in structure and magnetic response are being observed for oxygen deficits as low as 2 %. Finally, the progress in the preparation and characterization of thin epitaxial films will be reported.

DS 19.16 Tue 12:15 Poster A

The first principle study of Cu-based hybrids — •Pegah Zolfaghari[1], Gilles A de Wijs[1], and Robert A de Groot[1,2] — [1]Electronic Structure of Materials, Institute for Molecules and Materials, Faculty of Science, Radboud University Nijmegen, Heyendaalseweg 135, 6525 AJ Nijmegen, The Netherlands — [2]Solid State Materials for Electronics, Zernike Institute for Advanced Materials, Rijksuniversiteit Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands

Hybrids, organic-inorganic materials, in the perovskite-type layer structures with the general formula $(C_nH_{2n+1}NH_3)_2MCl_4$ in which $n = 0, 1, 2, ...$, and M represents a divalent transition metal ion, have been extensively studied in recent years. Among these series of hybrids, the copper compounds are the most interesting ones. Firstly, the divalent metal Cu^{2+} is a strong Jahn-Teller ion, as a result different structual transitions in these materials occur. Secondly, the magnetic intra-layer interactions are ferromagnetic.

The density functional (DFT) calculations were applied to study the $(NH_4)_2CuCl_4$ and $(C_2H_5NH_3)_2CuCl_4$ compounds. The magnetic and electronic properties were investigated. The calculations reveal that the compounds have a stable, layered ferromagnetic ground state that is consistent with experimental results.

DS 19.17 Tue 12:15 Poster A

Synthesis and magnetic properties of cobalt ferrite nanoparticles — •Morad F. Etier[1], Vladimir V. Shvartsman[1], Frank Stromberg[2], Joachim Landers[2], Heiko Wende[2], Fábio G. Figueiras[3], and Doru C. Lupascu[1] — [1]Institute for Materials Science, University of Duisburg-Essen, Essen, Germany — [2]Faculty of physics and Center for Nanointegration (CeNIDE) Duisburg-Essen, University of Duisburg-Essen, Duisburg, Germany — [3]Department of Physics, CICECO, University of Aveiro, Aveiro, Portugal

Cobalt ferrite is one of the most widely used materials in magnetic recording devices due to its high coercivity (about 5400 Oe), moderate magnetization (84 emu/g), and good chemical stability. Below Tc = 820 K cobalt ferrite is in a ferrimagnetic state. The magnetic properties of cobalt iron oxide nanoparticles mainly depend on the annealing temperature and particle size.

Nanoparticles of cobalt ferrite were successfully fabricated by the co-precipitation method. The crystal structure was confirmed by X-ray diffraction, the composition by energy dispersive spectroscopy, and phase changes by thermogravimetric differential thermal analysis. The particle morphology was analyzed by scanning electron microscopy. Magnetic properties were investigated by magnetometry and Mössbauer spectroscopy. Particle size is in the range of 24 to 44 nm. Both the particle size and agglomeration level are controlled by the amount of sodium hydroxide used. Dependence of remnant magnetization and coercive field on particle size is analyzed.

DS 19.18 Tue 12:15 Poster A

Magnetic and Electronic properties of Mn-stabilized Zirconia (MnSZ) — •Jan Zippel[1], Michael Lorenz[1], Anette Setzer[1], Holger Hochmuth[1], Pablo Esquinazi[1], Nikolai Sobolev[2], Alexandre Jacquot[3], and Marius Grundmann[1] — [1]Universität Leipzig, Fakultät für Physik und Geowissenschaften, Institut für Experimentlaphysik II, Linnéstrasse 5, 04103 Leipzig, Germany — [2]Universidade de Aveiro, Departamento de Fisica, Campus de Santiago, 3810-193 Aveiro, Portugal — [3]Fraunhofer Institut für Physikalische Messtechnik, Heidenhofstrasse 8, D-79110 Freiburg, Germany

The possibility to combine both, the electron spin as a new degree of freedom and the electron charge offers opportunities for a new generation of devices. As recently predicted [1], MnSZ is proposed as a ferromagnetic semiconductor with a Curie temperature T_C above room temperature. As recently shown, a Mn related ferromagnetism has not been observed yet [2]. By applying an annealing step in oxygen defficient ambient at about $T_{\mathrm{ann}} \approx 700°$ C to the MnSZ thin films grown by pulsed-laser deposition (PLD), we observe a ferromagnetic behavior in superconducting quantum interference device (SQUID) measurements at about $T = 60$ K. In addition, electron paramagnetic resonance (EPR) suggests a change of the Mn oxidation state from an EPR silent Mn^{3+} to Mn^{2+}. Seebeck-effect measurements verify a transition from p–type conductivity to n–type conductivity around 500 K. [1] S. Ostanin et *al.*, Phys. Rev. Lett. **98**, 016101 (2007). [2] J. Zippel et *al.*, Phys. Rev. B **82**, 125209 (2010).

DS 19.19 Tue 12:15 Poster A

The magneto-impedance of iron whiskers at low temperature — •Matthäus Langosch, Haibin Gao, and Uwe Hartmann — Institute of Experimental Physics, Saarland University, P. O. Box 151150, D-66041, Saarbrücken, Germany

In order to understand all aspects of the AC transport behavior of a ferromagnetic material in an external magnetic field at low temperature, iron single crystals (iron whiskers) were grown as specific samples to investigate the magneto-impedance (MI) effect at 4.2 K. The MI measurements were performed as a function of the magnitude of the driving current and its frequency. The chosen frequencies were up to 100 kHz, where domain wall motion takes place and contributes to the MI effect. The measured low temperature impedance changes are on the order of hundreds of percent and are much higher than that at room temperature. This behavior can mainly be attributed to a large mean free electronic path on the one hand and the skin effect on the other hand.

DS 19.20 Tue 12:15 Poster A

Structural and magnetic analysis of Vanadates — •Christine Tölzer[1], Johanna Brand[1], Masahiko Isobe[2], Karsten Binder[1], Timo Taetz[3], María Teresa Fernández-Díaz[5], Angela Möller[3,4], Yutaka Ueda[2], and Markus Braden[1] — [1]II. Institute of Physics, University of Cologne — [2]Institute for Solid State Physics, University of Tokyo — [3]Institute of Inorganic Chemistry, University of Cologne — [4]Department of Chemistry and Texas Center for Superconductivity, University of Houston — [5]Institute Laue-Langevin, Grenoble

We present the analysis of three different Vanadates: $InCu_{2/3}V_{1/3}O_3$, $Rb_2V_8O_{16}$ and ZnV_2O_4. The layered compound $InCu_{2/3}V_{1/3}O_3$ is a representative of the quasi two-dimensional S=1/2 honeycomb lattice due to the ordering of Cu and V. A Néel-temperature near 38 K was deduced from anomalies in the magnetic susceptibility. We have studied the magnetic structure in $InCu_{2/3}V_{1/3}O_3$ by neutron diffraction on the high-flux powder diffractometer D20. A rise in scattering upon cooling indicates magnetic ordering to set in near the anomaly observed in the susceptibility. Furthermore, we discuss the charge and orbital ordering in $Rb_2V_8O_{16}$ and in ZnV_2O_4, as analysed by single-crystal x-ray diffraction as function of temperature.

DS 19.21 Tue 12:15 Poster A

Normal and anomalous Hall effect in $NbFe_2$ — •Sven Friedemann[1], Manuel Brando[2], William J Duncan[3], Andreas Neubauer[4], Christian Pfleiderer[4], and Malte Grosche[1] — [1]University of Cambridge, Cavendish Laboratory, JJ Thomson Avenue, CB3 0HE Cambridge, United Kingdom — [2]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Strasse 40, 01187 Dresden, Germany — [3]Department of Physics, Royal Holloway, University of London, Egham TW20 0EX, United Kingdom — [4]Physik Department E21, Technische Universität München, James-Franck-Strasse, D-85748 Garching, Germany

The intermetallic system $NbFe_2$ exhibits ferromagnetic and antiferromagnetic order, which can be suppressed by slight changes to the composition within the $Nb_{1-y}Fe_{2+y}$ homogeneity range. A quantum critical point (QCP) arises at slight Nb excess of about $y = 0.015$. In proximity to its QCP $NbFe_2$ exhibits non-Fermi-liquid behaviour, which makes this material the first clear candidate for a three dimensional ferromagnetic QCP in a clean transition metal compound at ambient pressure. We present Hall effect measurements on several single crystals chosen from the $Nb_{1-y}Fe_{2+y}$ solution series. The data are analysed in terms of anomalous and normal contributions to the Hall voltage. We find anomalous contributions arising from both Side Jump and Skew Scattering with distinct changes in their relative strength as a function of Nb content. The normal contribution reflects the electronic structure.

DS 19.22 Tue 12:15 Poster A

First principles studies of complex magnetism in Mn nanostructures on Fe(001) surface — •ricardo noboru igarashi[1], angela burlamaqui klautau[2], and helena maria petrilli[1] — [1]Instituto de Física, Universidade de São Paulo, CP 66318, 05315-970, São Paulo, SP, Brazil — [2]Faculdade de Física, Universidade Federal do Pará, Belém, PA, Brazil

The magnetic properties of Mn nanostructures on Fe(001) surface have been studied using the noncollinear first-principles RS-LMTO-ASA (Real-Space Linear Muffin Tin Orbital Atomic Sphere Approximation) [1] method within density functional theory. We have considered a variety of nanostructures such adsorbed wires, pyramids, flat and intermixed clusters of sizes varying from two and nine atoms. Our calculations of interatomic exchange interactions reveal the long range nature of exchange interactions between Mn-Mn and Mn-Fe atoms. We have found that the strong dependence of these interactions of the local environment and the effect of spin-orbit coupling lead to the possibility of realizing complex magnetic structures such as helical and half skyrmion.

[1] S. Frota-Pessôa, Phys. Rev. B 69, 104401 (2004); Phys. Rev. B 46, 14570 (1992); P. R. Peduto, S. Frota-Pessôa and M. S. Methfessel, Phys. Rev. B 44, 13 283 (1991).

DS 19.23 Tue 12:15 Poster A

Incorporation of N codopants in Co:ZnO investigated by X-ray absorption spectroscopy — •Daniel Schauries[1], Andreas Ney[1], Verena Ney[1], Fabrice Wilhelm[2], Andre Rogalev[2], and Flora Yakhou[2] — [1]Fakultät für Physik, Universität Duisburg-Essen, Lotharstr. 1, D-47057 Duisburg, Germany — [2]European Synchrotron Facility, 6 Rue Jules Horowitz, BP 220, 38043 Grenoble Cedex, France

p-doping of ZnO in general remains a grand challenge for material science. In particular p-type ZnO is of interest to investigate the perspectives for obtaining RT-ferromagnetism in p-type Co:ZnO.

We have grown Co:ZnO:N(0001) on sapphire substrates using reactive magnetron sputtering from Co/Zn targets at Co concentrations of 10, 15 and 20% and different Ar : O_2 : N_2 sputter gas compositions.

The structure was studied by synchrotron-based element specific X-ray absorption spectroscopy. All edges were measured with the electric field of the X-rays perpendicular and parallel to the c-axis to obtain X-ray Linear Dichroism (XLD). Subsequently all spectra for the Zn, Co, O and N-K-edge were simulated with FDMNES[1] to determinate the positions of the species. While Co only occupies Zn-sites, the situation turned out to be more complex for N — for low N_2-concentration in the sputter gas probably incorporated N_2 was formed, high N_2-levels also led to the formation of substitutional N atoms on O-sites.

The resulting magnetic properties of Co:ZnO:N will be discussed as well. We greatfully acknowledge financial support from the DFG through the Heisenberg Programme.

[1] Y. Joly, Phys. Rev. B **63**, 125120-125129 (2001).

DS 19.24 Tue 12:15 Poster A

Polarized Neutron Reflectometry of Rare-Earth Nitride Thin Films — •Sebastian Brück[1,2], David Cortie[2], Josh Brown[3], Thomas Saerbeck[2], Clemens Ulrich[1], Frank Klose[2], and James Downes[3] — [1]School of Physics, University of New South Wales, Sydney, Australia — [2]Australian Nuclear Science and Technology Organization, Lucas Heights, Australia — [3]Department of Physics, Macquarie University, Australia

Rare-earth monopnictides like HoN, DyN, or ErN are semiconductors with typical band gaps between 0.73 and 1.3eV. The fact that they exhibit ferromagnetic ordering at low temperatures makes them possible candidates for an intrinsically ferromagnetic semiconductor. Thin, polycrystalline rare-earth nitride films of 15 to 40nm thickness were grown onto c-plane sapphire substrates using low-energy ion assisted deposition. A temperature- and field-dependent polarized neutron reflectometry study in combination with SQUID magnetometry was carried out to characterize the magnetic properties of these films in a depth resolved way. The investigated samples show a homogeneous distribution of the magnetic moment throughout the film with ferromagnetic ordering temperatures comparable to the bulk materials. ErN and HoN films do not show an opening of the magnetic hysteresis loop even for the lowest measured temperature of T=2K. DyN on the other hand clearly shows a coercive field and remnant magnetization at 5K.

DS 19.25 Tue 12:15 Poster A

ZnO Metal Semiconductor Field Effect Transistor with magnetic channel — •Tim Kaspar, Danilo Bürger, Ilona Skorupa, Vicki Kühn, Artur Erbe, Manfred Helm, and Heidemarie Schmidt — Helmholtz-Zentrum Dresden-Rossendorf, P.O. Box 510119, 01314 Dresden, Germany

We focus on the development of transparent semiconductor spintronics devices. Our work is motivated by the observation of s-d exchange inducted spin polarization in magnetic ZnO:(Co, Mn) thin films below 50 K and related magnetoresistance effect [1]. Our aim is to control the conductance in ZnO Metal Semiconductor Field Effect Transistors (MESFET) with magnetic channel by external electrical AND magnetic fields. The magnetic ZnO:(Co, Mn) channel layers have been deposited by pulsed laser deposition on c-plane sapphire substrates. Gate, source, and drain contacts have been structured by optical lithography. The gate contact has been fabricated by reactive sputtering of Ag/Au [2]. Source and drain contacts have been fabricated from high conducting transparent ZnO. The characteristics of the ZnO-based MESFETs with magnetic channel in external perpendicular magnetic fields ranged from -1.8T to +1.8T are presented.

[1] Qingyu Xu, *et al.*, Phys. Rev. Lett. **101**, 076601 (2008)

[2] H.Frenzel *et al.*, Appl. Phy. Lett. **92**, 192108 (2008

DS 19.26 Tue 12:15 Poster A

Anomalous hysteretic Hall effect in a ferromagnetic, Mn-rich, amorphous Ge:Mn nano-network — •Danilo Bürger, Shengqiang Zhou, Marcel Höwler, Xin Ou, György Kovacs, Helfried Reuther, Arndt Mücklich, Wolfgang Skorupa, Manfred Helm, and Heidemarie Schmidt — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, P.O. Box 510119, 01314 Dresden, Germany

The read out of the magnetization state in magnetic semiconductors by electrical Hall resistance measurements makes it possible to use ferromagnetic semiconductors in nonvolatile memories. In a previous work [1], we fabricated ferromagnetic Ge:Mn by Mn ion implantation and pulsed laser annealing (PLA) and observed hysteretic Hall resistance below 10 K. By applying different PLA conditions we fabricated a percolating, Mn-rich, amorphous Ge:Mn nano-network with hysteretic Hall resistance up to 30K. This nano-network is embedded in crystalline Ge:Mn between 5 nm and 40 nm under the sample surface. We applied chemical and physical etching to confirm the contribution of the nano-network to the magnetic properties. The nano-network has a significant influence on the correlation between magnetism and anomalous Hall resistance. In the future such nano-networks may be used to spin-polarize free charge carriers in semiconductors at room temperature. [1] S. Zhou *et al.*, Phys. Rev. B **81**, 165204 (2010)

DS 19.27 Tue 12:15 Poster A

Optical and Magneto-optical Properties of ZnO(0001) Single Crystals Implanted with Fe and Co Ions — •Scarlat Camelia[1], Zhou Shengqiang[1], Gordan Ovidiu[2], Fronk Michael[2], Zahn R. T. Dietrich[2], Helm Manfred[1], Schmidt Heidemarie[1], and Salvan Georgeta[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Germany — [2]Semiconductor Physics, Chemnitz University of Technology, Germany

ZnO is a transparent wide-band-gap semiconductor which has been intensively investigated in the view of (magneto-) and (opto-)electronic applications. In this work the (magneto-)optical properties of unimplanted ZnO(0001) single crystals and single crystals implanted with ^{57}Fe and Co ions were investigated at room temperature by means of Raman spectroscopy, spectroscopic ellipsometry, and magneto-optical Kerr effect (MOKE) spectroscopy. The ZnO (0001) single crystals were coimplanted with ^{57}Fe and Co ions at 623 K with same fluence respectively. After implantation the samples were annealed in a high-vacuum furnace at 1073 K for different annealing time. The Raman spectra measured in resonance with an excitation energy of 3.82 eV exhibit higher order scattering by LO phonons. The increase in the ratio between the second and the first order phonon peak intensities for long annealing time can be correlated with a reduction in the number of defects and with improved crystallinity. The implanted ZnO crystals exhibit magneto-optical activity in two broad spectral ranges centered around 3 eV and around 4.3 eV, the strength of which also varies significantly with the annealing time.

DS 19.28 Tue 12:15 Poster A

Bipolar resistive switching at manganite/manganite interfaces — •Christin Kalkert, Jon-Olaf Krisponeit, Vasily Moshnyaga, Bernd Damaschke, and Konrad Samwer — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-

Platz 1, 37077 Göttingen

Bipolar resistive switching stands for remanent switching of resistivity by application of electric fields reversible by opposite polarities. This phenomenon is observed in a wide variety of perovskite materials and holds the potential of creating new resistive random access memory devices. $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) manganite films were prepared by using the metalorganic aerosol deposition technique. On Al_2O_3 substrates the manganite films show nanocolumnar growth with different growth orientations as determined by x-ray diffraction and TEM analysis. The films were structured by electron beam lithography into LSMO paths/bridges between larger LSMO contact areas; after a second lithography step Au/Cr films were deposited onto the contact areas. These structures show bipolar resistive switching, which can also be induced and probed by means of conductive AFM. The C-AFM measurements show that the switching takes place at the manganite/manganite interfaces, i.e. at the boundaries of the nanocolumns. The resistive switching of the structures and the C-AFM measurements are discussed in terms of a local structural transformation at the manganite/manganite interfaces. (APL 99, 132512, (2011))

Financial support by DFG via SFB 602, TPA2 and the Leibniz Program is ackowledged.

DS 19.29 Tue 12:15 Poster A

Ultrafast Spin-Lattice Coupling in Transition Metal Oxides — •Lena Maerten, André Bojahr, Marc Herzog, Daniel Schick, and Matias Bargheer — Insitut für Physik und Astronomie, Universität Potsdam, Germany

Understanding the interplay of the electronic, lattice and spin degrees of freedom in solids is essential for devising future nanoelectronic applications. Nanostructured transition metal oxides provide an ideal test ground for studying the interaction of the contributing subsystems on an ultrafast time scale.

We use femtosecond optical and infrared pump probe spectroscopy and time resolved x-ray diffraction techniques to investigate the electronic and lattice dynamics in $SrRuO_3/SrTiO_3$ and $(LaSr)MnO_3/SrTiO_3$ superlattices. Sub-picosecond buildup of magnetostrictive stress has been found in a $SrRuO_3/SrTiO_3$ nanolayer [1]. We show additional temperature- and fluence-dependent reflectivity data revealing further insight into the demagnetization process and discuss the coupling of the magnetic and structural degrees of freedom for the different materials by means of x-ray diffraction results.

[1]C. v. Korff Schmising et al., PRB 78, 060404 (2008)

DS 19.30 Tue 12:15 Poster A

Colossal Magnetoelastic Effects at the Phase Transition of (La, Pr, Ca)MnO$_3$ — •Markus Michelmann, Christoph Meyer, Vasily Moshnyaga, and Konrad Samwer — I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37707 Göttingen

A strong coupling of charge, spin and lattice degrees of freedom in perovskite manganites, i.e. $(La, Pr, Ca)MnO_3$, results from the competition between the ferromagnetic double exchange and charge/orbital ordering, promoted by the electron-phonon interaction. Therefore, the paramagnetic-ferromagnetic (PM-FM) phase transition is clearly reflected in the behavior of the elastic constants. Here, we report ultrasound velocity and attenuation in polycrystalline $(La_{1-y}Pr_y)_{0.7}Ca_{0.3}MnO_3$ bulk samples ($y = 0$, 0.4, 0.5, 1) as a function of temperature, $T = 10 - 300$ K, and magnetic field, $B = 0 - 7$ T, with special focus on the hysteresis effects and metamagnetism at the 1st order PM-FM transition. Close to the Curie point modest magnetic fields, $B = 1 - 5$ T, induce a large increase of shear stiffness and a strong softening of bulk modulus by about 10%. A minimum in bulk modulus and a peak in longitudinal sound attenuation were observed at the phase transition and attributed to a coupling between the lattice and spin fluctuations. The magnitude of this softening is maximized at a certain temperature and magnetic field, indicating a critical end point of the magnetic transition. Support by Deutsche Forschungsgemeinschaft via SFB 602, TP A2 is acknowledged.

DS 19.31 Tue 12:15 Poster A

Magneto-optical Studies on Transition Metal doped Zinc Oxid — •Stephanie Jankowski[1], Sebastian Geburt[2], Carsten Ronning[2], and Wolfram Heimbrodt[1] — [1]Department of Physics and Material Science Center, Philipps- University Marburg, Renthof 5, D-35032 Marburg, Germany — [2]Physikalisch-Astronomische Fakultät, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, D-07743 Jena, Germany

We present the results of magneto photoluminescence on ZnO-bulk doped with the magnetic ions Co and Mn. The measurements have been performed in magnetic fields up to 7 Tesla in a temperature range 1.8-300 K. Zeeman spectroscopic in the excitonic region have been used to determine the g-factors of the samples. Normally the g-factor of II-VI diluted magnetic semiconductor is very high because of the Giant Zeeman effect. Even in case of transition metal doped ZnO surprisingly small Zeeman-splitting has been found. In comparison to other Mn- and Co-doped II-VI semiconductors the optical 3d intra-ionic transitions are very weak. The physical reasons for these phenomena will be discussed.

DS 19.32 Tue 12:15 Poster A

Microscopic and macroscopic studies on the magnetoelectric coupling in chiral multiferroics — Max Baum[1], •Jonas Stein[1], Simon Holbein[1], Thomas Finger[1], Navid Qureshi[1], Jeannis Leist[3], Joachim Hemberger[1], Petra Becker-Bohatý[2], Ladislav Bohatý[2], Götz Eckold[3], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Kristallographie, Universität zu Köln — [3]Institut für Physikalische Chemie, Universität Göttingen

In the chiral magnets $MnWO_4$ and $TbMnO_3$ ferroelectric polarisation is directly induced by the non-collinear magnetic structure. We present microscopic neutron scattering studies and macroscopic measurements of the ferroelectric polarisation and of the magnetic structure in these materials. Using a stroboscopic method the control of the chiral magnetism by an external electric field is analysed with polarised neutrons finding unexpectedly large relaxation times. Measurements of the pyrocurrent on $MnWO_4$ confirm these long time scales. In addition we discuss the magnetic excitations at the incommensurate zone centre of $MnWO_4$, a low energy mode should posses electromagnon character. The magnetic structure of $NaFe(WO_4)_2$ was studied by neutron diffraction. At zero magnetic field we find an incommensurate structure which transforms to commensurate order upon the application of moderate fields.

DS 19.33 Tue 12:15 Poster A

On the ferroelectric phase transition of boracites — •Michael Fechner and Nicola Spaldin — ETH Zurich, Department for Material Theory,CH-8093 Zurich, Switzerland

We present results of first-principles electronic structure calculations for the Cl and I boracites. The boracites[1] are a class of ferroelectric minerals with formula $Me_2B_7O_{12}X$, where Me is a bivalent metal (Fe, Co, Zn) and X a halogen (Cl, Br or I). All boracites are cubic at high temperature, and undergo a phase transition on cooling first to an orthorhombic phase and in some cases subsequently to a triclinic phase. Boracites with magnetic ions further develop magnetic ordering and become multiferroic. Here we investigate the mechanism for the ferroelectric phase transition from the cubic high symmetry phase to the orthorhombic ferroelectric intermediate and triclinic low temperature phase. Finally we found a dominant unstable phonon mode at the Γ point which drives the phase transition. However this mode couples with modes at the zone boundary making the boracites improper ferroelectrics.

[1] Nelmes, R., 1974. Structural Studies of Boracites - Review of Properties of Boracites. Journal Of Physics C-Solid State Physics, 7(21), pp.3840-3854.

DS 19.34 Tue 12:15 Poster A

XAS and XMCD of ultrathin Fe layers on BaTiO$_3$(001): Experiment and Theory — •Stephan Borek[1], Angelika Chassé[1], Guntram Fischer[1], Wolfram Hergert[1], Remya Kunjuvettil Govind[1], Karl-Michael Schindler[1], Vasili Hari Babu[2], Joachim Gräfe[2], Martin Welke[2], and Reinhard Denecke[2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg — [2]Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig

Promising candidates for switching the magnetization using voltages are multiferroic systems. As a model system we studied ultrathin Fe layers on $BaTiO_3(001)$. Using x-ray absorption spectroscopy as a powerful method to investigate structural, electronic and magnetic properties simultaneously, the circular dichroism in x-ray absorption (XMCD) and x-ray absorption as such were used to determine the remanent magnetization as a function of film thickness. The onset of ferromagnetism at a temperature of 150 K was found for 5±1 layers. Using a Heisenberg-model in the framework of Monte-Carlo-Simulations shows that up to 3 monolayers the critical temperature is around 170 K.

In addition the contribution of each layer could be separated using a fully relativistic multiple scattering formalism. Different magnetic structures and their impact on the spectroscopic properties, as well as the anisotropic behaviour of the multiferrroic systems have been investigated theoretically. The spin and orbital moments as obtained from the XMCD experiments and DMFT calculations will be compared.

DS 19.35 Tue 12:15 Poster A

Ferroelectricity and Magnetic Structure of Mn Moments in Multiferroic GdMnO$_3$ — •Enrico Schierle[1], Victor Soltwisch[1], Christoph Trabant[1,2], Alex Frano[1,3], Detlef Schmitz[1], Fabiano Yokaichiya[1,6], Andrej Maljuk[1,4], Dimitri Argyriou[1,5], and Eugen Weschke[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Germany — [2]II. Physikalisches Institut, Universität zu Köln, Germany — [3]MPI-FKF Stuttgart, Germany — [4]IFW, Dresden, Germany — [5]European Spallation Source, Lund, Sweden — [6]Laboratrio Nacional de Luz Sincrotron, Campinas-SP, Brasil

Orthorhombic REMnO$_3$ oxides can show strongly coupled ferroelectric (FE) and magnetic order, with FE polarization P induced by magnetic cycloids of the Mn spins[1,2]. However, from recent X-ray diffraction studies, there is growing evidence for a decisive role of ordering of the RE-4f moments as well and it seems that a large part of P can be explained by ionic displacements not necessarily connected with cycloidal magnetic order of Mn moments[3,4,5]. We employed Resonant Soft X-Ray Scattering at the Mn-L$_{2,3}$ resonance to prove the existence of a ferroelectric phase at the surface of GdMnO$_3$ even in zero external magnetic field and to examine its connection to the magnetic structure of the Mn moments in an element specific way.

[1] Kimura et al., Nature **426**, 55-58 (2003) [2] Kenzelmann et al., PRL **95**, 087206 (2005) [3] Schierle et al., PRL **105**, 167207 (2010) [4] Feyerherm et al., Journal of Physics: Conference Series **200**, 012032 (2010) [5] Walker et al., Science **333**, 1273 (2011)

DS 19.36 Tue 12:15 Poster A

Electronic and magnetic properties of LuFe$_2$O$_4$ — •Christine Derks[1], Karsten Kuepper[2], Manfred Neumann[1], Dharmalingam Prabhakaran[3], Stephen J. Blundell[3], Andrei Rogalev[4], and Fabrice Wilhelm[4] — [1]Fachbereich Physik, Universität Osnabrück, Germany — [2]Institut für Festkörperphysik, Universität Ulm, Germany — [3]Department of Physics, University of Oxford, United Kingdom — [4]ESRF, Grenoble, France

LuFe$_2$O$_4$ is a compound showing fascinating magneto electric coupling via charge ordering. Electronic and magnetic properties of the charge ordered phase of LuFe2O4 have been investigated by means of x-ray spectroscopic and theoretical electronic structure approaches [1]. Using hard x-ray radiation of the ESRF ID12 circular polarisation beamline, Fe K-edge and Lu L-edge spectra have been detected. The Fe K-edge spectra will be discussed in comparison to the former Fe L-edge spectra. The Lu L-edge spectra show very interesting XMCD signals from which a small magnetic moment could be deduced.

[1]Kuepper et al. Phys. Rev. B, Vol. 80, 22, 220409

DS 19.37 Tue 12:15 Poster A

Influence of the strength of the magnetoelectric coupling on the electric field induced magnetization reversal in a composite multiferroic chain — Paul P. Horley[1], Alexander Sukhov[2], Chenglong Jia[2], Eduardo Martinez[1], and •Jamal Berakdar[2] — [1]Centro de Investigacion en Materiales Avanzados (CIMAV S.C.), Chihuahua/Monterrey, 31109 Chihuahua, Mexico — [2]Institut für Physik, Martin-Luther Universität Halle-Wittenberg, 06120 Halle/Saale, Germany

A theoretical study of the multiferroic dynamics in a composite one-dimensional system consisting of unstrained BaTiO$_3$ multiferroically coupled to an iron chain is presented. The method [1] is based on the thermodynamical treatment of the magnetization and the polarization quantitatively described via the Landau-Lifshits-Gilbert and the Landau-Khalatnikov equations (both at T=0 K) coupled via an additional term in the total free energy. The coupling originates from the screening charge induced in the ferromagnet by the ferroelectric polarization in a very narrow interfacial layer. For real parameters corresponding to the rhombohedral phase of BaTiO$_3$ and for bcc iron and for a wide range of strengths of this coupling we predict the possibility of obtaining a well-developed hysteresis in the ferromagnetic part of the system induced by an external electric field. We also inspect the dependence of the reversal modes on the electric field frequency and predict a considerable stability of the magnetization reversal for frequencies in the range of 0.5÷12[GHz]. [1] A. Sukhov *et al.,* J. Phys.: Cond. Matter **22**, 352201 (2010); Ferroelectrics (at press).

DS 19.38 Tue 12:15 Poster A

Electric field controlled manipulation of the magnetization in BaTiO$_3$ based ferroelectric/ferromagnetic hybrid structures — •Stephan Geprägs, Matthias Opel, Sebastian T. B. Goennenwein, and Rudolf Gross — Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching

Multiferroic materials, which simultaneously possess at least two long-range ordering phenomena in the same phase, have attracted widespread interest over the last years. In particular, the coexistence and cross-coupling of ferroelectric and ferromagnetic ordering in magnetoelectric multiferroics could offer the possibility to electrically read and write the magnetic state in future non-volatile memory cells. Unfortunately, these materials are scarce in nature. Attractive alternatives are composite material systems, in which ferromagnetic and ferroelectric compounds are combined. Such extrinsic multiferroic structures enable large and robust magnetoelectric effects at room temperature due to the elastic coupling between the ferroic constituents.

Here, we report on the electric field control of the magnetization in ferromagnetic/ferroelectric hybrid structures based on BaTiO$_3$ single crystals, using different materials as ferromagnetic layer, such as polycrystalline Ni and Fe$_{50}$Co$_{50}$ as well as epitaxial Fe$_3$O$_4$ and Sr$_2$CrReO$_6$ thin films. In these hybrid structures, reversible and irreversible changes of the magnetization as a function of the applied electric field were found, which are discussed in the framework of a theoretical model based on molecular dynamics simulations.

DS 19.39 Tue 12:15 Poster A

Interfacial effects on $[(\mathrm{SrMnO}_3)_j/(\mathrm{LaMnO}_3)_k]_N$ multilayers — •Markus Waschk, Paul Zakalek, Alexander Weber, and Thomas Brückel — Jülich Centre for Neutron Science JCNS-2 and Peter Grünberg Institut PGI-4, Forschungszentrum Jülich GmbH, D-52425 Jülich

On the search for new storage devices, the combination of ferroelectric and ferromagnetic properties in metal-oxide layers opens a wide field of new non-volatile memory devices, which show low energy consumption. Here we combine LaMnO$_3$ (LMO) and SrMnO$_3$ (SMO), which both are antiferromagnetic bulk insulators, while a multilayer stack behaves as ferromagnetic conductor for very small bilayer thicknesses. The ferromagnetism of the lower LMO layer is induced by the interface to the upper SMO layer. The influence is strongly dependent on the roughness of the interface, and was not yet observed in the opposite boundary. Our multilayers are grown epitaxially on SrTiO$_3$ (STO) (100) single crystals by an oxygen-assisted Molecular Beam Epitaxy System and alternatively, to compare both preparation methods, by a high pressure oxide sputtering system. Within our very smooth layers with interfacial roughness of the order of a unit cell we study the influence of the interface quality on the magnetic behaviour. We present the preparation method from first steps to a complex multilayer and the results of our in-house characterisation methods. Further we show our first results of a polarized neutron reflectometry study at D-17 of the ILL in Grenoble which show depth resolved the magnetic properties of the single layers and interfaces.

DS 19.40 Tue 12:15 Poster A

Fe-Cr cation ordering in PLD grown thin-films of multiferroic double perovskite Bi$_2$FeCrO$_6$ — •Vikas Shabadi, Philipp Komissinskiy, Mehran VafaeeKhanjani, Aldin Radetinac, and Lambert Alff — Institut für Materialwissenschaft, Technische Universität Darmstadt, Petersenstraße 23, 64287 Darmstadt, Germany

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

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The authors would like to acknowledge the support from DAAD.

DS 19.41 Tue 12:15 Poster A

Chemical solution deposition of multiferroic La0.7Sr0.3MnO3, BaTiO3 thin films prepared by ink plotting — •Anke Kirchner[1], Melis Arin[2], Petra Lommens[2], Xavier Granados[3], Susagna Ricart[3], Bernhard Holzapfel[1], and Isabel van Driessche[2] — [1]IFW Dresden, Institute for Metallic Materials, Helmholtzstr. 20, 01069 Dresden, Germany — [2]SCRiPTs, Department of Inorganic and Physical Chemistry, Ghent University, Krijgslaan 281 (S3), 9000 Ghent, Belgium — [3]Materials Science Institute of Barcelona, CSIC-ICMAB, Campus Universitat Autònoma de Barcelona, 08193 Bellaterra, Spain

Ferroelectric BaTiO3 (BTO) as well as ferromagnetic La0.7SrMnO (LSMO) thin films were prepared by chemical solution deposition (CSD). Based on these, a multiferroic architecture stack of La0.7Sr0.3MnO3 / BaTiO3 layers was developed. Aqueous, environmentally friendly precursor solutions were formulated for both materials. These are used for ink plotting on SrTiO3 (100) substrates. Films were subjected to a subsequent thermal treatment at the corresponding crystallization temperature. The structural as well as the magnetic and electric properties are presented. The Curie temperature of the ferromagnetic LSMO layer with a film thickness of only 60 nm was determined to 360 K. The magnetization curve indicates a hysteresis loop with a saturation magnetization above 400 emu/cm3. The ferroelectric character of the BTO films was demonstrated by polarization curves.

DS 19.42 Tue 12:15 Poster A

Diffraction Anomalous Fine Structure of Ho_2PdSi_3 and $YMn_{2-\xi}Fe_\xi O_5$ — •Melanie Nentwich[1], Matthias Zschornak[1], Carsten Richter[1,2], and Dirk C. Meyer[1] — [1]TU Bergakademie Freiberg, Institut für Experimentelle Physik, Leipziger Straße 23, 09596 Freiberg — [2]Hamburger Synchrotronstrahlungslabor HASYLAB at DESY

Diffraction Anomalous Fine Structure (DAFS) is a site-selective method for studying local electronic structures. As an advantage over X–ray Absorption Fine Structure (XAFS) it is possible to differentiate between atoms of the same kind but different Wyckoff positions which is especially useful for site–ordered mixed valence systems. Here, this method was applied to study the substitution of Mn atoms with Fe on the octahedral and pyramidal sites in $YMn_{2-\xi}Fe_\xi O_5$ [2]. Further, the *c*–ordering of Pd substitutes on Si sites according to a super structure proposal from F. Tang et al. [1] was investigated for the intermetallic compound Ho_2PdSi_3. Theoretical modelling was performed using the FDMNES code [3]. The measurements of the experimental data have been carried out at beamline E2 of DESY/HASYLAB Hamburg.

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DS 19.43 Tue 12:15 Poster A

Synthesis and characterisation of $BaTiO_3$ nanopowders and $CoFe_2O_4/BaTiO_3$ nanocomposites — •Yanling Gao, Morad Etier, and Doru C. Lupascu — Institute for Materials Science, University Duisburg-Essen, Universitätsstrasse 15, 45141 Essen, Germany

Multiferroic materials have drawn much attention, because they display the coexistence of ferroelectric and magnetic properties. In this study, we have succeeded in the synthesis and characterization of the $BaTiO_3$ nanocrystals by the low cost and straightforward auto-combustion process of amorphous organic precursor. In the following, $CoFe_2O_4/BaTiO_3$ nanocomposites with core/shell structures were also obtained by using this process. The particles are systematically characterized by powder X-ray diffraction (XRD), scanning electron microscopy (SEM), thermogravimetric, differential thermal analyses (TGA/DTA), and infrared spectroscopy (IR). The XRD results confirm the presence of both the spinel and the perovskite phases. The SEM-EDX and the atomic force microscopy (AFM) micrographs of $CoFe_2O_4/BaTiO_3$ show two-phase composite nanostructures of a cobalt ferrite core coated with a $BaTiO_3$ shell. The weight fraction of $CoFe_2O_4$ and the size of nanocomposites are the keys to the dielectric and magnetic properties of $CoFe_2O_4/BaTiO_3$ nanocomposites.

DS 19.44 Tue 12:15 Poster A

Topology of spin polarization of the 5d states on W(110) and Al/W(110) surfaces — •Artem G. Rybkin[1], E. E. Krasovskii[2,3,4], D. Marchenko[5], E. V. Chulkov[2,4,6], A. Varykhalov[5], O. Rader[5], and A. M. Shikin[1] — [1]St. Petersburg State University — [2]University of the Basque Country, San Sebastián — [3]IKERBASQUE Bilbao — [4]Donostia International Physics Center — [5]Helmholtz-Zentrum Berlin — [6]Materials Physics Center, CSIC-UPV/EHU, San Sebastián

The spin polarization of W(110) and Al/W(110) surfaces is studied by spin- and angle-resolved photoemission. On both surfaces distinct $E(\mathbf{k}_\parallel)$ dispersions are identified with an unusual topology: a single spectral branch is spin polarized antisymmetrically relative to the $\bar{\Gamma}$ point, and two spin-polarized branches cross at $\bar{\Gamma}$. Based on *ab initio* theory coupled with one-step photoemission calculations, we show that the measured spin polarization is a property of the ground state and identify the effect as the counterpart of the recently discovered Rashba-polarized bulk states but with a distinct non-Rashba topology. We address also the question of topological protection.

DS 19.45 Tue 12:15 Poster A

STM studies on the ternary topological insulator $PbBi_4Te_7$ — •Andreas Eich, Alexander Ako Khajetoorians, Julian Hagemeister, Oswald Pietzsch, Jens Wiebe, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Jungiusstrasse 11, D-20355 Hamburg, Germany

Topological insulators are a new class of materials with a bulk band gap like an ordinary insulator but exhibit a gapless surface state where the spin and momentum are locked. This topological surface state which results from a combination of spin-orbit interactions and time-reversal symmetry exhibits exotic spin-dependent transport phenomena at the surface. Nevertheless, the electronic properties of these surface states can be influenced by adsorbates. By adding a third component to a binary topological insulator it is also possible to influence both the energetic position of the Dirac cone and the surface state localization. Here we show STM measurements of the structure of a ternary topological insulator, namely $PbBi_4Te_7$. It has a hexagonal unit cell and contains five-layer (5L) and seven-layer (7L)-blocks with the atomic layer sequence, Te-Bi-Te-Bi-Te (5L) and Te-Bi-Te-Pb-Te-Bi-Te (7L). Theory predicts that not only the position of the Dirac cone relative to the Fermi energy is changed but that the surface states are localized in the 7L-block, leading to buried surface-states in the case of a 5L-terminated surface. We review the growth properties of this crystal and comment on the topological properties of these layers.

DS 19.46 Tue 12:15 Poster A

Bose-Hubbard model on two-dimensional line graphs — •Johannes Motruk and Andreas Mielke — Institut für Theoretische Physik, Ruprecht-Karls-Universität Heidelberg, Philosophenweg 19, D-69120 Heidelberg

We investigate the positive hopping bosonic Hubbard Model on line graphs of finite 2-connected planar bipartite graphs. The model on these lattice geometries exhibits flat bands and the single- as well as many-particle ground states are highly degenerate. Using notions from graph theory, we are able to give a basis for the space of many-particle ground states. The particles in these states are localized on vertices of the line graph which are edges of the original graph belonging to edge-disjoint cycles. This construction works up to a certain critical filling factor at which the cycles are close-packed. We rigorously show the linear independence of these states and prove that they span the space of many-particle ground states.

Furthermore, we establish that the entropy per lattice site in the ground state with constant (except critical) filling factor remains finite in the thermodynamic limit. Some of our findings can be applied to spin models of quantum antiferromagnets at high fields on the considered lattices.

DS 19.47 Tue 12:15 Poster A

Growth, Annealing and Characterization of $Sr_3Fe_2O_{7-\delta}$ — •Darren Peets[1], Junghwa Kim[1], Andrey Maljuk[1,2], Chengtian Lin[1], and Bernhard Keimer[1] — [1]MPI-FKF, Heisenbergstr. 1, D-70569 Stuttgart — [2]IFW Dresden, Helmholtzstr. 20, D-01069 Dresden

Iron(IV)- and ruthenium(IV)-containing perovskite-related phases have proven rich in novel physics. $SrFeO_{3-x}$ exhibits a wide variety of unusual magnetic phases, from five distinct types of helical magnetism at $x = 0$ [1] to a phase with frustrated, disordered Fe^{4+} moments at $x = 0.25$ [2]. The Ru-based intergrowth phase $Sr_3Ru_2O_7$ exhibits metamagnetic quantum critical points in field. However, the magnetic phase diagram of its Fe^{4+} analogue $Sr_3Fe_2O_{7-\delta}$ remains largely unexplored. We report the crystal growth, oxygen annealing, and characterization of large single-crystalline samples of $Sr_3Fe_2O_{7-\delta}$ suitable for neutron diffraction experiments. This work lays the foundation for comprehensive doping-dependent studies of $Sr_3Fe_2O_{7-\delta}$'s magnetic phase diagram and magnetic excitations.

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DS 19.48 Tue 12:15 Poster A

Finite-temperature density-functional theory of the Hubbard model — •Tobias Müller and Gustavo Pastor — Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel

The finite temperature properties of the Hubbard model are investigated in the framework of lattice density-functional theory (LDFT). The single-particle density matrix γ_{ij} with respect to the lattice sites is considered as the basic variable of the many-body problem. Following Mermin's theorem the free energy $F = E - TS = K + W - TS$ at temperature T is regarded as a functional of γ, where $K[\gamma]$, $W[\gamma]$ and $S[\gamma]$ stand for the kinetic-energy, Coulomb-energy and entropy functionals, respectively. A finite-temperature extension of Levy's constraint search approach is formulated. In this framework exact numerical results for W and S are obtained as a function of the nearest-neighbor γ_{ij} and T for different system sizes at half-band filling. The properties of these functionals are discussed in some detail. On the basis of this analysis we propose a simple explicit approximation to $W[\gamma]$ and $S[\gamma]$ which is relevant to arbitrary lattices. The method is finally applied to one-dimensional systems and the accuracy of the derived equilibrium properties is discussed

DS 19.49 Tue 12:15 Poster A

Green function of the single-site full-potential scattering problem including scalar-relativistic and spin-orbit effects — •David Bauer, Phivos Mavropoulos, Rudolf Zeller, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich

We present a method for the solution of the scalar-relativistic equation for a finite-range non-spherical potential and with the option of including spin-orbit coupling. Our scope is to determine the Green function for the single-site scattering problem, which is used in the multiple-scattering Korringa-Kohn-Rostoker Green function method for electronic structure calculations of impurity atoms embedded in a crystalline host.

The Green function can be written in a semi-separable form where the regular and irregular radial solutions of the scalar-relativistic operator are used. Also the right- and left-hand-side solutions are needed, which are not necessarily identical and can differ for example when including spin-orbit coupling as a pertubative term. The radial functions are calculated by a direct solution of a generalized Lippmann-Schwinger (LS) integral equation by employing a Chebyshev expansion. To save computational time, we proceed in a two step approach. First a LS equation is solved for the spherically symmetric case. The result is used to determine the Green function of the spherical problem, which in a second step is used in a new LS equation that includes non-spherical and spin-orbit terms. The latter has a special structure which allows a reduction of the computational time.

DS 19.50 Tue 12:15 Poster A

Micromagnetic Simulations of Spin Dynamics in Magnetic Nanodots — •Robert Rückriem[1], Philipp Krone[1], Thomas Schrefl[2], and Manfred Albrecht[1] — [1]Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany — [2]St. Pölten University of Applied Science, St. Pölten, Austria

Micromagnetic simulations were performed to investigate the spin dynamics in a single magnetic nanodot varying diameter ($50 - 150$ nm), thickness ($5 - 20$ nm), saturation magnetization ($0.5 - 2.0$ T) and uniaxial anisotropy ($0 - 250$ kJ/m^3). Using a finite element based three step simulation technique, the spatial distribution of excited spin waves as well as their frequency spectra was obtained. The occurring spin wave modes were identified as edge modes which are strongly influenced by demagnetizing field effects [1] and center modes which oscillate in the whole nanodot. By changing the magnetic and geometric parameters of the nanostructure, the precession frequency can be tuned which is important for magnetic engineering for instance in the field of microwave assisted magnetic recording [2].

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DS 19.51 Tue 12:15 Poster A

Pairs of diverging-converging spin vortices in biquadratically interlayer exchange coupled elements — •Sebastian Wintz[1], Christopher Bunce[1], Anja Banholzer[1], Thomas Strache[1], Michael Körner[1], Sibylle Gemming[1], Artur Erbe[1], Jeffrey McCord[2], Jörg Raabe[3], Christoph Quitmann[3], and Jürgen Fassbender[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Christian-Albrechts-Universität zu Kiel, Kiel, Germany — [3]Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland

Spin structures have been a relevant topic of magnetism research for many years. In particular, magnetic vortices have attracted much attention, due to their non-trivial topology and the various dynamic modes they exhibit [1]. A magnetic vortex consists of a planar, flux-closing magnetization curl that turns out of the plane in the central nanoscopic core. For a single layer structure, the curl's radial components typically cancel each other out. Recent investigations show that this holds also true for multilayer vortex systems comprising bilinear interlayer exchange coupling (IEC) [2]. In this contribution we report on pairs of diverging-converging spin vortices occurring in biquadratically coupled systems. Using magnetic x-ray microscopy we directly observe that the individual vortices of such pairs possess a residual radial magnetization component. From this $\nabla \mathbf{M}_{xy} \neq 0$, an additional perpendicular magnetization divergence $\nabla \mathbf{M}_z$ is analytically deduced. We compare our continuous model with discrete micromagnetic simulations. [1] S.-B. Choe et al., Science 304, 420 (2004). [2] S. Wintz et al., Appl. Phys. Lett. 98, 232511 (2011).

DS 19.52 Tue 12:15 Poster A

Structural, electronic, and magnetic properties of CoO/Ni interfaces — •Udo Schwingenschlögl, Sergiy Grytsyuk, and Fabrizio Cossu — KAUST, PSE Division, 23955-6900 Thuwal, Kingdom of Saudi Arabia

We study the CoO/Ni interface. Since the lattice mismatch of Ni with respect to CoO is about 21% we use a large supercell for our first-principles calculations, which reduces the lattice mismatch to 0.8%. We investigate the structural, electronic, and magnetic properties of two CoO/Ni interfaces: (1) An O layer mediates the coupling between Ni and Co and (2) direct Ni-Co contact. Our results indicate that the magnetization is reduced by 19% in the first case, while in the second case it increases by 106% as compared to bulk Ni. The magnetic moments of the Ni atoms are larger if the exchange coupling is mediated by O atoms, while for direct contact with the Co atoms they become smaller than in the bulk. The Co 3d local density of states of the second interface shows surprisingly small deviations from the corresponding bulk results, although the first coordination sphere is no longer octahedral.

DS 19.53 Tue 12:15 Poster A

Exchange-bias effects in Co/$YMnO_3$ bilayer: Magnetization and magneto-transport measurements — •J. Barzola-Quiquia, A. Lessig, C. Zandalazini, G. Bridoux, and P. Esquinazi — Division of Superconductivity and Magnetism, University of Leipzig, D-04103 Leipzig, Germany

The exchange bias effects in a bilayer composed by the antiferromagnetic o-$YMnO_3$ and ferromagnetic Co thin films have been investigated through SQUID magnetometry and magneto-transport measurements. Magnetization hysteresis loops and magneto-transport properties show pronounced asymmetries in the field and magnetization axis. Both exchange bias parameters, the exchange bias field $H_E(T)$ and the magnetization shift $M_E(T)$, vanish around the Néel temperature $T_N \simeq 45$ K. The magnetization shift is also measured by a shift in the longitudinal and Hall resistances showing a similar temperature dependence as the one obtained from magnetization measurements. Because the o-$YMnO_3$ film is highly insulating, our results demonstrate that the M_E shift is related to the pinned moments within the ferromagnetic Co layer at the interface.

DS 19.54 Tue 12:15 Poster A

Perpendicular exchange bias in ferrimagnetic spin valves — •Radu Abrudan[1], Ilie Radu[2], Detlef Schmitz[3], Hartmut Zabel[1], and Florin Radu[3] — [1]Institut für Experi-

mentalphysik/Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]Radboud University Nijmegen, Institute for Molecules and Materials, Heyendaalseweg 135, 6525 AJ Nijmegen,The Netherlands — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Albert-Einstein-Strasse 15, 12489 Berlin, Germany

Exchange bias effect refers to the shift of the hysteresis loop of a ferromagnet which is in direct contact to an antiferromagnet. For applications in spintronics a robust and tunable EB effect is required. We present experimental evidence for perpendicular EB in ferrimagnetic spin valves in a DyCo$_5$/Ta/Fe$_{76}$Gd$_{24}$ prototype trilayer, where the DyCo$_5$ alloy plays the role of a hard ferrimagnet and the Fe$_7$6Gd$_{24}$ is a soft ferrimagnet. Taking advantage of the tunability of the exchange coupling between the ferrimagnetic layers by means of thickness variation of an interlayer spacer, we show that perpendicular exchange bias can be induced with desirable absolute values at room temperature with no field cooling procedure. Moreover, the shift of the hysteresis loop can be reversed with relatively low magnetic fields of several hundred Oersteds. This flexibility in controlling a robust perpendicular EB at room temperature may be of crucial importance for applications.

DS 19.55 Tue 12:15 Poster A

Renormalization of exchange coupling parameters in systems with coexisting strong and induced magnetic moments — •Phivos Mavropoulos, Marjana Ležaić, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich

In magnetic systems with coexisting strong and induced (weak) magnetic moments, it is often the case that the magnetic excitations change the direction and magnitude of the weak moments but only the direction of the strong moments. It is also often the case that the energy landscape can be parametrised by a quadratic dependence on the weak-moments magnitude in addition to a Heisenberg expression for the strong-moments direction. We show that under these conditions the weak moments can be completely eliminated as degrees of freedom in favour of renormalized exchange coupling parameters among the strong moments. We further show that this renormalization is also valid at elevated temperatures. The thermodynamic properties (including all correlation functions) of the full system, where the strong and weak moments are independent degrees of freedom, can be derived from the correlation functions of the renormalized system, where only the strong moments are accounted for as degrees of freedom. A prerequisite for the latter theorem is a quadratic measure in the phase space of the weak moments. The theorem justifies certain schemes for the derivation of exchange parameters and can also be of practical use for reducing the numerical load in calculations.

DS 19.56 Tue 12:15 Poster A

Coupling Single Molecule Magnets to Ferromagnetic Substrates — Alberto Lodi Rizzini[1], Cornelius Krull[1], •Timofey Balashov[1], Jerald Kavich[1], Aitor Mugarza[1], Piter Miedema[2], Pardeep Thakur[3], Violetta Sessi[3], Svetlana Klyatskaya[4], Mario Ruben[4], Sebastian Stepanow[5], and Pietro Gambardella[1] — [1]ICN, Barcelona, Spain — [2]Utrecht University, Utrecht, The Netherlands — [3]ESRF, Grenoble, France — [4]Institute of Nanotechnology, KIT, Germany — [5]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

We investigate the interaction of TbPc$_2$ single molecule magnets (SMMs) with ferromagnetic Ni substrates. Using element-resolved x-ray magnetic circular dichroism, we show that TbPc$_2$ couples antiferromagnetically to Ni films through ligand-mediated superexchange. This coupling is strongly anisotropic and can be manipulated by doping the interface with electron acceptor or donor atoms. We observe that the relative orientation of the substrate and molecule anisotropy axes critically affects the SMM magnetic behavior. TbPc$_2$ complexes deposited on perpendicularly magnetized Ni films exhibit enhanced magnetic remanence compared to SMMs in the bulk. Contrary to paramagnetic molecules pinned to a ferromagnetic support layer, we find that TbPc$_2$ can be magnetized parallel or antiparallel to the substrate, opening the possibility to exploit SMMs in spin valve devices.

DS 19.57 Tue 12:15 Poster A

Zero bias anomalies and magnon excitation in tunnel junctions with magnetic and nonmagnetic electrodes — •Volker Drewello, Zoë Kugler, Günter Reiss, and Andy Thomas — Universität Bielefeld, Fakultät für Physik, Dünne Schichten und Physik von Nanostrukturen, Universitätsstr. 25, 33615 Bielefeld

In order to understand the tunneling spectra of magnetic tunnel junctions, tunnel junctions are fabricated in which one or both ferromagnetic electrodes were replaced by non-magnetic metal (tungsten). The bias dependence of these junctions is investigated with high accuracy by inelastic electron tunneling spectroscopy. Both types of junctions exhibit a zero bias anomaly that is different in size and sign compared to those of magnetic tunnel junctions, that is, junctions with two ferromagnetic electrodes. A pronounced difference is also found depending on the material that the electrons tunnel into, which is attributed to the excitation of magnons.

DS 19.58 Tue 12:15 Poster A

Electrical characterization of nanoscaled CoFeB|MgO|CoFeB-based magnetic tunneljunctions (MTJs) for thermal spin-transfer-torque (TST) — •Johannes Christian Leutenantsmeyer[1], Marvin Walter[1], Vladyslav Zbarsky[1], Patrick Peretzki[2], Henning Schuhmann[2], Michael Seibt[2], and Markus Münzenberg[1] — [1]I. Physikalisches Institut, Georg-August-Universität Göttingen, 37077 Göttingen — [2]IV. Physikalisches Institut, Georg-August-Universität Göttingen, 37077 Göttingen

MTJs are of general interest because of their quantum mechanical properties such as the tunnel-magnetoresistance (TMR), spin-transfer-torque and the recently measured magneto Seebeck effect.

Here we present the studies about our nanoscaled MTJs. The junctions are grown in UHV at base pressures around 5×10^{-10} mbar. The thin films are deposited by magnetron sputtering (Ta, CoFeB) and E-Beam evaporation (MgO, Ru). After annealing, the samples are patterned with bondpads via optical lithography, which enable us to contact sub-micron-scaled junctions. The MTJ itself is written by e-beam lithography and etched by argon-ion milling. With a high resolution e-beam resist, we reach a junction size of approximately 50 nm. The smaller junctions require the transition to thinner barriers (down to 3 monolayers), which we develop for the observation of new phenomena, like the theoretically predicted TST. Characterization shows TMR of up to 230% and large magneto Seebeck effect.

We gratefully acknowledge the funding of Deutsche Forschungsgemeinschaft through SFB 602 and SPP SpinCaT.

DS 19.59 Tue 12:15 Poster A

Spin transport and tunnel magnetoresistance of MgO-based magnetic tunnel junctions with different CoFeB compositions — •Vladyslav Zbarsky[1], Marvin Walter[1], Gerrit Eilers[1], Markus Münzenberg[1], Patrick Peretzki[2], Michael Seibt[2], and Johannes Leutenantsmeyer[1] — [1]I. Phys. Inst., Universität Göttingen, Germany — [2]IV. Phys. Inst., Universität Göttingen, Germany

The optimization of MTJs is necessary for increasing the TMR and therefore is very important for the production of MRAM devices. The quality of the tunnel barrier of our CoFeB/MgO/CoFeB MTJs is essential for getting high TMR. For this reason we minimized the roughness of MgO layer on the TMR. Another important parameter which we could optimize is the choice and preparation of the buffer layer. For example we compared two sorts of Ta buffer layers: prepared via magnetron sputtering and via e-beam evaporation. Already by optimizing these two parameters we could increase the TMR from 80% to above 220%. The next important step is further optimization of annealing parameters, because annealing influences the crystallisation behaviour of our MTJs. In this case, we investigate the influence of the annealing temperatures and annealing duration on the TMR. For the magneto-Seebeck effect a strong dependence on the choice of CoFeB composition is theoretically predicted. A change in the composition is of strong interest since the Fe to Co ratio gradually tunes the Fermi level by electron doping. In this context, we investigate the behaviour of TMR and spin transport for different CoFeB alloys.

DS 19.60 Tue 12:15 Poster A

Domain wall dependent magnetoresistance at zero field in electromigrated ferromagnetic nanocontacts. — •Mohamad-Assaad Mawass[1,5], Robert M. Reeve[1], Jakoba Heidler[2], Jan Rhensius[2,3], Laura J. Heyderman[2], Regina Hoffmann[4], André Bisig[2,3], and Mathias Kläui[1,2,3] — [1]Johannes Gutenberg-Universität Mainz, Mainz, Germany — [2]Paul Scherrer Institut, Villigen, Switzerland — [3]Universität Konstanz, Konstanz, Germany — [4]Physikalisches Institut and DFG-Center for Functional Nanostructures, Karlsruhe Institute of Technology, Karlsrue, Germany — [5]Max-Planck-Institut für Intelligente Systeme, Stuttgart, Germany

Magnetotransport measurements of magnetic nanocontacts have been studied with the aim to understand the interactions between spin-polarized charge carriers and magnetization on the nanoscale. Here, we study the evolution of magnetoresistance (MR) in electromigrated ferromagnetic break junctions obtained in clean ultra-high vacuum (UHV) conditions. While previously permalloy (Ni80Fe20) nanocontacts with variable constriction width have been investigated [A. Patra et al., PRB 82, 134447 (2010)], the question of the influence of the alloy nature on the observed MR effects remains. The in-situ controlled electromigration of notched half ring structures under UHV conditions for pure Ni and Fe contacts was investigated and similarly large effects could be observed. In particular, large MR effects at remanence are found in contacts that approach the atomic limit. Additionally, our measurements show a sign-change of the MR at low conductance levels and this is compared to recent theoretical predictions.

DS 19.61 Tue 12:15 Poster A

Anomalous Hall effect as a Fermi surface property — •Alexander Mook[1], Falko Pientka[1,2], Ingrid Mertig[1,3], and Peter Zahn[1] — [1]Institut für Physik, Martin-Luther-Universität, Von-Seckendorff-Platz 1, D-06120 Halle — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle — [3]Fachbereich Physik, Freie Universität, D-14195 Berlin

Already Haldane has shown in a seminal paper that the intrinsic anomalous Hall conductivity can be expressed as an integral over the Fermi surface as expected for a Fermi liquid property [1].

The anomalous Hall conductivity can be expressed either by a volume integral of the occupied states in the Brillouin zone or a Fermi surface integral with a thorough treatment of the Brillouin zone boundaries. We implemented both methods and applied them to a tight-binding Hamiltonian including exchange splitting and spin-orbit coupling.

Our investigations show that both results agree well. Details of the integration procedure have to be optimized to obtain a satisfying agreement for cases where avoided band crossings occur close to the Fermi level. The surface integration replaces the time consuming volume integration over the Fermi sea [2]. The method is applicable to advanced ab initio electronic structure schemes which provide besides the band energies also the Berry curvature.

[1] F. D. M. Haldane, *Phys. Rev. Lett.* **93**, 206602 (2004). [2] M. Gradhand, D. V. Fedorov, F. Pientka, P. Zahn, I. Mertig, and B. L. Göyrffy, *Phys. Rev. B* **84**, 075113 (2011).

DS 19.62 Tue 12:15 Poster A

Structural, electronic and transport properties of platinum-based chains: an ab initio study — •Ilia Sivkov, Kun Tao, and Valeri Stepanyuk — Max-Planck-Institut für Mikrostrukturphysik Weinberg 2, D-06120 Halle, Germany

We have investigated the structural, electronic and magnetic properties of platinum-based chains. Both pure platinum chains and chains with 3d impurities have been considered. The calculations of these properties were performed using methods based on the density functional theory.We show that the magnetic anisotropy energy of such chains strongly depends both on their shape, and on the impurities involved. Furthermore, transport calculations based on the non-equilibrium Green's function formalism have been performed.

DS 19.63 Tue 12:15 Poster A

Magnetic and transport properties of a series of dinucklear Nickel(II) complexes — •Claudia Loose[1], Torsten Hahn[1], Jens Kortus[1], Jochen Lach[2], and Berthold Kersting[2] — [1]TU Bergakademie Freiberg, Fakultät für Chemie und Physik — [2]TU Leipzig, Fakultät für Chemie und Mineralogie

Using first-principle density functional theory (DFT) we examined four different dinucklear Nickel(II) complexes [1] in order to obtain the electronic and magnetic structure with a special focus on spin-dependent transport through these molecules.

We compare results from different exchange correlation functionals (PBE/B3LYP) as implemented in two different packages (NRL-MOL/ORCA). Furthermore we investigate the transport properties of those complexes using methods of the non equilibrium Green's function formalism (NEGF).

[1] Coord. Chem. Rev. 253 (2009) 2244 - 2260

DS 19.64 Tue 12:15 Poster A

Optimization of spin-valve structures for spin-pumping experiments — •Christian Swoboda, Nils Kuhlmann, Andreas Vogel, Toru Matsuyama, and Guido Meier — Institut für Angewandte Physik und Zentrum für Mikrostrukturforschung, Universität Hamburg, Jungiusstrasse 11, 20355 Hamburg, Germany

In recent years, high-frequency phenomena of magnetic nanostructures have been studied intensively since they are expected to provide new technological applications as well as fundamental understanding of spin dynamics. Currently, the combination of magnetization dynamics and spin transport, the spin-pumping effect [1, 2], is of great interest. First experimental results including the detection of pure spin currents have been presented [3]. The aim of our work is to build an all-metal lateral spin-valve [4], where the spins are injected into an adjacent normal-metal via a ferromagnet with precessing magnetization at ferromagnetic resonance (spin-pumping). The lateral spin-valve device enables to detect and to quantify the pure spin current via a second ferromagnet. Besides the basic concept of a lateral spin-valve device operated by spin-pumping, we present a detailed study of the magnetization dynamics of the ferromagnetic electrodes. We optimized geometry and center-to-center distance of the electrodes in order to enhance the spin-pumping efficiency.

[1] Y. Tserkovnyak et. al., PRL 88, 117601 (2002); [2] A. Brataas et. al., PRB 66, 060404 (2002); [3] M.V. Costache et. al., PRB 78, 064423 (2008); [4] A. Vogel et. al., APL 94, 122510 (2009)

DS 19.65 Tue 12:15 Poster A

Spin density distribution and Hanle lineshapes of injected spins into n-GaAs — •Bernhard Endres, Mariusz Ciorga, Robert Wagner, Sebastian Ringer, Martin Utz, Dominique Bougeard, Dieter Weiss, Christian H. Back, and Günther Bayreuther — Universität Regensburg

Spin extraction into a ferromagnetic GaMnAs contact from an n-GaAs channel across an Esaki diode structure was measured by cross-sectional imaging of the spin polarization in GaAs [1,2]. The resulting spin density distribution in the 1 μm thick GaAs channel shows a strong bias dependence with the maximum polarization at the contact edge opposite to the maximum charge current. This behavior cannot be described by a frequently used one-dimensional model whereas two-dimensional numerical simulations of the electron drift and spin diffusion reproduce the observed distribution quite well. Even at the nominally field-free contact edge electron drift must be taken into account because of the inhomogeneous current density. As a consequence, if Hanle measurements are fitted with a one-dimensional drift-diffusion function as usually done they yield spin lifetimes which may strongly depend on the distance to the contact and the applied bias voltage. In contrast, a two-dimensional fit including the nonuniform current density provides spin lifetimes nearly independent of bias and contact distance. The remaining variations can be explained by electric fields around the contact area. [1] P. Kotissek et al., Nature Phys. 3, 872 (2007) [2] B. Endres et al., J. Appl. Phys. 109, 07C505 (2011)

DS 19.66 Tue 12:15 Poster A

Fe_3O_4/ZnO: A high-quality magnetic oxide-semiconductor heterostructure by reactive deposition — •Ozan Kirilmaz[1], Sebastian Brück[1,2], Markus Paul[1], Andreas Müller[1], Eberhard Goering[3], Jo Verbeeck[4], He Tian[4], Michael Sing[1], and Ralph Claessen[1] — [1]Experimentelle Physik 4, Universität Würzburg, D-97074 Würzburg, Germany — [2]University of New South Wales, School of Physics, Sydney NSW 2052, Australia — [3]Max Planck Institute for Intelligent Systems, D-70569 Stuttgart, Germany — [4]Electron Microscopy for Materials Science, University of Antwerp, 2020 Antwerp, Belgium

Magnetite (Fe_3O_4) is ranked among the most promising materials to be used as a spin injector into a semiconducting host. We demonstrate epitaxial growth of Fe_3O_4 films on ZnO which presents a further step for polarized spin injection into semiconductors. Regarding volume properties of the films, X-ray photoelectron spectroscopy evidences that the iron-oxide is phase-pure and stoichiometric magnetite. Diffraction measurements indicate highly oriented epitaxy and complete structural relaxation. The magnetic behavior shows a slow approach to saturation at high fields in comparison with bulk crystals. The typical (111) surface structure of Fe_3O_4 is observed already at the early growth stage. Due to island growth, domain boundaries form upon coalescence of the islands. The island growth enables partial relaxation of the misfit strain. X-ray resonant magnetic reflectometry reveals that only the very first monolayers of Fe_3O_4 at the interface exhibit a reduced magnetization, presumably related to the presence of the ZnO substrate.

DS 19.67 Tue 12:15 Poster A

Spin Injection and Spin Transport in Zinc Oxide — •Matthias Althammer, Eva-Maria Karrer-Müller, Sebastian T. B. Goennenwein, Matthias Opel, and Rudolf Gross — Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching

The wide bandgap semiconductor zinc oxide is interesting for semiconductor spintronics because of its small spin-orbit coupling implying a large spin coherence length. We investigate the injection, transport, and detection of spin-polarized charge carriers in ZnO utilizing all-electrical, vertical spin valve devices with ferromagnetic electrodes. Using pulsed laser deposition and electron-beam evaporation, we fabricated epitaxial multilayers of TiN/Co/ZnO/Ni/Au on (0001)-oriented Al_2O_3 substrates with different thicknesses of the ZnO spacer layer ranging from 5 nm to 100 nm. The multilayers were patterned into vertical mesa structures with junction areas between 100 μm^2 and 400 μm^2. Magnetotransport measurements show a clear spin valve behavior. The switching fields correspond to the coercive fields of the ferromagnetic layers as determined by SQUID magnetometry. For a ZnO thickness of 15 nm, the magnetoresistance (MR) increases from 0.8% at 200 K to 8.5% at 1.8 K. We analyze the maximum MR at low temperatures as a function of the ZnO thickness in the framework of a two spin channel model with a spin-dependent interface resistance and obtain a spin drift length for ZnO of 14.3 nm.

This work was supported by the Deutsche Forschungsgemeinschaft via SPP 1285 (project no. GR 1132/14).

DS 19.68 Tue 12:15 Poster A

Spindynamics of microstructured permalloy systems — •Sven Stienen[1], Ralf Meckenstock[1], Jürgen Lindner[1], Nathalie Reckers[1], Kai Wagner[1], Florian Römer[1], Zheng Duan[2], and Michael Farle[1] — [1]Universität Duisburg-Essen, Fakultät für Physik and CeNIDE, Lotharstraße 1, 47057 Duisburg — [2]University of California, Department of Physics and Astronomy, Irvine, USA

We model a ferromagnetic resonance (FMR) measurement by micromagnetic simulations using the 3D Object Orientated Micromagnetic Framework (OOMMF) code to investigate spinwave modes in permalloy (Py) microstripes. Dispersion relations (3-12GHz) were calculated with different directions (0°/90°) of the external magnetic field (0-400mT) applied in the sample plane. The major magnetic anisotropy in the Py-stripe is the demagnetisation field. The simulations allow the visualization and identification of the excitations in the time and space domain. Quasi uniform, edge and not-aligned modes are observed. The simulations were compared with the FMR results obtained by anisotropic magneto resistance[1]. The position and shape of all modes can be explained by specific aspects of the demagnetisation field and are in qualitativly good agreement with simulations. This work has been supported by the Deutsche Forschungsgemeinschaft (DFG) via SFB 491.

[1]A. Banholzer et al, Nanotechnology, 22,(2011) 295713

DS 19.69 Tue 12:15 Poster A

Imaging of magnetisation dynamics of coupled vortices in trilayer systems — •Anja Banholzer[1], Sebastian Wintz[1], Christopher Bunce[1], Thomas Strache[1], Michael Körner[1], Arthur Erbe[1], Aleksandr Puzic[2], Jörg Raabe[2], Christoph Quitmann[2], Kilian Lenz[1], and Jürgen Fassbender[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [2]Paul Scherrer Institut, 5232 Villigen, Switzerland

Magnetic vortices recently gained interest as potential storage media. Different control methods are used to manipulate the vortex states. We now use scanning transmission x-ray microscopy (STXM) to image the magnetic configurations within the different layers of a Co/Cu/NiFe trilayer system. The dominant coupling mechanisms here are the magneto-dipolar interaction and interlayer exchange coupling. The corresponding magnetization configurations under a static magnetic field, as well as ac magnetic fields are investigated. The emerging motion of the core is tunable by the amplitude and frequency of the field. The interactions of the two cores and their individual resonance frequencies are studied. This implies a corresponding resistance change of different configurations at different magnetic fields and currents as well as the displacement of the core.

DS 19.70 Tue 12:15 Poster A

Oersted field contribution on the magnetic vortex core dynamics probed by homodyne detection — •June-Seo Kim[1,5], Martin Stärk[1], Mathias Kläui[1,5], Florian Kronast[2], Roland Mattheis[3], Christian Ulysse[4], and Giancarlo Faini[4] — [1]Fachbereich Physik, Universität Konstanz, Universitätsstr. 10, D-78457 Konstanz, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [3]Institut für Photonische Technologien e.V., Jena, Germany — [4]Phynano Team, Laboratoire de Photonique et de Nanostructures, CNRS, Marcoussis, France — [5]Institut für Physik, Johanes Gutenberg-Universität Mainz, D-55099, Mainz, Germany

When injecting spin-polarized currents into magnetic discs, both spin torque and Oersted fields can manipulate magnetic vortex structures. The Oersted field contribution due to the inhomogeneous current distribution in the magnetic vortex core structure is experimentally determined by using a homodyne detection scheme. We find that the amplitude of the vortex core gyration increases for vortices located close to the current injection contacts due to the enhancement of the Oersted field contribution. From systematic phase measurements as a function of microwave frequency, two remarkable phenomena are observed: (i) the trajectory of the vortex core gyration is distorted by the interaction with the disc edge leading to non-linear oscillations (ii) the interplay between spin torque and Oersted field depends sensitively on the exact vortex core position.

DS 19.71 Tue 12:15 Poster A

Ultrafast, layer-selective dynamics of interlayer exchange-coupled Fe-Ru-Ni-trilayers — •Dennis Rudolf[1], Patrik Grychtol[1], Roman Adam[1], Bastian Heller[1], Moritz Plötzing[1], Christian Weier[1], Claus M. Schneider[1], Chan La-O-Vorakiat[2], Emrah Turgut[2], Henry C. Kapteyn[2], Margaret M. Murnane[2], Stefan Mathias[3], Martin Aeschlimann[3], Justin M. Shaw[4], Hans Nembach[4], and Thomas J. Silva[4] — [1]Peter Grünberg Institut, PGI-6, Research Center Jülich, 52425, Jülich, Germany — [2]Department of Physics and JILA, University of Colorado, Boulder, Colorado 80309-0440, USA — [3]University of Kaiserslautern and Research Center OPTIMAS, 66606, Kaiserslautern, Germany — [4]Electromagnetics Division, National Institute of Standards and Technology, Boulder, Colorado, 80305-3328, USA

Using ultrafast light pulses of laser-generated high harmonics between 20 eV and 70 eV, we investigated static and dynamic properties of interlayer exchange-coupled thin Fe-Ru-Ni-trilayers with varying Ru thickness. In the static case we observed layer-selective switching of Fe- and Ni-layers. We studied the magnetization dynamics on the fs-timescale using a pump-probe technique with 1,5 eV-pump and high harmonics-probe and observed layer-selective dynamics of Fe- and Ni-layers at the M absorpion edges (54 eV for Fe and 66 eV for Ni). A comparison of the demagnetization times for parallel and antiparallel magnetization alignment of the Fe- and Ni-layers provides insight into the role of exchange interaction and spin transport in femtomagnetism.

DS 19.72 Tue 12:15 Poster A

Element-resolved Ultrafast Spin Dynamics in Multi-component Ferromagnets and Ferrimagnets — •Andrea Eschenlohr[1], Ilie Radu[1,2], Christian Stamm[1], Kadir Vahaplar[2], Torsten Kachel[1], Niko Pontius[1], Rolf Mitzner[1], Karsten Holldack[1], Alexander Föhlisch[1], Florin Radu[1], Richard F. L. Evans[3], Thomas A. Ostler[3], Johan Mentink[2], Roy W. Chantrell[3], Arata Tsukamoto[4,5], Akiyoshi Itoh[4], Andrei Kirilyuk[2], Alexey V. Kimel[2], and Theo Rasing[2] — [1]Helmholtz Zentrum Berlin für Materialien und Energie GmbH, Germany — [2]Radboud University Nijmegen, The Netherlands — [3]University of York, UK — [4]Nihon University, Chiba, Japan — [5]Japan Science and Technology Agency, Saitama, Japan

With 100 fs soft x-ray pulses generated by the Femtoslicing facility at the BESSY II storage ring we measure element-resolved transient x-ray magnetic circular dichroism in ferromagnetic NiFe alloys, as well as ferrimagnetic GdFeCo alloy after laser excitation. We find time constants of demagnetization that are not only different for each magnetic sublattice in our alloy samples, but also different from the time constants found for respective pure element samples. Supported by phenomenological considerations and atomistic simulations we conclude that sub-picosecond magnetization dynamics is sensitive to both the magnetic moment and exchange interaction between the sublattices in multi-component magnets.

DS 19.73 Tue 12:15 Poster A

Gyration of magnetic vortices in anharmonic potentials — •Christian Adolff, Michael Martens, Thomas Kamionka, Ulrich Merkt, and Guido Meier — Institut für Angewandte Physik und Zentrum für Mikrostrukturforschung, Universität Hamburg, Jungiustr. 11, 20355 Hamburg, Germany

Magnetic vortices inherently form in soft ferromagnetic thin-film elements. They can be described as quasiparticles in confining potentials with eigenfrequencies in the sub-gigahertz range [1, 2]. We investigate the excitation of magnetic vortices in permalloy squares with side lengths of up to five micrometers. Strongly excited vortex cores move near to the edges of the squares where significant deviations from a parabolic potential occur. Analyzing the eigenfrequency of the vortex for different geometries, i.e. side lengths and thicknesses, gives insight into isotropic and anisotropic terms of the potential. These are studied by means of ferromagnetic resonance spectroscopy, micromagnetic simulations and analytical calculations.
[1] A. Thiele, J. Appl. Phys. 45, 377 (1974)
[2] B. Krüger et al., Phys. Rev. B 76, 224426 (2007)

DS 19.74 Tue 12:15 Poster A

Magnetization dynamics in Ni on the picosecond timescale — •Martin Lüttich[1], Jakob Walowski[1], Andreas Mann[1], Markus Münzenberg[1], Unai Atxitia[2], and Oksana Chubykalo-Fesenko[2] — [1]I. Physikalisches Institut, Universität Göttingen — [2]Instituto de Ciencia de Materiales de Madrid

Magnetization dynamics of polycrystalline nickel films are measured using the all-optical pump-probe technique for various pump pulse fluences. The parallel treatment of photons, electrons, phonons and magnetic correlations of the system amounts a challenge to the microscopic theoretical description. At the same time different length and time scales are involved.

We investigate the influence of hot electrons on the relative demagnetization. Performing the experiment for different pump fluences, we measure a higher relative demagnetization at higher fluences. These results are compared to simulations with the Landau-Lifshitz-Bloch equation, which is based on a thermal model, and featured by the consideration of two electron temperature dependent relaxation times $\tau_\perp$ and $\tau_{||}$. The electron temperature needed as input for the simulations is extracted from experiments.

DS 19.75 Tue 12:15 Poster A

Ultrafast Demagnetization Dynamics in $Ni_{1-x}Pd_x$ alloys — •Moritz Plötzing[1], Patrik Grychtol[1], Roman Adam[1], Claus M. Schneider[1], Hans Nembach[2], Justin Shaw[2], Tom Silva[2], Oliver Schmitt[3], Daniel Steil[3], Mirko Cinchetti[3], and Martin Aeschlimann[3] — [1]Peter Grünberg Institut, PGI-6, Research Center Jülich, 52425, Jülich, Germany — [2]Electromagnetics Division, National Institute of Standards and Technology, Boulder, Colorado 80305-3328, USA — [3]University of Kaiserslautern and Research Center OPTIMAS, 67663, Kaiserslautern, Germany

In the presented work, we investigated alloys of Ni and Pd with varying mixing ratios focusing on the magnetization dynamics on different timescales. For this purpose, we characterized the samples using a vibrating sample magnetometer and ferromagnetic resonance in order to determine the Curie temperature T_C and the picosecond dynamics, respectively. The latter is described by the Gilbert damping parameter α. Both quantities depend strongly on the stoichiometry and can be tuned very precisely over a wide range by changing the Pd concentration. Additionally, we carried out a thorough investigation of the laser-induced demagnetization time τ_M on the femtosecond timescale employing a time-resolved MOKE setup. According to the theoretical model published in [1], the dynamics on both timescales is related and the proportionality is mainly defined by T_C. Using the measured values for α and τ_M, we study the applicability of the theory for a ferromagnetic d-alloy and consequently the underlying fundamental processes.

[1] Koopmans et al., Phys. Rev. Lett. 95, 267207 (2005)

DS 19.76 Tue 12:15 Poster A

Ultrafast magnetization dynamics of FePt:Cu — •Daniel Steil[1], Sabine Alebrand[1], Oliver Schmitt[1], Mirko Cinchetti[1], Martin Aeschlimann[1], Fabian Ganss[2], Christoph Brombacher[2], and Manfred Albrecht[2] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Institute of Physics, Chemnitz University of Chemnitz, 09107 Chemnitz, Germany

$L1_0$ ordered FePt compounds with out of plane anisotropy are one future candidate as a storage layer for the next generation of hard disc drives, due to their very high anisotropy energy. As these compounds typically have very high coercivity, they are best used in combination with heat assisted recording (HAMR) [1]. We have studied the demagnetization dynamics in the alloy system FePt:Cu following impulsive laser excitation. In particular we also investigated the helicity dependence of the magnetization dynamics. By adding copper to FePt it is possible to tune anisotropy and Curie temperature, which allows to study the influence of both parameters on magnetization dynamics. We find a fast and strong demagnetization for all sample compositions, leading to a long lasting multidomain state for high enough excitation fluences in remanence. Additionally we observe a small influence of light helicity on the magnetization dynamics for at least one of the samples, whose origin will be discussed.

Funding by the EU within the FP7 project UltraMagnetron is kindly acknowledged.

[1] D. Weller et al., Annu. Rev. Mater. Sci. 30, 611-644 (2000)

DS 19.77 Tue 12:15 Poster A

Angular and Temperature dependent Ferromagnetic Resonance (FMR) measurements on FeRh thin films — •Eduardo Mancini, Federico Pressacco, Markus Härtinger, Georg Woltersdorf, and Christian Back — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Regensburg, Deutschland

We report the results of FMR investigations performed on $Fe_{0.5}Rh_{0.5}$(30 nm)/MgO below and above the critical temperature (around 400 K) at which the magnetic order changes from the antiferromagnetic- to the ferromagnetic phase. From these measurements we extract the amplitude, the position and the linewidth of the resonance line. For the amplitude the heating and cooling branches display the hysterestic behavior which is expected for this material with a difference in their critical temperatures of about 10 K. In the ferromagnetic phase (T=450 K), we observe an easy plane anisotropy for the magnetization from the analysis of the resonance position as a function of the external field orientation. From the linewidth of the resonance we extract the damping of the magnetization and discuss its temperature dependence in the neighborhood of the critical temperature.

DS 19.78 Tue 12:15 Poster A

Time-resolved Scanning-Kerr-Microscope on Rolled-Up-Ferromagnetic-Microstructures — •Daniel Mellem, Sebastian Mansfeld, Jan-Niklas Toedt, Felix Balhorn, Lennard Moldenhauer, Wolfgang Hansen, Detlef Heitmann, and Stefan Mendach — Institut für Angewandte Physik, Jungiusstr. 11, D-20355 Hamburg

Our time-resolved Scanning-Kerr-Microscope (TR-SKM) [1] is used to directly image propagating spin waves. We introduce the working principle of our Microscope and present first measurements of spin waves in rolled-up ferromagnetic structures, which were recently introduced as a novel type of flexible spin wave resonator by our group [2].

We gratefully acknowledge support by the DFG via SFB668 and GrK 1286.

[1] S. Mansfeld et al., Physical Review Letters, in press (2011)
[2] F. Balhorn et al. PRL 104, 037205, 2010

DS 19.79 Tue 12:15 Poster A

Spin-Wave Confinement in Rolled-Up Permalloy Nano-Stripes in Various Magnetization Configurations — •Lennart Moldenhauer, Felix Balhorn, Daniel Mellem, Sebastian Mansfeld, Wolfgang Hansen, Detlef Heitmann, and Stefan Mendach — Institut für Angewandte Physik und Zentrum für Mikrostrukturforschung, Universität Hamburg, Jungiustr. 11, 20355 Hamburg, Germany

A variety of planar systems consisting of magnetic nano- and micro-stripes have recently been investigated in terms of their magnetodynamic behavior [1]. Using the concept of self-rolling strained layers [2] we realized rolled-up Permalloy (Py) stripes.

We studied the spin-wave behavior in these three dimensional self-organized structures in different magnetic configurations and for varying geometrical stripe parameters via broadband microwave absorption spectroscopy. We discuss our measurements in terms of azimuthal and axial spin-wave confinement. We compare our results to previous experiments on planar stripes and rolled-up films [3].

[1] J. Topp et al., PRB **78**, 024431 (2008); [2] V. Y. Prinz et al., Physica E **6**, 828-831 (2000); [3] F. Balhorn et al., PRL **104**, 037205 (2010)

DS 19.80 Tue 12:15 Poster A

Ultrafast magnetic dynamics in EuTe thin films — •Niko Pontius[1], Christoph Trabant[1,2], Enrico Schierle[1], Eugen Weschke[1], Torsten Kachel[1], Christian Schüssler-Langeheine[1], Rolf Mitzner[1], Günther Springholz[3], and Karsten Holldack[1] — [1]Helmholtz-Zentrum Berlin — [2]II. Physikalisches Institut, Universität zu Köln — [3]Institut für Halbleiterphysik, Johannes Kepler Universität, Linz, Austria

Ultrafast control of magnetic materials and structures are a key prerequisite for developing advanced magnetic storage devices with increased speed and decreased dimensions. To this end, investigations of confined magnetic structures behaviour apart from equilibrium with sufficient spatial and temporal resolution under as defined conditions as possible are essential.

Here we investigate the fs temporal non-equilibrium evolution of the antiferromagnetic (AFM) order in EuTe thin films through resonant soft x-ray diffraction after laser excitation. Momentum resolved scans across the Bragg reflection provide information on the thin film magnetic profile evolution during the ultrafast quenching and recovery of the AFM order. They reveal that the magnetic profile is modified in a completely different way than for elevated temperatures in thermal equilibrium. Since the AFM structure of EuTe sensitively depends on the ionic distances, this study also provides new information on the interplay between structural and magnetic degrees of freedom. The measurements were performed at the FemtoSPEX facility at the HZB.

DS 19.81 Tue 12:15 Poster A

Temperature dependence of the magnon dispersion relation in low-dimensional transition-metal systems: A first-principles investigation — •Waldemar Töws and Gustavo M. Pastor — Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel

The influence of Stoner excitations on the spin-wave spectrum of one- and two-dimensional 3d transition metals has been investigated. The physical situations represented by the Stoner excitations correspond to extreme nonequilibrium states, which can be induced by strong ultrashort laser pulses. In this work we quantify to what extent an important increase of the electronic temperature T_e describing Stoner excitations affects the stability of magnetism within the metal. For this purpose, we perform numerical calculations in the framework of *ab initio* density-functional theory with a generalized gradient approximation to the exchange and correlation energy. The free energy of frozen-magnon states as a function of spin-wave vector q and T_e have been systematically studied for V, Fe, Co and Ni wires and monolayers with various nearest-neighbor distances. First of all, we demonstrate that the local magnetic moments are extremely stable even at temperatures T_e much larger than the Curie temperature T_C. The T_e-dependence of the magnetic couplings between the local moments is quantified by fitting the effective exchange couplings J_{ij} to the free-energy dispersion relation in the framework of a classical spin model. One actually finds that electronic temperatures T_e well above T_C are needed to change the nature of the magnetic order within the metal. The consequences for the theory of laser-induced magnetization dynamics are discussed.

DS 19.82 Tue 12:15 Poster A

Time Resolved Scanning Kerr Microscopy of Structures in thin ferromagnetic Films — •Jan-Niklas Toedt, Sebastian Mansfeld, Jesco Topp, Kim Martens, Daniel Mellem, Wolfgang Hansen, Detlef Heitman, and Stefan Mendach — Institute of Applied Physics, University of Hamburg

We study the behavior of planar Damon-Eshbach spin-waves in thin structured ferromagnetic films utilizing time resolved scanning Kerr microscopy (TR-SKM) [1]. We have investigated spin waves incident on a range of structures including gratings, double slits and modulated films. We show that the underlying physics can be explained by the anisotropy of the dispersion relation leading, e.g., to sub wavelength imaging [2, 3].

We gratefully acknowledge support by the DFG via SFB 668, SFB 508, GrK 1286, and by the City of Hamburg via the Cluster of Excellence Nano-Spintronics.

[1] Freeman et al., Journal of Applied Physics **79**, 5898 (1996); [2] Liu et al., Science **315**, 1686 (2007); [3] Mansfeld et al., Physical Review Letters, in press (2011) - arXiv:1108.5883v1

DS 19.83 Tue 12:15 Poster A

Field-induced magnetization dynamics in dot patterned CoB/Pt multilayer structures — •F. Büttner[1,2,3,4], C. Moutafis[2,3], A. Bisig[1,2,3,6], C.M. Günter[4], J. Geilhufe[5], M. Schneider[4], C. v. Korff Schmiesing[4], M. Hantschmann[4], M. Riemeier[4], J. Mohanty[4], S. Schaffert[4], J. Franken[7], R. Lavrijsen[7], H. J. M. Swagten[7], H. Stoll[8], M. Weigand[5,8], M. Kläui[1,2,3,6], and S. Eisebitt[4,5] — [1]Uni Mainz, 55128 Mainz, Germany — [2]PSI, 5232 Villigen, Switzerland — [3]EPF Lausanne, 1015 Lausanne, Switzerland — [4]TU Berlin, 10623 Berlin, Germany — [5]HZB, 12489 Berlin, Germany — [6]Uni Konstanz, 78457 Konstanz, Germany — [7]TU Eindhoven, 5612 AZ Eindhoven, Netherlands — [8]MPI für Metallforschung, 70569 Stuttgart, Germany

The controlled movement of nanometer sized magnetic domains on the (sub-) nanosecond time scale is of key importance for the development of new magnetic devices in storage and computing technology. While magnetization dynamics in in-plane magnetized materials has been intensely studied, domain sizes are too large for most state-of-the-art applications. In out-of-plane materials, however, we find narrow domains and domain walls, but these are much more sensitive to local pinning, thus making controlled displacements extremely challenging. We present here high resolution magnetic images of low pinning CoB/Pt multilayer structures and demonstrate the suitability of this material for controlled and reproducible field-induced dynamics of the magnetic domains on the nanosecond time scale.

DS 19.84 Tue 12:15 Poster A

Spin-wave tunneling through a mechanical gap in microstructured $Ni_{81}Fe_{19}$-stripes — •Thomas Langner[1], Björn Obry[1], Philipp Pirro[1], Thomas Brächer[1,2], Katrin Vogt[1,2], Britta Leven[1], and Burkard Hillebrands[1] — [1]TU Kaiserslautern, Fachbereich Physik and Forschungszentrum OPTIMAS, Erwin-Schrödinger-Str. 56, 67663 Kaiserslautern — [2]Graduate School Materials Science in Mainz, Gottlieb-Daimler-Straße 47, 67663 Kaiserslautern

The manipulation of the propagation properties of spin waves is of high importance to develop systems that can transport information using the spin wave as information carrier. One way to manipulate these properties is the use of magnetic tunnel barriers. We investigated the tunneling of spin waves through a mechanical gap in microstructured stripes made of $Ni_{81}Fe_{19}$. The focus of this work is on the investigation of the transmission of spin waves with varying wavelengths through a tunnel barrier with respect to the position of the gap. It is shown that quantization effects play an important role in the transmission behavior of tunneling spin waves in microscaled systems. The region between the excitation antenna and the gap acts as a spin-wave resonator. It has a large influence not only on the excitation properties but also on the transmission characteristics. We present Brillouin light scattering microscopy measurements revealing a strong influence of pinning effects of standing spin-wave modes inside this resonator on the tunneling efficiency.

DS 19.85 Tue 12:15 Poster A

Spin-wave logic elements based on ferromagnetic microstructures — •Jan Westermann[1], Philipp Pirro[1], Thomas Brächer[1,2], Björn Obry[1], Katrin Vogt[1,2], Roland Neb[1], Britta Leven[1], and Burkard Hillebrands[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, TU Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Graduate School Material Science in Mainz, 67663 Kaiserslautern, Germany

The investigation of propagating spin waves in micron-sized metallic ferromagnetic structures is subject of different experimental studies due to their potential application in spin-wave logic devices. Using the amplitude and the phase of the spin waves, these devices may provide outstanding performance, especially when operated with multiple frequencies.

We present micro-magnetic simulations focused on the feasibility of micro-structured spin-wave logic elements as well as an experimental investigation of short wavelength spin waves. The controlled excitation and the propagation of those spin waves is essential for efficiently working spin-wave logic elements. To analyze the excitation spectrum we use phase resolved Brillouin Light Scattering Microscopy to observe the spin waves in single micro-structures. For these experiments, we excite spin waves using different kinds of microwave antennas which show geometry dependent excitation spectra. Our experimental and numeric investigations show that magnetic micro-structures are promising candidates for wave-logic based elements. Financial support by Carl-Zeiss-Foundation, MAINZ and DFG is gratefully acknowledged.

DS 19.86 Tue 12:15 Poster A

Quantitative modeling of elastically driven ferromagnetic resonance — •Matthias Pernpeintner[1], Mathias Weiler[1], Lukas Dreher[2], Hans Huebl[1], Christian Heeg[1], Rudolf Gross[1], Martin S. Brandt[2], and Sebastian T. B. Goennenwein[1] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Walter Schottky Institut, Technische Universität München, 85748 Garching, Germany

In conventional ferromagnetic resonance (FMR) experiments, an external radio frequency magnetic field drives the magnetization precession. Recently, it has been shown that FMR can be excited all elastically by means of coherent phonons [1]. In this acoustically driven FMR, the magnetoelastic coupling of surface acoustic waves (SAW) in the GHz frequency range with a thin ferromagnetic film is exploited.

Here we show that acoustically driven FMR can be phenomenologically modeled using a modified Landau-Lifshitz-Gilbert approach in which the SAW induces an internal, virtual magnetic driving field. In a quantitative analysis, the magnetization dynamics are calculated as a function of external magnetic field magnitude and orientation. Full quantitative agreement of this simulation and SAW transmission experiments performed in a Ni/LiNbO$_3$ hybrid device is shown, using a set of parameters consistent with literature data.

This opens the path for further experimental studies of resonant magnon-phonon coupling and acoustic spin current generation using elastically driven magnetization dynamics.

[1] M. Weiler *et al.*, Phys. Rev. Lett. **106**, 117601 (2011).

DS 19.87 Tue 12:15 Poster A

Microscopic magnetic structuring of spin-wave wave- guides by ion implantation in a Ni$_{81}$Fe$_{19}$ layer — •Thomas Meyer[1], Björn Obry[1], Philipp Pirro[1], Thomas Brächer[1,2], Roland Neb[1], Julia Osten[3], Thomas Strache[3], Jürgen Fassbender[3], and Burkard Hillebrands[1] — [1]FB Physik and Landesforschungszentrum OPTIMAS, TU Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Graduate School Materials Science in Mainz, 67663 Kaiserslautern, Germany — [3]Institut für Ionenstrahlphysik und Materialforschung, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Ion implantation of ferromagnetic films has proven to be a promising tool for the fabrication of fully planar samples with a microscopic magnetic substructure. A waveguide-like propagation of spin waves in a Ni$_{81}$Fe$_{19}$ film which was locally patterned by ion implatation could be observed. The investigations have been performed using Brillouin light scattering microscopy on samples patterned with varying ion fluences. Further investigations on the coupling behaviour of two parallel stripes in this fully planar structures have been performed. The presented fabrication technique of spin-wave waveguides provides much lower stray fields and better heat conduction. Especially the latter is a matter of interest when the objects are exposed to intense microwave fields (excitation of spin waves) or investigated by laser spectroscopy like Brillouin light scattering. Financial support by the DFG (GRK 792) is gratefully acknowledged.

DS 19.88 Tue 12:15 Poster A

Thermally modulated ferromagnetic resonance in planar microresonator — •Puchong Kijamnajsuk[1,2], Christian Schöppner[1], Sven Stienen[1], Detlef Spoddig[1], Ralf Meckenstock[1], and Josef Pelzl[2] — [1]Universität Duisburg-Essen, Standort Duisburg, Institut für Physik und CeNIDE, AG Farle, Lotharstr. 1, 47048 Duisburg — [2]Institute of Experimental Physics, Ruhr University Bochum

A novel approach based on the combination of two scanning thermal near field techniques: the thermally modulated ferromagnetic resonance (FMR) by the probe of a scanning thermal wave microscope and the 3ω-signal from the same thermal probe. The simultaneous detection of the thermally modulated microwave absorption and of the 3ω-response of the nano-probe offers a means to control the thermal contact between probe and sample. To enhance the sensitivity of the FMR detection for the single 30nm x 30nm x 30nm ferromagnetic Heusler alloy Ni$_{45}$Mn$_{37}$In$_{13}$Co$_5$, we have designed a microresonator setup. The constant amplitude microwave field is generated inside the resonator at the position of the sample at a fixed frequency 14GHz. To observe the FMR we apply the fixed external magnetic field and modulate the sample temperature by joule heating from the probe. With the microresonator we demonstrate the detection of FMR of a single nano-sized cube.

DS 19.89 Tue 12:15 Poster A

Broadband Electron Spin Resonance Experiments using superconducting Coplanar Waveguides — •Conrad Clauss[1], Daniel Bothner[2], Lapo Bogani[1], Marc Scheffler[1], Dieter Koelle[2], Reinhold Kleiner[2], and Martin Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart, D-70550 Stuttgart, Germany — [2]Physikalisches Institut - Experimentalphysik II and Center for Collective Quantum Phenomena in LISA+, Universität Tübingen, D-72076 Tübingen, Germany

In recent years superconducting coplanar devices operating at microwave/GHz frequencies are employed in more and more experimental studies.

Here, we present electron spin resonance (ESR) experiments using a superconducting coplanar waveguide to provide the RF field to drive the spin flips. In contrast to conventional ESR studies this allows broadband frequency as well as magnetic field swept observation of the spin resonance.

We show experimental data of the spin resonance of the organic radical NitPhoMe (2-(4'-methoxyphenyl)-4,4,5,5-tetra-methylimidazoline-1-oxyl-3-oxide) for frequencies in the range of 1 GHz to 40 GHz and corresponding magnetic fields up to 1.4 T (for g=2). In addition we show the temperature dependence of the ESR signals for temperatures up to 30 K, which is well above the critical temperature of the niobium superconductor.

DS 19.90 Tue 12:15 Poster A

Studying magnetic nanostructures and the local magnetic induction of bulk samples by micro-Hall magnetometry — •Merlin Pohlit[1], Pintu Das[1], Adham Amyan[1], Yuzo Ohno[2], Hideo Ohno[2], and Jens Müller[1] — [1]Physikalisches Institut, Goethe-Universität, Frankfurt (M), Germany — [2]Laboratory for Nanoelectronics and Spintronics, Tohoku University, Sendai, Japan

Hall magnetometers based on high-mobility two-dimensional-electron systems in GaAs/AlGaAs heterostructures are powerful tools for studying individual magnetic structures on the micro- and nanoscale [1]. In particular, the devices can be used in a wide temperature and magnetic field range. Besides the possibility to position magnetic structures directly on top of the lithographically defined Hall crosses, bulk magnetic and superconducting samples may be placed on the magnetometers for local magnetic induction measurements. Here, a series of adjacent Hall crosses allows for spatially-resolved measurements with micron-size resolution. The versatility of the devices can be demonstrated by different measuring techniques including eight-terminal Hall gradiometry, magnetic flux noise measurements and the use as susceptometers. We discuss various examples for these methods, e.g. on the ferromagnetic semimetal EuB$_6$, where two consecutive transitions occur at 15.5K and 12.6K.These are related to electronic and magnetic phase separation and bulk magnetic ordering, but the details are not yet fully understood. We perform stray field calculations in order to simulate our results and find good agreement with the experimental data. [1] P. Das et al., APL 97, 042507 (2010)

DS 20: Application of thin films

Time: Wednesday 9:30–11:30 Location: H 0111

DS 20.1 Wed 9:30 H 0111

Towards attosecond pulse shaping in the water window — •Alexander Guggenmos[1,2], Michael Hofstetter[1,2], Ferenc Krausz[1,2], and Ulf Kleineberg[1,2] — [1]Fakultät für Physik, Ludwig-Maximilians-Universität München, Garching, Germany — [2]Max-Planck-Institut für Quantenoptik, Garching, Germany

Attosecond pulses pave the way towards the direct observation of electron dynamics in atoms, molecules or solid surfaces/nanostructures with a never before achieved temporal precision. Having the tunability for shaping these generated pulses from high harmonic radiation, serves as key for getting even deeper physical insight into these dynamics utilizing pump-probe experiments. Aperiodic broadband multilayer XUV mirrors are key components to fulfill these requirements and to offer for each experiment its perfectly tailored attosecond pulse due to controlling spectral resolution, center energy, temporal resolution or to compress chirped pulses to their fourier limit. Extending the current technology to the water window range around 300-500 eV may enable on the one hand a complete new sort of experiments as the in-vitro investigation of bio-materials on the attosecond time scale but on the other hand limits the scope for perfectly matched pulses due to fabrication limits of aperiodic multilayer designs.

We will present first investigations of multilayer XUV optics for the water window range which can control spectral and temporal resolution and even compress attosecond pulses with a high precision of reproducibility. Simulations and optimizations of multilayer systems as well as experimental results of XUV measurements are presented.

DS 20.2 Wed 9:45 H 0111

Single-Shot Imaging of Transient Reflectivity Changes for Temporal Jitter Characterization in Ultrafast X-ray Pump-Probe Experiments — M. Beye[3], M. Bionta[2], S. de Jong[2], A. Galler[1], C. Graves[2], J. Gruenert[1], M. Holmes[2], O. Krupin[1,2], •B. Li[1], R. Marvel[4], M. Minitti[2], A. Reid[2], and W. F. Schlotter[2] — [1]European XFEL GmbH, Hamburg, Germany — [2]SLAC National Accelerator Laboratory, CA 94025, USA — [3]Helmholtz Zentrum Berlin, Germany — [4]Vanderbilt University, Nashville 37235, USA

The X-ray Free-Electron-Laser sources will enable frontier research in the studies of extremely small structures (angstrom resolution) and extremely fast phenomena (<10 fs) at the same time. The origin of a Self-Amplified Spontaneous Emission-based FEL is the shot noise in the electron bunch, and thus each individual FEL pulse is different in terms of pulse energy, spectrum, wavefront, temporal properties etc. Measuring the temporal profile of the ultrafast FEL pulse remains a very challenging topic [1-2]. Here we report on recent results from a research campaign at the LCLS SXR instrument, where single-shot images of the cross-correlation of XFEL pulses and infrared laser pulses are measured and analyzed. The X-ray induced transient change of optical reflectivity is observed and the time delay in-between the X-ray pulses and optical laser pulses could also be derived preliminarily.

[1] Nature Photonics, 2, 165 (2008). [2] J. Phys. B: At. Mol. Opt. Phys., 43, 194010 (2010).

DS 20.3 Wed 10:00 H 0111

Fabrication of multilayer Laue lenses for high resolution hard x-ray microscopy — •Liese Tobias[1], Radisch Volker[1], Ruhlandt Aike[2], Krüger Sven Philip[2], Giewekemeyer Klaus[2], Osterhoff Markus[2], Salditt Tim[2], and Krebs Hans-Ulrich[1] — [1]Institut für Materialphysik, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Institut für Röntgenphysik, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

High resolution microscopy using both soft and hard x-rays is highly useful for biological and material sciences. Especially for spatial resolutions in the 10 nm range, highly-precise optical devices like Kirkpatrick-Baez mirrors, waveguides, compound refractive lenses or zone plates are required. As an alternative to conventional zone plates, also multilayer structures are applied, mostly fabricated by sputter-slice technique so far. However, multilayer zone plates (MZP) and Laue lenses (MLL) can also be fabricated by a combination of pulsed laser deposition (PLD) and focused ion beam (FIB) [1,2]. In this contribution, we show the design of a multilayer Laue lens for efficient focusing of hard x-rays in one dimension, the necessary optimization steps for the W/Si multilayer deposition, and the FIB fabrication from the deposited multilayer. First synchrotron experiments demonstrate the application for high resolution microscopy below 10 nm.

[1] T. Liese, V. Radisch and H.-U. Krebs, Rev. Sci. Instr. 81 (2010) 073710; [2] T. Liese,V. Radisch, I. Knorr, M. Reese, P. Großmann, K. Mann and H.-U. Krebs, Appl. Surf. Sci. 257 (2011) 5138.

DS 20.4 Wed 10:15 H 0111

LTO and LFP Thin Film Electrodes — •Frank Berkemeier, Wunde Fabian, Köhler Mathias, and Schmitz Guido — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm Str. 10, 48161 Münster, Germany

Thin films of lithium titanium oxide (LTO) and lithium iron oxide (LFP) were prepared by reactive ion beam sputtering, in a thickness between 50 and 500 nm. After preparation, the structure of the layers was investigated by X-ray diffraction (XRD) and transmission electron microscopy (TEM). To characterize the electrochemical properties of the layers, i.e. their capability to reversibly intercalate/deintercalate lithium, cyclic voltammetry (CV) and galvanostatic intermittent titration technique (GITT) was performed. It was found that in both cases, the electrochemical performance strongly depends on the conditions during sputtering, i.e. substrate temperature and oxygen partial pressure. When using optimum deposition conditions, reversible capacities of about 88 mAh/g (LTO) and 40 mAh/g (LFP) were found. Using LTO and LFP films that match each other with respect to their capacity, the electrochemical functionality of the films was demonstrated, combining both materials in a galvanostatic cell, and performing continuous CV measurements. In addition to these performance tests, the diffusion coefficient of lithium inside the films was determined by GITT, using thin film approach. Due to the well-defined thickness of the films, this approach can be used quite reliably, and shows in case of e.g. LTO that the diffusion coefficient of lithium only slightly depends on concentration within the regime of reversible cycling.

DS 20.5 Wed 10:30 H 0111

The Dependence of Field Effect Mobility on Layer Thickness in Ultra-Thin Film, Solution Processed, Indium Zinc Oxide TFTs — •Daniel Walker[1], Marc Häming[2], Alexander Issanin[2], Andreas Klyszcz[2], Mareiki Kaloumenos[2], Christian Melzer[1], Heinz von Seggern[1], Rudolph Hoffmann[2], Klaus Bonrad[2], and Peer Kirsch[2] — [1]TU Darmstadt, FB Materialwissenschaften, D-64287 Darmstadt, Germany — [2]Merck TU Darmstadt Laboratories, D-64287 Darmstadt, Germany

Indium-Zinc Oxide and related inorganic semiconductors are generating significant interest due to their transparency and large field effect mobilites for use in both next generation LCD backplane and flexible electronics. In our solution processed devices which have an ultra-thin active layer, between 5 and 20nm thick, we have found that films of equal thickness have dramatically different field-effect mobility and on-off ratios depending on subtle changes in the method of depositing the layer although the subsequent annealing step where the layer itself is formed remains the same. In some cases the mobilities more than double and exceed 10cm2/Vs. Furthermore we have seen that increasing the layer thickness results in an overall decrease in field effect mobility. The mechanism behind these effects is unclear and examining such thin films presents its own challenges. This talk will discuss different experimental techniques, from electronic measurements to SPM used to examine the obtained films and proposes possible mechanisms behind the enhanced transistor characteristics due to the preparation route.

DS 20.6 Wed 10:45 H 0111

Fabrication and characterisation of CNT via interconnects for application in integrated circuits — •Holger Fiedler[1], Sascha Hermann[1], Stefan E. Schulz[1,2], and Thomas Gessner[1,2] — [1]Chemnitz University of Technology, Center for Microtechnologies (ZFM), 09126 Chemnitz, Germany — [2]Fraunhofer Research Institute for Electronic Nano Systems (ENAS), 09126, Germany

Carbon nanotubes (CNT) have special properties, like high electrical and thermal conductivity as well as a strong resistance towards electromigration. This is why CNTs are potential candidate to replace copper in integrated circuits as interconnect material. We designed and fabricated CNT vias based on a metal/CNT hybrid technology. Via structures were patterned using a damascene process flow. Multiwall carbon nanotubes (MWCNT) were vertically grown in vias by chemical vapour deposition on a metallic substrate. Site-selectivity is achieved by employing surface-catalyst interactions to restrict CNT growth to the vias. The gaps between the CNTs were filled with silicon dioxide by decomposition of tetraethylorthosilicate. This is stabilizing the CNT arrays for a subsequent chemical mechanical planarization (CMP). Employing CMP provides two major benefits. Firstly, all shells of the MWCNT can be contacted and therefore contribute to the number of conductive paths. Secondly, due to the flatter surface after CMP, the deposition of the top contact layer is homogeneous, which significantly improves the metal-CNT contact. IV characteristics were obtained from 440 structures per wafer. 95% of the dies investigated show a resistance below 1 kΩ.

DS 20.7 Wed 11:00 H 0111

Unabhängige Temperaturkontrolle bei der Abscheidung von MPCVD-Diamantschichten — •Reinhard Remfort, Nicolas Wöhrl und Volker Buck — Universität Duisburg Essen und CeNIDE, 47057 Duisburg, Deutschland

Die MPCVD (Microwave Plasma Chemical Vapor Deposition) bietet eine etablierte Möglichkeit zur Herstellung großflächiger und besonders reiner bzw. gezielt dotierter Diamantschichten. Die Erzeugung solch maßgefertigter Diamantschichten erfordert eine genaue Kontrolle der Prozessparameter die im allgemeinen jedoch nicht unabhängig voneinander einstellbar sind. Eine besonders wichtige Variable ist die Substrattemperatur, da sie unter anderem maßgeblich die Morphologie der wachsenden Schicht bestimmt. Die Substrattemperatur ist stark abhängig von Plasmaparametern welche selbst wieder von den restlichen Prozessparametern abhängen. Um die Substrattemperatur unabhängig von diesen Parametern kontrollieren zu können, wurde eine Aerosolkühlung mit entsprechender Steuerung in den Substrathalter einer MPCVD-Anlage eingebracht. Die zur Regelung notwendige Temperaturmessung des Substrates erfolgt berührungslos mittels eines Pyrometers seitlich über ein im MW-Resonanzraum angebrachtes Periskop. Die Anordnung ermöglicht daher eine plasmaunabhängige Temperaturmessung. Einzelne Parameter wie zum Beispiel der Abstand des Substrates vom Plasma, können variiert werden ohne dabei die Substrattemperatur zu beeinflussen. Infolge dieser, von anderen Parametern unabhängigen Temperaturkontrolle, wird ein weiterer Freiheitsgrad für die Maßfertigung von Diamantschichten gewonnen.

DS 20.8 Wed 11:15 H 0111

Biofunctionalization of diamond like carcon layers — •Sven Möller[1], Jana Sommerfeld[1], Thomas Keller[2], and Carsten Ronning[1] — [1]Institute of Solid State Physics, University of Jena, Helmholtzweg 3, 07743 Jena — [2]Institute of Material Science and Technology, University of Jena, Löbdergraben 32, 07743 Jena

Diamond like carbon (DLC) is known to be a promising material for various biomedical applications. Due to this capability we have investigated its interaction with biological material like proteins. The DLC layers in this work have been prepared via mass separated ion beam deposition (MSIBD) on silicon substrates. For this purpose, carbon ions were accelerated with a voltage of 30 kV, separated by a 90° sector magnet and focused by a system of electron lenses. For deposition on the substrate, the ions were decelerated afterwards down to a few hundred eV. The ion energy at the end of the deposition process works as an indicator for the sp^3 content respectively the diamond likeness of the layer. Furthermore the surface can be changed by ion beam irradiation additionally in order to create regions with different surface properties. A solution containing the designated proteins were applied to the substrate, which has been analyzed afterwards using several techniques like atomic force microscopy for roughness measurements and contact angle measurements to study the wettability.

DS 21: Micro- and nanopatterning (jointly with O)

Time: Wednesday 11:45–13:45 Location: H 0111

DS 21.1 Wed 11:45 H 0111

Investigation of the Fe incorporation in ion-beam induced patterning on Si (100) — •behnam khanbabaee[1], andreas biermanns[1], marina cornejo[2], dietmar hirsch[2], frank frost[2], and ullrich pietsch[1] — [1]Universität Siegen, Festkörperphysik,Siegen, Germany — [2]Leibniz-Institut für Oberflächenmodifizierung e. V. (IOM), Leipzig, Germany

Ion beam erosion of semiconductor surfaces can modify the surface and depends on main sputtering parameters; different surface topographies such as ripple or dot like pattern are fabricated on the surface. Recent experiments have shown that the incorporation of foreign metallic atoms during the sputtering process plays a crucial role in pattern formation on surfaces. In the result of investigation we report on the depth profile of Fe atoms incorporated in sputtering process on Si (100) with low energy Kr ion beam. X-ray reflectivity (XRR) measurements determine the concentration profile of Fe atoms. X-ray absorption near edge spectroscopy (XANES) at the Fe K-edge (7112 eV) shows the formation of Fe rich silicide near surface region. X-ray photoelectron spectroscopy (XPS) shows a shift in the binding energy of Si2p levels at the surface compared top bulk confirming the formation of different phases of Fe-silicide on top and below the surface. The depth profiles obtained by XRR are compared to results obtained by complementary secondary-ion mass spectrometry (SIMS).

DS 21.2 Wed 12:00 H 0111

Threshold sputter depth for nanopattern formation and "zero" sputter yield ion beam irradiation of amorphous carbon — •Omar Bobes, Kun Zhang, and Hans Hofsäss — II. Phys. Institut, Uni Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The question whether sputtering is actually needed for pattern formation by ion beam erosion is still under debate. Therefore, we investigate the minimal required sputter depth which corresponds to the transition from a flat surface to a nanostructured surface for ion energies up to 10 keV. Especially, we chose ion beam irradiation under conditions where the sputter yield approaches zero. This can be achieved by using a light substrate materials such as carbon and heavy ions with energies not exceeding 100 eV, e.g., for 100 eV Xe^+-ions at 60° angle of incidence the sputter yield is to 0.002. In order to distinguish between sputter effect and the effect of displacement of recoil atoms for the pattern formation, low energy He^+-ion irradiation has been used and compared with Xe^+-ion irradiation. He^+-ions are unique, because they provide a small and almost constant sputter yield in the energy region between 500 eV and 1200 eV for amorphous carbon, but the displacement yield changes by a factor of two. One can choose the energies of Xe^+- and He^+-ions in such a way, either resulting in similar sputter yields or in similar displacement yield. The first results of such experiments will be presented.

DS 21.3 Wed 12:15 H 0111

Is silicide formation the decisive factor in impurity induced ion beam pattern formation? — Sven Müller[1], •Martin Engler[1], Frank Frost[2], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Cologne, Germany — [2]Leibniz-Institut für Oberflächenmodifizierung e.V., Leipzig, Germany

Metal co-deposition during ion beam erosion of Si induces nanoscale patterns. Here we present the results of a comparative study of Pd and Ag co-deposition during 2 keV Kr^+ ion irradition of Si(001) at normal incidence. Co-deposition was conducted by e-beam evaporation and by sputter deposition from an adjacent target, which was hit by the eroding ion beam simultaneously with the Si surface.

The collision kinetics of Ag and Pd are almost identical due to their similar atomic masses (Ag: 107.9 amu, Pd: 106.4 amu) and nuclear charges (Ag: $Z = 47$, Pd: $Z = 46$). There should be differences in pattern formation If chemistry is of relevance it, since Ag is almost insoluble in Si and forms no silicides, while Pd forms a number of silicides with substantial enthalpy of formation.

We find that for Ag co-deposition no patterns are formed while a sequence of patterns forms for Pd co-deposition which depends strongly on the flux ratio of arriving Pd atoms to Kr^+ ions.

Most surprising, pattern formation with Pd not only ceases for low, but also for high flux ratios. We therefore speculate that under the conditions used, phase separation through spinodal decomposition triggers the formation of the most pronounced patterns.

DS 21.4 Wed 12:30 H 0111

Innovative FIB specific Nanopatterning Strategies for Optimized Photonic Crystal Nanofabrication — •Frank Nouvertne and Achim Nadzeyka — Raith GmbH, Konrad Adenauer Allee 8, D-44263 Dortmund, Germany

The physical interactions underlying ion beam lithography (IBL) are quite complex as it brings in both sputtering and redeposition effects. Sputtering, the key mechanism for focused ion beam milling, is a complex process that depends on several factors, such as crystal orientation, surface topography, surface diffusion, ion implantation, and the stoichiometry of the solid. Redeposition is a less desirable mechanism that is ubiquitous in focused ion beam milling and has a similar complexity as sputtering. These additional physical complexities associated with the IBL technique call for more flexible beam deflection strategies than are typically available for EBL.

This talk will focus on the optimization of a photonic crystal fabricated by a FIB milling process, controlled by ELPHY MultiBeam, a new generation of nanofabrication pattern generators (PG). This newly developed PG allows for a huge variety of different directional and repetitive patterning strategies, which - in combination with a dedicated automatic drift compensation functionality - enables the required, most precise pattern placement accuracy and highest stability for this long term photonic crystal nanofabrication process over several hours.

DS 21.5 Wed 12:45 H 0111

Photonic Crystal Gratings for High-Speed Energy-Efficient Laser Sources — •Philip Wolf[1], Werner Hofmann[1], Norbert Grote[2], and Dieter Bimberg[1] — [1]IFKP & Center of Nanophotonics, TU Berlin — [2]Heinrich Hertz Institute, Fraunhofer, Berlin

Recently, VCSELs with highest modulation speeds [1] and highest energy efficiencies have been demonstrated [2]. Furthermore, a novel nano-photonic element, the so-called sub-wavelength or high-contrast grating (HCG) has been successfully applied in various VCSEL structures [3-5]. This special photonic crystal can be understood as a multi-mode Fabry-Pérot interferometer being able to replace a thick distributed Bragg-mirror [3]. It has been demonstrated that a HCG can improve the modal behavior of this type of lasers [4]. We expect that this technology will enable us to demonstrate VCSEL of superior bandwidth and energy efficiency. The challenge is to implement this technology into cutting-edge high-speed device designs. Here, we like to show our new concept and present recent breakthroughs in fabrication of these photonic crystals using electron beam lithography and dry-etching with our ICP-reactor.

[1] Hofmann, W. et al.: "44 Gb/s VCSEL for optical interconnects," OFC 2011, PDPC5, 2011. [2] Moser, P. et al.: "81 fJ/bit energy-to-data ratio of 850 nm VCSEL for optical interconnects," APL, 98, 2011. [3] Chang-Hasnain, C.J. et al.: "High-Contrast Grating VCSELs," IEEE J. Sel. Top. Quantum Electron., 15, 2009. [4] Hofmann, W. et al.: "Long-Wavelength High-Contrast Grating VCSEL," IEEE Photon. J., 2, 2010. [5] Il-Sung Chung et al., IEEE PTL, 20, pp. 105, 2008.

DS 21.6 Wed 13:00 H 0111

Nanopatterning by molecular polygons — •Stefan-Sven Jester, Eva Sigmund, Natalia Shabelina, Stephan M. Le Blanc, and Sigurd Höger — Rheinische Friedrich-Wilhelms-Universität Bonn, Kekulé-Institut für Organische Chemie und Biochemie, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany

Self-assembly of rigid molecules at the solution/solid interface interface allows an efficient approach towards two-dimensional supramolecular crystalline surface patterns. In-situ scanning tunneling microscopy yields a submolecularly resolved insight into the adlayer structures and thus a conclusion on the driving forces for their formation. Of particular interest is how the nanoscale architectures depends on the symmetry and dimensions of the molecular building blocks and their substituents. One approach to tailored adlayers is based on the adsorption of shape-persistent arylene-alkynylene macrocycles at the interface of 1,2,4-trichlorobenzene and HOPG. The molecules are accessible from organic synthesis and can be widely substituted with functional groups. Recent work has focused on macrocycles involving dithiophene corner building blocks connected via linear phenylene-ethynylene-butadiynylene units that can be viewed as molecular polygons of distinct symmetry (i.e. triangles, squares, pentagons, and hexagons), so that concepts of discrete geometry can be applied to design tailorable nanoscale surface patterns. The results gain insight into the 2D crystallization of nanoscale pentagons, binary mixtures of triangles and hexagons, and how large periodicities of several 10 nm may become accessible.

DS 21.7 Wed 13:15 H 0111

Rapid Prototyping of Hierarchical Gecko-Mimicking Nano- and Microstructures using Multiphoton Absorption — •Michael Röhrig[1], Michael Thiel[2], Matthias Worgull[1], and Hendrik Hölscher[1] — [1]Karlsruhe Institute of Technology, P.O. Box 3640, 76021 Karlsruhe, Germany — [2]Nanoscribe GmbH, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopolds., Germany

Applying 3D direct laser writing, we designed hierarchical gecko-type structures which match the elastic modulus and the relevant length scale of the gecko's setae very closely. These setae, delicate hairs covering the gecko's toes, originate the famous ability of geckos to climb effortlessly walls and ceilings. The setae are consisting of beta-keratine, a stiff material with Young's modulus of around 1 - 4 GPa. Due to their hierarchical design, they are very compliant and can achieve a very high real contact area even to rough substrates. Thus, the van der Waals forces cause high adhesion that enables geckos to stick to nearly every surface. Mimicking the gecko-effect is therefore pursued by groups all over the world. However, such structures are mostly based on soft materials that usually have some drawbacks, like degradation or rapid contamination. Hence, we used 3D direct laser writing to structure stiff materials. 3D direct laser writing is a rapid prototyping method based on multiphoton absorption that allows for the fabrication of arbitrary three-dimensional structures down to the nanometer scale. Measuring the adhesion by using atomic force microscopy, we could show that hierarchy is indeed favorable for artificial gecko-inspired structures made of stiff materials on the nanometer scale.

DS 21.8 Wed 13:30 H 0111

Time and space resolved pump-probe investigations on induced ablation of thin films with femtosecond laser pulses — •Stephan Rapp, Matthias Domke, and Heinz P. Huber — Munich University of Applied Sciences

An about 500 nm thin molybdenum film acts as p-contact for CIGS thin film solar cells, which has to be separated to serially interconnect the sub cells of a solar panel. The Mo can be structured either by irradiating the Mo from the front side or from the glass substrate side, resulting in a selective removal or a lift-off of an intact Mo cap, respectively. To investigate the underlying physical effects, a pump-probe setup is used for time- and space resolved microscopy. Several series of pictures are taken with time delays between femto- and microseconds, showing the complete temporal evolution of laser ablation (lift-off). The front side irradiation with fluences up to 5.0 J/cm^2 leads to thermal effects after a few picoseconds and after 100 ps ring systems appear. This suggests a bulging of the material. After 3 ns a shock wave crosses the sample with velocities from 675 to 3950 m/s. The substrate side irradiation with fluences up to 1.0 J/cm^2 initiates a decrease of the sample reflectivity due to heating for delay times up to 10 ps. Ring systems are formed after 4 ns and a model was created to determine the bulging height by analyzing these Newton′s rings. After the bulging a lift-off of an intact Mo cap can be observed at times between 10 and 40 ns for fluences above the ablation threshold which was determined to 0,6 J/cm^2.

DS 22: Trends in atomic layer deposition I (Focused session – Organizer: Nielsch)

Time: Wednesday 15:00–17:15 Location: H 0111

Invited Talk DS 22.1 Wed 15:00 H 0111

Trends in Atomic Layer Deposition — •Helmut Baumgart — Dept. of Electrical and Computer Engineering, Old Dominion University, Norfolk, Virginia 53529, USA — Applied Research Center at Thomas Jefferson National Accelerator Labs, Newport News, Virginia 23606, USA

Atomic Layer Deposition (ALD) is recognized by the International Technology Roadmap for Semiconductors (ITRS) as the preferred method to deposit technologically important thin films of novel high-k dielectric metal oxides or semiconducting metal oxides for CMOS and MEMS technology with Angstrom accuracy. ALD has been accepted by the microelectronics industry for mainstream Integrated Circuit (IC) processing technology primarily for high-k and metal gate stack engineering and DRAM capacitor development. Continuous device scaling serves as the technology driver and the trend is to develop very high-k oxides by ALD such as perovskites for future applications. In order to extend Moore*s Law another trend in CMOS technology is the increased interest in 3-D devices such as FIN-FETs and nanowire MOSFETs, which call for ALD technology for the realization of Gate-All-Around structures. There is an increasing demand for new and more complex nano-scaled films that are deposited with uniform composition, high conformality and superior thickness accuracy over increasingly severe surface topographies with high aspect ratios. An overview of recent trends in ALD thin film technology will be presented with examples in IC and non IC applications.

Topical Talk DS 22.2 Wed 15:30 H 0111

Energy conversion devices made using ALD — •Julien Bachmann — University of Hamburg, Hamburg, Germany

The interconversion of solar, electrical, and chemical forms of energy relies on the separation and recombination of charge carriers at interfaces. Because the transport of electrons, holes, and ions to and from the interface may be the factor limiting the overall device efficiency, nanostructuring often serves to increase the specific surface area of a device without elongating the diffusion distances excessively. The unique ability of atomic layer deposition to coat substrates of complex geometries — highly porous ones in particular — makes it particularly suited to the preparation of model systems in which to study the influence of geometric parameters on the efficiency of energy conversion devices.

We applied ALD to the creation of extremely thin antimony sulfide absorber layers in solar cells based on nanocrystalline titanium oxide. As a result, we were able to found an optimal thickness of the intrinsic absorber which maximizes the photovoltaic efficiency. In the area of electrolysis, we established the preparation of structured iron oxide surfaces the specific area of which is defined by cylindrical pores. The current density obtained for the oxidation of water at such electrodes depends on pore length and diameter linearly.

Topical Talk DS 22.3 Wed 16:00 H 0111

Role of substrate chemistry in ALD revealed by in-situ techniques — •Massimo Tallarida, Marcel Michling, Chittaranjan Das, Daniel Friedrich, Matthias Städter, and Dieter Schmeisser — Brandenburgische Technische Universität Cottbus, Konrad-Wachsmann-Allee 17, 03046 Cottbus, Germany

We show recent results of our in-situ investigations where the role of substrate chemistry in ALD is outlined. While the usual strategy to develop new properties of ALD films is to find new precursors or new procedures, the influence of substrate chemistry on the growth properties of ALD films has been often underestimated. This has principally a technical reason, as the usual characterization methods (QMS, FTIR, ellipsometry) are only weakly sensitive to the substrate, and a characterization of substrates before ALD is often not possible. Thanks to the use of in-situ characterization methods, including photoemission and X-ray absorption spectroscopy with synchrotron radiation, we are able to determine chemical properties of substrates before ALD and after either half or complete ALD cycles. The substrate chemistry influences the standard Al_2O_3 ALD with TMA and water [1,2], as well as the TiO_2 ALD with TTIP and either water, O_2 or O_2-plasma.

[1] M. Tallarida, K. Kukli, M. Michling, M. Ritala, M. Leskelä and D. Schmeisser, Chem. Mater. **23**, 3159 (2011);

[2] M. Tallarida, C. Adelmann, A. Delabie, S. van Elshocht, M. Caymax, and D. Schmeisser, Appl. Phys. Lett. **92**, 042906 (2011).

DS 22.4 Wed 16:30 H 0111

Highly Efficient Embedded Transmission Gratings — Stephan Ratzsch[1], •Frank Fuchs[2], Adriana Viorica Szeghalmi[1], Ernst-Bernhard Kley[1], and Andreas Tünnermann[2] — [1]Institut für Angewandte Physik, Friedrich-Schiller-Universität Jena, 07745 Jena — [2]Institut für optische Feinwerktechnik, Fraunhofer-Gesellschaft, 07745 Jena

We present a new approach for realization of a highly efficient transmission grating for TM polarized light operating at 1030 nm wavelength. It had been theoretically shown that it is possible to reach 100 % diffraction efficiency for a fused silica grating embedded within a high refractive index material. High quality, homogenous and void free coatings are required to achieve high optical efficiency. Plasma enhanced atomic layer deposition (PEALD) meets the enormous demands posed by these embedded gratings; however, film thickness homogeneity (less than 2% non-uniformity) and low surface roughness are essential. Titanium (IV) oxide (TiO2) is a potential candidate for the high index embedding material because of its adequate optical properties in the near infrared spectral range. The grating parameters (period, height, line width, etc.) have been optimized by rigorous coupled wave analysis (RCWA). These parameters depend on the refractive index of the titania layer. Therefore the refractive index and extinction should be precisely controlled. The refractive index of titania deposited by thermal ALD processes is generally highly sensitive to the temperature of the substrate. In contrast, the titania films produced by PEALD between 80°C and 210°C have a high refractive index.

DS 22.5 Wed 16:45 H 0111

Optical applications of atomic layer deposition thin films — •Adriana Szeghalmi[1], Thomas Weber[1], Mato Knez[2], Ernst Bernhard Kley[1], and Andreas Tünnermann[1] — [1]Institute of Applied Physics, Friedrich Schiller University, Jena, Germany — [2]Max-Planck Institute of Microstructure Physics, Halle (Saale) Germany

Thin films produced by atomic layer deposition (ALD) are very promising optical layers for the development of highly efficient optics. Here, a broad overview of optical elements developed based on ALD thin films and multilayers will be presented. ALD nanolaminates with a period below 10 nm have very low interlayer diffusion and roughness and can be applied as X-ray mirrors. Nanostructured optical elements can highly benefit of conformal ALD coatings. Metal wire polarizer elements for UV applications with high polarization extinction ratio at ca. 250 nm wavelength have been obtained by a frequency doubling technique using ALD deposition of iridium. Coating high aspect ratio linear gratings with high refractive index dielectric materials, guided mode resonance grating (GMRG) optics can be easily achieved. These resonant waveguides respond by a large spectral shift of the guided mode resonance peak in the reflectance or transmittance spectra to changes of the local dielectric environment. These elements find application as filters, mirrors, sensors, etc. The optical properties and sensitivity of GMRG optics have been optimized by rigorous coupled wave approach calculations. Using highly sensitive GMRG elements, the ALD growth of sub-nanometer thin films has been monitored in situ for the first time.

DS 22.6 Wed 17:00 H 0111

Templated ALD for Synthesis of Magnetic Nanotube Suspensions — •Robert Zierold[1], Zhenyu Wu[2], Carl E. Krill III[2], and Kornelius Nielsch[1] — [1]University of Hamburg — [2]Ulm University

Commercial ferrofluids usually consist of spherical, superparamagnetic nanoparticles suspended in a carrier liquid. The application of an external magnetic field, however, can trigger network formation and a concomitant increase in the liquid's viscosity—its so-called *magnetoviscosity*. Herein, we show how magnetic nanotubes can be prepared by ALD in porous alumina templates. In this process, the iron oxide deposited from the reaction of ferrocene with ozone is sandwiched between two silica layers (APTES, water, ozone) for protective reasons. The combination of a template, the sub-nm layer thickness control afforded by ALD, and proper adjustment of the H_2 reduction parameters for the converting amorphous iron oxide to magnetite allow the experimentalist to tailor all geometric tube parameters (length, diameter, wall thickness) as well as the type of magnetism manifested by the nanotubes—superparamagnetism/ferromagnetism. Viscosity measurements performed on mixtures of commercial ferrofluids (consisting of spherical particles) with nanotubes reveal a significant enhancement in the strength of the magnetoviscous effect compared to samples without additives. The different fluid-mechanical properties of such *hybrid* ferrofluids might pave the way for new engineering applications.

Financial support was provided by the state of Hamburg through the Excellence Cluster "Nanotechnology in Medicine"

DS 23: Trends in atomic layer deposition II (Focused session – Organizer: Nielsch)

Time: Wednesday 17:30–19:45 Location: H 0111

Invited Talk DS 23.1 Wed 17:30 H 0111

Functional complex oxide materials by atomic layer deposition — •Maarit Karppinen — Laboratory of Inorganic Chemistry, Department of Chemistry, Aalto University, Finland

Complex oxides of 3d transition metals play central roles in many important future applications related to e.g. spintronics and sustainable energy technologies. The apparent examples include but are not limited to the emerging spintronic devices based on manganese oxides, high-Tc superconductors based on copper oxides, next-generation thermoelectric devices based on cobalt oxides, solid-oxide fuel cells based on a tailored combination of various oxide materials, Li-ion batteries based on oxides of cobalt, manganese, iron, titanium, etc. The present lecture is a short summary of the ALD (Atomic Layer Deposition) research carried out on various complex oxide materials in our laboratory, such as hexagonal and orthorhombic forms of $RMnO_3$ (R = rare earth element) [1,2], $[Ca_2CoO_3]_{0.62}[CoO_2]$ [3], and $MnCo_2O_4$ [4]. All the fundamental elements of basic research on such thin-film materials are discussed: (i) ALD process development to obtain high-quality thin films of the desired metal composition, (ii) post-deposition treatments to obtain the desired phase in crystalline form and to control the oxygen stoichiometry, and (iii) basic chemical and physical property characterizations of the films.

[1] K. Uusi-Esko, J. Malm & M. Karppinen, Atomic layer deposition of hexagonal and orthorhombic $YMnO_3$ thin films, Chem. Mater. 21, 5691 (2009).
[2] K. Uusi-Esko & M. Karppinen, Extensive series of hexagonal and orthorhombic $RMnO_3$ (R = Y, La, Sm, Tb, Yb, Lu) thin films by atomic layer deposition, Chem. Mater. 23, 1835 (2011).
[3] J. Lybeck, M. Valkeapää, S. Shibasaki, I. Terasaki, H. Yamauchi & M. Karppinen, Thermoelectric properties of oxygen-tuned ALD-grown $[Ca_2CoO_3]_{0.62}[CoO_2]$ thin films, Chem. Mater. 22, 5900 (2010).
[4] K. Uusi-Esko, E.-L. Rautama, M. Laitinen, T. Sajavaara & M. Karppinen, Control of oxygen nonstoichiometry and magnetic property of $MnCo_2O_4$ thin films grown by atomic layer deposition, Chem. Mater. 22, 6297 (2010).

Topical Talk DS 23.2 Wed 18:00 H 0111

Uniform ZnMnO and ZnCoO films grown by Atomic Layer Deposition — •Marek Godlewski[1,2], Małgorzata Łukasiewicz[1], Aleksandra Wójcik-Głodowska[1], Elzbieta Guziewicz[1], and Bartłomiej Witkowski[1] — [1]Institute of Physics PAS, Al. Lotników 32/46, 02-668 Warsaw, Poland — [2]Dept. Mathematics and Natural Sciences College of Science, UKSW, Dewajtis 5,

Despite many efforts, origin of a ferromagnetic (FM) response in ZnMnO and ZnCoO is still not clear. It is believed that FM response reported for these two alloys is due to inclusions of foreign phases (TM oxides), defects or metal accumulations, rather than volume properties of investigated samples. Thus, control of uniformity of investigated samples is crucial.

Atomic Layer Deposition (ALD) enables deposition of uniform ZnMnO and ZnCoO films. This is possible by reduction of a growth temperature, selection of Mn and Co precursors, and use of optimized ratios of the relevant ALD cycles, as will be discussed in details. Importantly, uniform films of ZnMnO and ZnCoO remain paramagnetic even at increased concentration of magnetic ions. Magnetic investigations show the FM response for films deposited on purpose with a non-uniform Mn (Co) distribution. This enables us to discuss the origin of FM in ZnMnO and ZnCoO.

The research was partially supported by the grant Innovative Economy (POIG.01.01.02-00-008/08) and FunDMS Advanced Grant.

Topical Talk DS 23.3 Wed 18:30 H 0111

Atomic layer deposition of oxide thin films for non-volatile memory applications — •Susanne Hoffmann-Eifert — Peter-Grünberg Institut (PGI-7), Forschungszentrum Jülich and Jülich-Aachen Research Alliance (JARA-FIT), Germany

The fast growing market for portable electronic devices demands for non-volatile memory circuits with high speed data access and high reliability in combination with low power consumption. One promising concept is the resistive switching random access memory (RRAM). Films from transition metal oxides sandwiched between metal electrodes often show binary stable electric resistance states which can be switched by applying a certain voltage. Decisive for a stable device operation are a homogeneous microstructure and a controlled defect density in the oxide films of a few nm in thickness. Atomic layer deposition (ALD) can fulfill these requirements by its unique surface-reaction controlled self-limiting growth.

The talk will comprise recent results on ALD transition metal oxide thin films integrated into cross point MIM structures for future resistive switching applications. TiO2 thin films were grown from water based thermal ALD processes utilizing different alkoxide and amide based Ti sources. For ZrO2 thin films an amide type precursor was used in ozone and water based ALD processes. In addition, selected works on ALD HfO2, Nb2O5 and Ta2O5 thin films utilized in switching cells will be summarized. The examples highlight the importance of atomic layer deposition for the new non-volatile memory concept of resistive switching RAM.

DS 23.4 Wed 19:00 H 0111

Investigation of Morphology and Resistive Switching in ZrO2/TiO2 Films Grown by Atomic Layer Deposition — •Irina Kärkkänen[1], Mikko Heikkilä[2], Jaakko Niinistö[2], Mikko Ritala[2], Markku Leskelä[2], and Susanne Hoffmann-Eifert[1] — [1]Peter Grünberg Institute, Research Center Jülich , 52425 Jülich, Germany — [2]Laboratory of Inorganic Chemistry, University of Helsinki, Finland

Thin films from transition metal oxides have become of increasing interest for various applications, especially in high-k and resistive switching devices. In this work, we studied the influence of processing on the structural, morphological and electrical properties of ZrO2 and combination of ZrO2/TiO2 in the form of laminates and bilayers. The films were deposited from Zr(NEtMe)4 (TEMAZ) and Ti(OiPr)4 (TTIP) by atomic layer deposition using ozone or water as the oxygen sources. Deposition temperatures were 200°C, 240°C, and 280°C. The films were characterized with x-ray diffraction, x-ray reflectometry, atomic force microscopy, scanning electron microscopy, and electrical measurements. Differences in structure and electrical properties were found depending on type of oxygen source. Ozone grown ZrO2 films showed an(111) oriented cubic structure, whereas the ones deposited with water were polycrystalline with a cubic/tetragonal mixed phase in thicker films. Resistive switching of metal-insulator-metal structures was scrutinized. Structures like Pt/ZrO2/Ti/Pt, Pt/ZrO/TiO2/Ti/Pt, and Pt/TiO2/ZrO2/Ti/Pt showed different kinds of resistive switching behavior.

DS 23.5 Wed 19:15 H 0111

ALD of metal oxides and fluorides for optical applications — •Matti Putkonen[1,2], Adriana Szeghalmi[3], Mato Knez[3], and Timo Sajavaara[4] — [1]Beneq Oy, P.O. Box 262, FI-01511 Vantaa, Finland — [2]Laboratory of Inorganic Chemistry, Aalto University School of Science and Technology P.O. Box 16100, FI-00076 Aalto, Espoo, Finland — [3]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle (Saale), Germany — [4]Department of Physics, P.O. Box 35 (YFL), FI-40014 University of Jyväskylä, Finland

Atomic layer deposition (ALD) is a mature technology and there is increased number of ALD enabled applications, such as optical coatings.

For high index materials there are several possibilities but for low index materials deposited by ALD the selection is still more limited. The lack of industrially viable process for low refractive index materials, such as SiO_2 and metal fluorides is still the limiting factor.

In this presentation we show data concerning the SiO_2 deposition by thermal and plasma ALD using novel precursors as well as deposition of metal fluorides by using chemistry based on the traditional metal oxide ALD chemistry using either fluorinated metal β-diketonates or fluorinated hydrocarbons as a fluorine source. [1] The depositions were carried out by using Beneq TFS 200 and P400 ALD tools. The films were analyzed by TOF-ERDS, RBS, XRD and AFM. Optical properties of the deposited films were also measured at UV region. In this presentation we also discuss the ALD process requirements when these processes are transferred to large surface area coatings.

1. M. Putkonen et. al. J. Mater. Chem. 21 (2011) 14461.

DS 23.6 Wed 19:30 H 0111

Thermoelectric Characterization of Sb_2Te_3 Thin Films Deposited by ALD — •Sebastian Zastrow[1], Christian Schumacher[1], Matthias Regus[2], Stephan Schulz[3], and Kornelius Nielsch[1] — [1]University of Hamburg — [2]University of Kiel — [3]University of Duisburg-Essen

Thermoelectric materials can be used as temperature sensors or peltier cooling devices as well as to recover a part of the massive losses of energy due to the waste heat generated in fossil-fuel driven power plants and vehicles. Antimony Telluride (Sb_2Te_3) is a p-doped semiconductor and in the focus of interest for room temperature applications because of its thermoelectric peak performance at around 350 K. However, thermoelectric properties of Sb_2Te_3 ALD thin films have not been reported yet. Based on the work of Pore *et al.*, Sb_2Te_3 is deposited with a home-made reactor on SiO_2 by using $(Et_3Si)_2Te$ and $SbCl_3$. The surface roughness as well as the growth rate depend strongly on the deposition temperature as reported by Cu *et al.* To check the preferential growth directions and the composition, XRD and EDX measurements are carried out. The thermoelectric properties are influenced by the deposition parameters. Therefore, spatial scans of the Seebeck coefficient are performed and the electrical resistivity is measured. In order to enhance the thermoelectric performance, a first optimization by short annealing processes is done under helium atmosphere up to 570 K.

The authors would like to thank the "Karl-Vossloh-Stiftung".

DS 24: Organic electronics and photovoltaics: electronic properties I (jointly with CPP, HL, O)

Time: Wednesday 9:30–11:15 Location: H 2032

DS 24.1 Wed 9:30 H 2032

Design of novel dielectric surface modifications for perylene thin-film transistors — •Christian Effertz[1], Ingolf Segger[1], Philip Schulz[1], Arno Classen[2], Carsten Bolm[2], and Matthias Wuttig[1,3] — [1]I. Physikalisches Institut (IA), RWTH Aachen, 52056 Aachen — [2]Institut für Organische Chemie (IOC), RWTH Aachen, 52056 Aachen — [3]JARA FIT, Forschungszentrum Jülich, 52425 Jülich

Dielectric surface modifications (DSMs) can improve the performance of organic thin-film transistors (OTFTs) significantly. To gain a deeper understanding of this performance enhancement and to facilitate high mobility transistors, perylene based OTFTs utilizing novel dielectric surface modifications have been produced. Novel DSMs, which are based on derivates of tridecyltrichlorosilane (TTS) with different functional end-groups have been applied to tailor the adhesion energy of perylene. The resulting samples were characterized by electronic transport measurements, scanning probe microscopy and x-ray diffraction (XRD). Measurements of the surface free energy of the modified dielectric enabled the calculation of the adhesion energy of perylene upon these novel DSMs by the equation-of-state approach. These calculations demonstrate the successful tailoring of the adhesion energy. The insight gained in this study was used to carefully choose further novel DSMs based on polymers. Utilizing these novel DSMs, perylene thin-films and TFTs with a superior film quality, in terms of crystallinity and morphology, as well as performance, in terms of mobility, have been produced[1]. [1]: Effertz, C., et. al. (2011), Adv. Func. Mater. doi: 10.1002/adfm.201101299

DS 24.2 Wed 9:45 H 2032

Intermolecular hybridization governs molecular electrical doping — •Ingo Salzmann[1], Georg Heimel[1], Steffen Duhm[2], Martin Oehzelt[3], Patrick Pingel[4], Benjamin George[3], Alexander Schnegg[3], Klaus Lips[3], Ralf-Peter Blum[1], Antje Vollmer[3], and Norbert Koch[1,3] — [1]Humboldt Universität zu Berlin, Germany — [2]Chiba University, Japan — [3]Helmholtz Zentrum Berlin, Germany — [4]Universität Potsdam, Germany

Strong molecular acceptors in organic semiconductor (OSC) films are typically used for molecular electrical p-type doping assuming electron transfer from OSC to dopant. Positive polarons in the fundamental OSC gap are thus expected and could be observable in ultraviolet photoelectron spectroscopy (UPS) as emission feature at, or close to the Fermi Energy (E_F) with *reduced* ionization energy (IE), which, however, has not been observed to date. We present a study on the prototypical OSC/p-dopant pair pentacene (PEN) and tetrafluorotetracyano-quinodimethane (F4-TCNQ) up to 1:1 ratio [1]. The IE of 1:1 mixed (amorphous) films is *increased* and larger than possible for pure PEN, while all states occur well below E_F in UPS. We suggest OSC/dopant frontier molecular orbital hybridization forming a doubly occupied bonding and an empty anti-bonding supramolecular hybrid orbital with reduced fundamental gap, which is in fact found by optical absorption measurements and corroborated by density-functional theory (DFT) calculations. Based on similar results for various OSCs, common doping-related observations are discussed within this framework. [1] I. Salzmann, G. Heimel et al., *Phys. Rev. Lett.*, in press.

DS 24.3 Wed 10:00 H 2032

Effect of molecular p-doping on hole density and mobility in P3HT and MEH-PPV — •Patrick Pingel and Dieter Neher — Institute of Physics and Astronomy, University of Potsdam, D-14476 Potsdam

Molecularly doped semiconducting polymers can exhibit exceptionally high electrical conductivity, making them suitable for use in solution-processed organic circuitry. Recently, p-doping of conjugated polymers with the strong molecular acceptor tetrafluorotetracyanoquinodimethane, F_4TCNQ, has been introduced.

Here, we present a detailed study of the doping efficiency and carrier mobility in thin layers of poly(3-hexylthiophene), P3HT, and poly(2-methoxy-5-(2'-ethylhexyloxy)-p-phenylene vinylene), MEH-PPV, doped with F_4TCNQ over a wide range of concentrations. Investigation of these layers with impedance spectroscopy in a metal-insulator-semiconductor (MIS) geometry allowed us to determine both charge carrier density and mobility as a function of doping ratio.

We show that the density of mobile holes increases strictly linearly with increasing F_4TCNQ concentration, but the mobilities in P3HT and MEH-PPV exhibit non-monotonic dependencies on doping concentration. This behavior can be fully explained by a model originally developed by Arkhipov et al. [Phys. Rev. B **72**, 235202 (2005)], which predicts that the Coulomb potential of a doping-induced negative counterion acts as a trapping center for holes. Thus, energetical disorder in the polymer layer is effectively increased upon chemical doping.

DS 24.4 Wed 10:15 H 2032

Investigation of the degradation processes in small molecule solar cells using impedance spectroscopy — •André Döring, Lorenzo Burtone, Martin Hermenau, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany

The purpose of this work is to correlate the impedance spectra (IS) of different solar cell structures - composed of small molecules - with the degradation processes that take place under different aging conditions.

The materials chosen for the optically active bulk-heterojunction layer are ZnPc as donor and C_{60} as acceptor, often used in small-molecule solar cells. In addition to the bulk-heterojunction, doped electron and hole transport layers forming a p-i-n structure are used. Concomitant with the measurement of the IS, the characteristic parameters of the device (i.e. j_{SC}, V_{OC}, FF, PCE, EQE) are monitored during the degradation and correlated to the changes in the IS.

Analyzing the IS gives the possibility to identify different electrical processes that take place in the device. At the beginning of the aging process, we observe an initial improvement of the solar cell parameters, in conjunction with a decreasing trap response in the IS spectra. To investigate in more details the role of trap states for the solar cell performance, simplified structures are prepared. We identify in this way the trap location, type and density inside the solar cell structure. The devices are also exposed to controlled atmospheric conditions to investigate whether oxygen or water vapor is more responsible for the observed change in the electrical properties of the solar cell.

DS 24.5 Wed 10:30 H 2032

IR spectroscopic investigation of the MoO_3 doping efficiency in CBP — •Tobias Glaser[1,4], Sven Tengeler[1,4], Sebastian Beck[1,4], Daniela Donhauser[2,4], Bernd Lunkenheimer[3,4], Andreas Köhn[3,4], and Annemarie Pucci[1,4] — [1]Universität Heidelberg, Kirchhoff-Institut für Physik, INF 227, 69120 Heidelberg — [2]Technische Universität Braunschweig, Institut für Hochfrequenztechnik, Schleinitzstraße 22, 38106 Braunschweig — [3]Universität Mainz, Institut für Physikalische Chemie, Jakob-Welder-Weg 11, 55128 Mainz — [4]InnovationLab GmbH, Speyerer Str. 4, 69115 Heidelberg

A major challenge towards high-efficiency and low-voltage organic electronic devices such as OLEDs is to overcome the low bulk conductivity of the organic films. P-type doping with transition-metal oxides like tungsten oxide and molybdenum oxide has proven to increase the charge carrier concentration in hole transporting materials. But the doping efficiency of only a few percent is rather low and the reason for the low efficiency is not fully understood yet. We investigated doping of the ambipolar charge transport material 4,4'-Bis(N-carbazolyl)-1,1'-biphenyl (CBP) with MoO_3 using FTIR-spectroscopy in ultrahigh-vacuum. Comparison of the measured spectra of films with different MoO_3-concentration to DFT-calculations reveals the amount of charge transfer from CBP to MoO_3 but also shows that most of the CBP molecules are still in the neutral state. Also the impact of substrate temperature during the evaporation process is investigated.

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

DS 24.6 Wed 10:45 H 2032

Agglomeration of MoO_3 doped into organic thin films studied by TEM-spectroscopy and Tomography — •Daniela Donhauser[1,2], Katrin Schultheiss[1,2], Levin Dieterle[1,2], Martin Pfannmöller[3], Rasmus R. Schröder[3], Tobias Glaser[4,2], Bernd Lunkenheimer[5,2], Michael Kröger[1,2], and Wolfgang Kowalsky[1,2] — [1]Institut für Hochfrequenztechnik, Technische Universität Braunschweig — [2]InnovationLab GmbH, Heidelberg — [3]CellNetworks, Universität Heidelberg — [4]Kirchhoff-Institut für

Physik, Universität Heidelberg — [5]Institut für Physikalische Chemie, Johannes Gutenberg-Universität Mainz

Electrochemical doping is essential to overcome limitations in organic devices imposed by low intrinsic conductivity and high injection barriers at the contacts. Materials with very deep lying HOMO-levels like CBP (4,4'-Bis(N-carbazolyl)-1,1'-biphenyl) can be doped with transition metal oxides, e.g. MoO_3. In such systems a very low doping efficiency has been found for which the physical origin is not understood. With TEM spectroscopy we could show that agglomeration of MoO_3 in the CBP-matrix is most likely the reason for the low doping efficiency. Using TEM tomography we observed that MoO_3 forms filament-like structures perpendicular to the substrate. Combining our results with FTIR-measurements, which indicate a charge carrier localization at single molecules, we can model the charge transport to occur at the interface of the MoO_3 filaments and the organic matrix.

DS 24.7 Wed 11:00 H 2032

Depth Profiling of Organic Electronic Materials by Gas Cluster Ion Beam — •Andrey Lyapin — Physical Electronics GmbH, Fraunhoferstr. 4, D-85737, Ismaning, Germany

The development of new electronic devices incorporating organic materials, such as Organic Light Diodes (OLED) and Organic Photovoltaics (OPV) is rapidly increasing. To control quality, performance and lifetime of these devices, it is necessary to characterize the layered structures and the dopant distributions in the thin organic materials. Conventional surface analysis techniques such as XPS and ToF-SIMS, combined with mono-atomic ion beam sputtering, have been widely used for chemical depth profiling of inorganic thin films. However, this approach has not been successful for the depth profiling of organic materials due to the loss of chemical information during the sputtering process. Recent cluster ion beam developments utilizing C_{60}^{+} ions have also had limited success for the depth profiling of OLED and OPV structures due to similar modification of chemical and molecular information as a function of sputter depth. The use of surface-sensitive techniques will be discussed for chemical and molecular characterization of OLED and OPV materials in combination with newly developed Gas Cluster Ion Beam (GCIB) source to achieve non-destructive chemical/molecular characterization beyond the surface and through the device. The GCIB source with an average of 2500 Ar atoms per single charged ion has shown dramatic results that both simplify and improve upon the analysis of OLED and OPV materials with a C_{60}^{+} cluster ion beam.

DS 25: Organic electronics and photovoltaics: electronic properties II (jointly with CPP, HL, O)

Time: Wednesday 11:30–13:00 Location: H 2032

DS 25.1 Wed 11:30 H 2032

Point of inflection in IV curves due to degradation of cathode-organic interface — •Sidhant Bom, Nivedita Yumnam, and Veit Wagner — Jacobs University Bremen, School of Engineering and Science, Campus Ring 1, 28759 Bremen, Germany

The formation of point of inflection in IV curves is very well known in the field of organic photovoltaics. However, the opinion on this matter is diverse and conflicting. In an attempt to understand this phenomenon, we carried out series of experiments in which we were able to emulate the s-shape in the IV curve. In this study P3HT:PCBM bulk heterojunction solar cells were fabricated in between ITO/PEDOT:PSS and aluminum electrodes. Storing a completely fabricated cell in different environments resulted in a remarkable difference in the degradation of device parameters. Storing in vacuum completely stopped the degradation process while storing in an air tight container with nitrogen ambient showed extreme degradation within 24 hours with a severe s-shape in the IV curve. Interface modification at the cathode by inserting an additional thin C_{60} layer resulted in a similar s-shaped curve in contrast to the standard device. The data are explained by a model introducing a variable potential barrier at the aluminum cathode.

DS 25.2 Wed 11:45 H 2032

Dye Sensitised Solar Cells with Carotenoid Molecules — •Gino Günzburger[1], Res Jöhr[1], Biljana Bozic Weber[2], Catherine Housecroft[2], Edwin Constable[2], Hubert Hug[3], Petra Buchwald Hunziker[3], Ernst Meyer[1], and Thilo Glatzel[1] — [1]University of Basel, Department of Physics, Switzerland — [2]University of Basel, Department of Chemistry, Switzerland — [3]DSM Nutritional Products Ltd., NRD CH, Kaiseraugst, Switzerland

We report the analysis of long time stable dye sensitized solar cells using organic carotenoid-based dyes (crocetin, torularhodin and bixin). The particular properties of natural dyes require sensitisation in anhydrous solvents as well as cell assembly under inert gas atmosphere. Furthermore, the exposure to UV light, and the heat-transfer to the sensitised layers was minimized. However, a standard KI based electrolyte was still employed.

The cells were prepared and characterised by IV- and QE-measurements without any anti-reflective or light incoupling foils, or additional light-scattering titania layers. In contrast to the expectations the present cells yield relatively high efficiencies and stability (colour and efficiency was unchanged over a period of days or even weeks). The measured efficiencies under 100 mW/cm^2 AM1.5 simulated sun light at 25°C were 1.23%, 0.40% and 0.75% for the crocetin, torularhodin and bixin cells, respectively. Comparable literature values for crocetin dyes are 0.56% and thus lower by a factor of more than 2. [1].

[1]Yamakazi et al. Solar Energy 81 (2007)

DS 25.3 Wed 12:00 H 2032

High Performance Organic Transistors and Circuits with Patterned Polypyrrole Electrodes — •Liqiang Li, Harald Fuchs, and Lifeng Chi — Physikalisches Institut, Universität Münster, Münster, Germany

Electronic circuits based on organic transistors have sparkled considerable research interests due to their unique applications. One of the key prerequisites to convert the high potential to real applications is the preparation and patterning of appropriate electrode materials. Until now, a variety of electrode materials have been utilized for organic devices, among which conducting polymer electrodes have been proposed to be a promising alternative to replace metal electrodes, as they are endowed with unique features which may embody some advantages of organic circuits. However, high performance and stable devices with pure polypyrrole electrodes, especially n-type transistors and complementary circuits, are not reported.

Here we demonstrate the high performance p-/n-type organic transistors and complementary inverter circuits by using patterned PPY as pure electrode. Remarkably, both transistors and inverters with PPY electrodes show good stability under continuous operation and long-term storage conditions. Furthermore, PPY electrodes also exhibit good applicability in solution-processed and flexible devices. All these results indicate the great potential of PPY electrodes in solution-processed, all-organic, flexible, transparent, and low-power electronics.

DS 25.4 Wed 12:15 H 2032

Design rules for charge-transport efficient host materials for OLEDs — •Falk May[1], Björn Baumeier[1], Denis Andrienko[1], and Christian Lennartz[2] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]BASF SE, GVC/E - B009, Ludwigshafen, Germany

The use of blue phosphorescent emitters in organic light emitting diodes (OLEDs) imposes demanding requirements on a host material. Among these are large triplet energies, the alignment of levels with respect to the emitter, the ability to form and sustain amorphous order, material processability, and an adequate charge carrier mobility. A possible design strategy is to choose a pi-conjugated core with a high triplet level and to fulfill the other requirements by using suitable substituents. Bulky substituents, however, induce large spatial separations between conjugated cores, can substantially reduce intermolecular electronic couplings, and decrease the charge mobility of the host. In this work we analyze charge transport in amorphous bis(triphenylsilyl)dibenzofuran, a typical deep-blue OLED host material, and show that mesomeric effects delocalize the frontier orbitals over the substituents recovering strong electronic couplings without inducing significant variations of local dipole moments, which otherwise would lead to additional energetic disorder, site energy correlations, and undesirable current filaments. By linking electronic structure, molecular packing, and mobility we provide a pathway to the rational design of hosts with high charge mobilities.

DS 25.5 Wed 12:30 H 2032

Octithiophene on Au(111): Coverage dependent adsorption geometry and exciton dynamics — •Lea Bogner[1], Erwan Varene[1], Yan Pennec[2], and Petra Tegeder[1] — [1]Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin, Germany — [2]University of British Columbia, department of Chemistry and Physics, Vancouver, B.C. V6T 1Z4, Canada

Semiconducting organic molecules exhibit promising properties for applications in optoelectronic devices such as organic photovoltaic cells or organic light emitting diodes. In order to fully understand and improve the functionalities of organic semiconductors the investigation of adsorption properties, electronic structure and charge carrier dynamics at their interfaces with inorganic substrates plays a crucial role.

Octithiophene (8T) is the longest unsubstituted oligothiophene synthesized up to now and possesses the highest carrier mobility. Whereas several surface science studies on sexithiophene interfaces may be found in literature, little is known so far about 8T.

The adsorption geometry, electronic structure and exciton dynamics as function of 8T coverage have been investigated by means of scanning tunnelling microscopy (STM), high-resolution electron energy loss spectroscopy (HREELS) and time-resolved two-photon photoemission (2PPE). We found that 8T undergoes a change in the adsorption geometry from flat-lying in the sub-monolayer regime to a tilted configuration for the mono- and bilayer coverage. The photoemission intensities of the HOMO and HOMO-1 features as well as the exciton decay dynamics exhibit a strongly coverage dependent behavior.

DS 25.6 Wed 12:45 H 2032

Local Investigations on Air-stable n-Channel Perylene Diimide Based OFETs on Surface Modified SiO$_x$ Dielectric — •Franziska Lüttich[1], Daniel Lehmann[1], Harald Graaf[1,2], Christian von Borczyskowski[1], and Dietrich R. T. Zahn[1] — [1]Chemnitz University of Technology, Institute of Physics, Germany — [2]Now at University Kassel, Institute of Chemistry, Germany

Organic semiconducting materials are interesting for low-cost and flexible applications like organic light-emitting diodes, organic solar cells, and organic field-effect transistors (OFETs). Stability and low mobilities are the most limiting properties for these applications. Surface modifications changing the surface energy of the dielectric in OFETs influences the orientation of the organic molecules and therefore the mobilities. The surface energy can be determined by water contact angle measurements.

In order to investigate the influence of the surface energy we used OFET substrates from Fraunhofer IPMS and varied the water contact angle of the 100 nm thick dielectric of thermal silicon dioxide in the range from 20° to 55°. Thereafter the air-stable Polyera ActivInk$^{\text{TM}}$ N1200 (PDI8-CN$_2$) was deposited by spin coating. The topography was determined using an Atomic Force Microscope (AFM). The electrical characterization was performed by DC measurements and additionally locally resolved by Kelvin Probe Force Microscopy (KPFM) to obtain an insight in the local surface potential and the contact resistances. The determined electron mobility were found to change with varying water contact angle.

DS 26: Thin film characterization: structure analysis and composition (Ion assisted methods and analysis)

Time: Wednesday 15:00–16:30 Location: H 2032

DS 26.1 Wed 15:00 H 2032

Investigation of the effect of the incorporated Fe atoms in the ion-beam induced nanopatterns on Si (001) — •behnam Khanbabaee[1], Andreas Biermanns[1], Marina Cornejo[2], Frank Frost[2], and Ullrich Pietsch[1] — [1]Universität Siegen, Festkörperphysik,Siegen, Germany — [2]Leibniz-Institute für Oberflächenmodifizierung e. V. (IOM), Leipzig, Germany

Ion beam erosion of semiconductor surfaces can modify the surface and depends on main sputtering parameters; different surface topographies such as ripple or dot like pattern are fabricated on the surface. Recent experiments have shown that the incorporation of foreign metallic atoms during the sputtering process plays a crucial role in pattern formation on surfaces. In the result of investigation we report on the depth profile of Fe atoms incorporated in sputtering process on Si (100) with low energy Kr ion beam. X-ray reflectivity (XRR) measurements determine the concentration profile of Fe atoms. X-ray absorption near edge spectroscopy (XANES) at the Fe K-edge (7112 eV) shows the formation of Fe rich silicide near surface region. X-ray photoelectron spectroscopy (XPS) shows a shift in the binding energy of Si2p levels at the surface compared top bulk confirming the formation of different phases of Fe-silicide on tope and below the surface. The depth profiles obtained by XRR are compared to results obtained by complementary secondary-ion mass spectrometry (SIMS).

DS 26.2 Wed 15:15 H 2032

Pattern transfer on fused silica samples using sub-aperture reactive ion beam etching — •André Miessler and Thomas Arnold — Leibniz-Institut für Oberflächenmodifizierung (IOM), Permoserstrasse 15, D-04318 Leipzig, Germany

In comparison to sole Ar ion beam sputtering Reactive Ion Beam Etching (RIBE) reveals the main advantage of increasing the selectivity for different kind of materials due to chemical contributions during the material removal. Therefore RIBE is qualified to be an excellent candidate for pattern transfer applications. The goal of the present study is to apply a sub-aperture reactive ion beam for pattern transfer on large fused silica samples. Concerning this matter, the etching behavior in the ion beam periphery plays a decisive role.

Using a Kaufman-typed ion source with NF$_3$ as reactive gas, XPS measurements of the modified surface exposes impurities like Ni, Fe and Cr, which belongs to chemically eroded material of the plasma pot and a layer formation of silicon nitride, handicaps the etching process mainly in the beam periphery where the sputtering contribution decrease. These side effects influence the pattern transfer of trench structures, produced in AZ MIR 701 photoresist by lithography on a 2" fused silica plate, by changing the selectivity due to modified chemical reactions of the resist layer. Concerning this we investigate a RF-Ion source for sub aperture reactive ion beam applications and finally we examine the pattern transfer on large fused silica plates using NF$_3$-sub-aperture RIBE.

DS 26.3 Wed 15:30 H 2032

In situ X-Ray Reflectivity measurements during DC Sputtering of Vanadium Carbide thin films — •Marthe Kaufholz[1], Baerbel Krause[1], Sunil Kotapati[1], Sven Ulrich[2], Michael Stüber[2], and Tilo Baumbach[1] — [1]ISS, Karlsruher Institute for Technology — [2]IAM-AWP, Karlsruher Institute for Technology

Vanadium Carbide (VC) is a promising candidate for new hard coatings used e.g. in medical applications. For optimising the coating properties, the relation beween the microstructure formation, deposition conditions and mechanical properties has to be understood. In situ X-Ray Reflectivity (XRR) is a powerful tool to investigate the changes in thickness, electron density and roughness during deposition. In situ XRR measurements during sputtering were performed at ANKA (MPI-Beamline). Several VC films were deposited on Si with different growth conditions. Before and after deposition a full specular XRR curve was taken. During sputtering, the intensity changes e.g. due to the thickness increase were measured at fixed angular position of the detector. For the analysis of the angle - and time-dependent XRR a simulation tool is used based on the Parratt Algorithm. This tool can be adapted to other materials and deposition techniques. First measurements show that the electron density of the thin films depends strongly on the plasma properties during the deposition. This might give the possibility of a controlled growth of layers with different electron density by tuning the plasma conditions.

DS 26.4 Wed 15:45 H 2032

Composition and microstructure of r.f. magnetron sputter-deposited Cr-Zr-O thin films — •Stefanie Spitz, Michael Stüber, Harald Leiste, and Sven Ulrich — Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM-AWP), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Cr-Zr-O thin films were synthesised by reactive r.f. magnetron sputtering in an argon-oxygen atmosphere at a pressure of 0.4 Pa. While keeping the substrate temperature constant at 500 °C, the r.f. substrate bias was systematically varied between 0 V and -200 V to investigate the effect of ion bombardment during film growth on microstructure and phase formation. Following a combinatorial approach for thin film deposition by using a segmented Cr-Zr-sputter-target, thin films of five different elemental compositions from Cr-rich to Zr-rich could be obtained in one deposition process.

The evolution of the microstructure and phase formation has been studied by X-Ray Diffraction (XRD) and Transmission Electron Microscopy (TEM). In addition, a Rietveld simulation was done on selected films. The elemental composition of the films was analysed by Electron Probe Micro-Analysis (EPMA).

XRD reveals nanocrystalline microstructures for all films. It is shown that at low substrate bias and high Cr content thin films with a corundum structure are obtained. With increasing substrate bias and increasing Zr content ZrO_2 like structures are observed, even the high temperature cubic and tetragonal phases.

DS 26.5 Wed 16:00 H 2032

Sputter Yield Amplification upon reactive sputtering of TiO_2 — •Rüdiger M. Schmidt[1], Tomas Kubart[2], Michael Austgen[1], Dominik Wagner[1], Thomas Nyberg[2], Andreas Pflug[3], Sören Berg[2], and Matthias Wuttig[1] — [1]I. Institute of Physics, RWTH Aachen University, Germany — [2]Solid State Electronics, The Ångström Laboratory, Uppsala University, Sweden — [3]Fraunhofer IST, Braunschweig, Germany

Titanium Dioxide (TiO_2) is a material with attractive properties which have led to various applications such as anti-reflective coatings or self cleaning surfaces. One of the most frequently applied deposition techniques used for TiO_2 is reactive magnetron sputtering. Unfortunately TiO_2 suffers from a comparatively low deposition rate when reactively sputtered. To increase the deposition rate, Sputter Yield Amplification (SYA) can be used through recoil of the sputtering species at implanted heavy dopants below the target surface. Here we present experimental results showing a large increase of the TiO_2 deposition rate when doped with Tungsten. Although SYA has been proposed earlier, the production of doped targets was complicated. We have built a designated sputter deposition tool which enables systematic studies of SYA. In this study the rate increase by SYA is investigated for two different dopants, namely Tungsten and Bismuth. Our experiments show that the rate increase of TiO_2 by Bismuth is surprisingly low. Tungsten on the other hand results in a large rate increase of 160% in DC and 220% in HiPIMS mode. A number of additional experiments have been carried out to verify and explain this observation.

DS 26.6 Wed 16:15 H 2032

Characteristics of TiCrN films deposited by inductively coupled plasma assisted DC magnetron sputtering — •Byungchul Cha, Ahram Kwon, Uoochang Jung, and Hyungho Jo — Korea Institute of Industrial Technology, 1274, Jisa-Dong, Gangseo-Gu, Busan 618-230, Korea

In this study, Titanium Chromium Nitride (TiCrN) films were deposited on 316L stainless steel by inductively coupled plasma assisted DC magnetron sputtering. The effects of the N2/Ar gas ratio and the power of the ICP source on the properties of the TiCrN films were investigated. The thickness of films decreased with the increase nitrogen content in the inlet gas. The TiCrN film deposited at the 0.3 gas ratio showed maximum hardness of 3900 HK0.3 and excellent corrosion resistance. Increasing the ICP power during the sputtering, the hardness and the compressive stress of the TiCrN films increased, but the thickness of the films decreased linearly. XRD results of the TiCrN films showed the preferred orientation of (111), (200) and (220). The surface roughness of the TiCrN films analyzed by atomic force microscope decreased with the increase ICP power.

DS 27: Thin film characterization: structure analysis and composition (post growth analysis XRD, etc..)

Time: Wednesday 16:30–17:30 Location: H 2032

DS 27.1 Wed 16:30 H 2032

Molecular beam epitaxy of Ge-Sb-Te thin films on Si substrates — •Alessandro Giussani[1], Perumal Karthick[1], Peter Rodenbach[1], Michael Hanke[1], Wolfgang Braun[1,2], Raffaella Calarco[1], and Henning Riechert[1] — [1]Paul Drude Institut für Festkörpelektronik, Hausvogteiplatz 5-7, 10117 Berlin — [2]CreaTec Fischer Co. GmbH, Industriestr. 9,74391 Erligheim, Germany

Owing to their phase-change properties, Ge-Sb-Te thin films, i.e., Ge2Sb2Te5 (GST), are being intensively studied for new concepts of non-volatile memory. The deposition technique commonly employed is sputtering, leading to poly-crystalline layers. Here it is shown that molecular beam epitaxy allows for the preparation of highly ordered Ge-Sb-Te films even on strongly lattice-mismatched substrates like Si. In situ reflection high-energy diffraction and quadrupole mass spectrometry are utilized to monitor the growth process in real time. Ex situ x-ray diffraction, atomic force microscopy and secondary electron microscopy, and x-ray fluorescence are used to investigate the structural properties, the surface morphology, and the stoichiometry of the grown films, respectively. As main result, single crystalline GST layers can be achieved on Si(111) substrates with epitaxial relationships GST[111]//Si[111] and GST<-110>//Si<1-10> in the growth direction and in-plane, respectively. The growth on Si(001) instead produces (111)-oriented films with weak texture. GST thin films with a high structural order are expected to exhibit superior electrical/switching properties to the poly-crystalline layers deposited by sputtering.

DS 27.2 Wed 16:45 H 2032

Structural properties of MBE-grown $Bi_2Se_xTe_{3-x}$ layers — •Steffen Schreyeck[1], Christian Kehl[1], Nadezda V. Tarakina[1], Tanja Borzenko[1], Claus Schumacher[1], Grzegorz Karczewski[2], Jean Geurts[1], Karl Brunner[1], and Laurens W. Molenkamp[1] — [1]Universität Würzburg, Experimentelle Physik III, Würzburg, Germany — [2]Institute of Physics, Polish Academy of Sciences, Warsaw, Poland

$Bi_2Se_xTe_{3-x}$ (V_2VI_3) alloy layers, a material system with topological insulator (TI) properties, were grown by molecular beam epitaxy on H-passivated Si(111) at $T_S=300°C$. We varied the Se-flux at constant Bi- and Te-flux to obtain $Bi_2Se_xTe_{3-x}$ samples with x ranging from 0 to 3 (flux ratio $\frac{VI}{V}$ from 24 to 65). The crystal forms quintuple layers (QLs) VI(2)-V-VI(1)-V-VI(2), with Van-der-Waals bonds between the QLs. The streaky RHEED patterns, TEM and high-resolution X-ray diffraction (HRXRD) show good crystal quality for all compositions. The Se content x was determined by HRXRD assuming validity of Vegard's law. A comparison of flux ratios yield a highly preferred incorporation of Se rather than Te. Lattice dynamics was analysed by Raman spectroscopy from the even-symmetry optical phonon modes $E_g(2)$, $A_{1g}(1)$ and $A_{1g}(2)$. The mode frequencies are essentially determined by the atomic masses in the VI(2) positions and by the V-VI bonding forces. The essentially constant mode frequencies for Se-content x between 0 and 1 strongly indicate a preferential incorporation of Se in the VI(1) position, which is not involved in the vibrational motion, i.e. the realisation of an ordered Bi_2SeTe_2 phase (Te-Bi-Se-Bi-Te).

DS 27.3 Wed 17:00 H 2032

X-ray Resonant Reflectivity study of Transition Metal Oxides — •Sebastian Macke[1], Jorge Hamann-Borrero[2], Abdullah Radi[3], Ronny Sutarto[4], George Christiani[1], Gennady Logvenov[1], George Sawatzky[3], Bernhard Keimer[5], and Vladimir Hinkov[1] — [1]Max-Planck-UBC Centre for Quantum Materials, Vancouver, Canada — [2]Leibniz Institute for Solid State and Materials Research Dresden, Dresden — [3]University of British Columbia, Vancouver, Canada — [4]Canadian Light Source, Saskatoon, Canada — [5]Max Planck Institute for Solid State Research, Stuttgart

X-ray resonant reflectometry (XRR) is the ideal tool to study the depth resolved and element-specific electronic structure of multilayer films. Besides of the structural parameters of the thin film like thickness and roughness one is sensitive to the optical constants which includes effects like magnetic profiles, element density profiles, electronic reconstruction [1] and strain effects. By changing angle, energy and polarization of the incoming beam reflectivity maps can be measured leading in principle to an accurate picture of the depth resolved electronic states of thin films. Due to the complex physics of reflectometry this measurement method needs sophisticated tools to analyze the results quantitatively. In this work the issues arising with this method are addressed and discussed. It can be shown by fitting a simple system of a one layer system of PrNiO3 grown on an LSAT substrate that one can obtain from the maps the optical constants of the layers and the element specific density profiles.

[1] E. Benckiser et. al., Nature Materials 10, 189 (2011)

DS 27.4 Wed 17:15 H 2032

Growth of lead-free piezoelectric thin films of 0.92 ($Bi_{0.5}Na_{0.5}TiO_3$)-0.8 $BaTiO_3$ (BNT-BT) by pulsed laser deposition — •Mehrdad Baghaie Yazdi, Christian Bausch, Torsten Granzow, Wook Jo, and Lambert Alff — Technische Universität Darmstadt, Darmstadt, Deutschland

Pulsed laser deposition (PLD) is one of the most versatile methods for growing complex oxide thin films. We have investigated the growth of the lead free piezoceramic BNT-BT (0.92 ($Bi_{0.5}Na_{0.5}TiO_3$)-0.8 $BaTiO_3$). By adjusting the growth conditions, it was possible to grow a multitude of different phases out of a single phase BNT-8BT polycrystalline target. All epitaxial films were grown on (100) $SrTiO_3$ substrates, then reproduced on conducting STO:5%Nb to be used as bottom electrode. These thin films were studied by various X-ray diffraction methods and electrical properties were determined using a custom thin film measurement set-up.

DS 28: Thin film characterization: structure analysis and composition (Spectroscopy)

Time: Wednesday 17:45–19:45 Location: H 2032

DS 28.1 Wed 17:45 H 2032

X-ray absorption and resonant photoelectron spectroscopy of epitaxial Fe-doped $SrTiO_3$ — •Annemarie Köhl[1], Christian Lenser[1], Dariusz Kajewski[2], Jurek Kubacki[2], Chencheng Xu[1], Sebastian Wicklein[1], Jacek Szade[2], and Regina Dittmann[1] — [1]Peter Grünberg Institut 7, Forschungszentrum Jülich GmbH, Germany — [2]A.Chelkowski Institute of Physics, University of Silesia, Katowic, Poland

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

Thin film samples with Fe concentration of 2 at.% and 5 at.% were prepared by pulsed laser deposition at varying substrate temperatures. The surface morphology of the films is studied with AFM. X-ray absorption spectroscopy is performed in total-electron and auger-electron yield offering different probing depths. Significant variations of the Fe-L edge between bulk and interface as well as after annealing are observed and discussed in terms of integration into the lattice and evolution of secondary phases. Resonant photoelectron spectroscopy at the absorption edge of Ti, O and Fe was used to determine the spectral contributions to the valence band. Most noteworthy we find significant spectral weight above the valence band, which can be attributed to Fe-states.

DS 28.2 Wed 18:00 H 2032

Quantitaive and wavelenght dispersive x-ray fluorescence spectrometry of buried nanostructures — •Rainer Unterumsberger, Beatrix Pollakowski, Falk Reinhardt, Matthias Müller, and Burkhard Beckhoff — Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin, Germany

Quantitative X-Ray Fluorescence (XRF) spectrometry with synchrotron radiation is a well-established method for thickness determination of thin layers. The combination of Grazing Incidence X-Ray Fluorescence (GIXRF) and XRF spectrometry enables the possibility of near surface quantification of lowest depositions as well as buried nanolayer quantification. In this work quantitative XRF and GIXRF was compared and the advantages and limits of both methods will be presented. The sample systems consist of buried boron-carbon nanolayers varying in thickness and covered with 2.5 nm silicon dioxide. In addition, some of these sample systems were analyzed by X-Ray Emission Spectrometry (XES) employing a wavelength dispersive spectrometer combined with a refocussing optic optimised for a high detection efficiency, which allows for the investigation of buried nanolayers. This method will be used for the investigation of the chemical speciation and the impact of the chemical state on atomic fundamental parameters, which are relevant for the reliabilty of the thickness determination employing XRF.

DS 28.3 Wed 18:15 H 2032

X-Ray induced characterization of ion implantation depth profiles — •Philipp Hönicke and Burkhard Beckhoff — Physikalisch-Technische Bundesanstalt (PTB), Abbestr. 2-12. 10587 Berlin, Germany

An X-ray induced characterization method using Grazing Incidence X-Ray Fluorescence (GIXRF) analysis has been applied to the characterization of various ion implantations into silicon, germanium and gallium arsenide. Multiple implanted species with nominal fluences between 1x10^{14} cm^{-2} and 1x10^{16} cm^{-2} and implantation energies between 0.5 keV and 150 keV have been characterized using this method. The depth profiling with GIXRF analysis is based on the in depth changes of the X-ray Standing Wave (XSW) field intensity. The XSW field arises between the primary and the reflected beam and is dependent on the incident [1]. The implantation depth profile is convolved with this intensity distribution and creates a specific fluorescence curve when a GIXRF measurement is performed. The GIXRF measurements have been carried out at the laboratory of the PTB at BESSY using monochromatized synchrotron radiation of well-known radiant power and spectral purity [2]. The results obtained with this method show good agreement with secondary ion mass spectrometry and medium energy ion scattering [1] as well as grazing exit X-ray fluorescence [3] investigations.

[1] P. Hönicke et al., Anal. Bioanal. Chem. 396(8), 2825-2832 (2010)
[2] B. Beckhoff et al., Anal. Chem. 79, 7873-7882 (2007)
[3] Y. Kayser et al., Spectrochim. Acta B 65, 445-449 (2010)

DS 28.4 Wed 18:30 H 2032

Direct Fourier imaging of distortions in $LaAlO_3$ Films — •Christoph Schlueter[1], Tien-Lin Lee[2], Carmela Aruta[3], and Jörg Zegenhagen[1] — [1]ESRF,Grenoble, France — [2]Diamond Light Source Ltd, Didcot, UK — [3]CNR-SPIN, Naples, Italy

The formation of a quasi-2dimensional electron gas at interface of SrTiO3 (STO) and LaAlO3 (LAO) attracted considerable attention in the recent years. The polar LAO layer was expected to cause the build-up of an electric potential. Distortions in the overlayer are discussed as one possible response of the system. The highly sensitive X-ray standing wave (XSW) imaging technique is well suited to study theses films because of its chemical and spacial resolution.

LAO thin films below (2uc) and above (6uc) the critical thickness for conductivity were studied at the hard X-ray photo electron spectroscopy end station of ID32 at the ESRF. The XSW modulated core level photo electron yield was recorded for the five elements present in film and substrate for seven different Bragg reflections. Subsequent analysis provided for each reflection and element the amplitude and phase of one Fourier coefficient of the elemental atomic distribution function. The three dimensional real space image of the atomic distribution for each of the elements is reconstructed by direct Fourier inversion. The reconstructed 3D images obtained by this model free approach reveal significant atomic displacements.

DS 28.5 Wed 18:45 H 2032

Chemical Depth Profiles of Ternary Pd Alloys by HAXPES and First Spectra Simulations — •Julius Kühn[1,3], An-

dreas Lippitz[1], Thomas Gross[1], Mihaela Gorgoi[2], Sebastian Linke[3], Werner Moritz[3], and Wolfgang Unger[1] — [1]BAM Federal Institue of Materials Research and Testing, Berlin, Germany — [2]Helmholtz Zentrum Berlin, BESSY II, Berlin, Germany — [3]Department of Physical Chemistry, Humboldt-Universität zu Berlin, Germany

The catalytic activity of Pd is well known. By alloying with other transition metal the resistivity against poisoning due to sulfur can be improved. In our study we investigated the chemical states of a PdNiCo ternary thin film alloy used as the catalytically active layer in a hydrogen sensor by hard X-ray photo electron spectroscopy (HAXPES). The new technique offers the possibility to study the first nanometers of the sample by increasing the excitation energy from 2010 eV to 6000 eV to perform a non-destructive chemical state depth profiling across the surface of the alloy layer down to 18 nm. We studied the influence of hydrogen and hydrogen sulfide exposure and temperature treatments on the chemical composition of the alloy surface. In addition hard XP-spectra of PdNiCo alloys were calculated by the Simulation of Electron Spectra for Surface Analysis (SESSA) software and compared to experimental data. By doing this evidence for segregation phenomena at the ternary alloy surface is derived.

DS 28.6 Wed 19:00 H 2032

Factor Analysis and Advanced Inelastic Background Analysis in XPS: Unraveling time dependent contamination growth on multilayers and thin films — •Sina Gusenleitner[1,2], Tina Graber[2], Dirk Ehm[2], and Friedrich Reinert[1,3] — [1]Physikalisches Institut, Experimentelle Physik VII und W. C. Röntgen Research Center for Complex Material Systems, Universität Würzburg, 97074 Würzburg — [2]Carl Zeiss SMT GmbH, 73447 Oberkochen — [3]Karlsruhe Institut für Technologie, Gemeinschaftslabor für Nanoanalytik, 76021 Karlsruhe

In order to follow and understand time dependent contamination growth on multilayer mirrors for extreme ultraviolet (EUV) lithography applications, particular heterosystems were investigated with various spectroscopic methods like X-ray Photoemission Spectroscopy (XPS) and Reflection Electron Energy Loss Spectroscopy (REELS). Diverse capping layers can be used to terminate EUV multilayer mirrors to protect the underlaying multilayer stack, one very promising is Ru. In XPS problems encounter when analyzing spectra as the signals of Ru and C overlap. Further, Ru is not only present as pure metal, but also in its oxidized state. Disentangling the overlapping XPS spectra is achieved by application of Factor Analysis (FA) yielding not only the spectra of each component but also the according weights. Thus a model for the time dependent contamination growth can be developed. This model was cross checked by advanced inelastic background analysis. Both methods display an eminent way to unravel overlapping datasets and deducing multilayer composition models.

DS 28.7 Wed 19:15 H 2032

Structure determination of monolayer FeO(111) films on Ag(001) — •Daniel Bruns[1], Irena Kiesel[2], Steffen Jentsch[1], Soeren Lindemann[1], Christian Otte[1], Timo Kuschel[1], and Joachim Wollschlaeger[1] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück — [2]Technische Universität Dortmund, Fakultät Physik/DELTA, Maria-Goeppert-Mayer-Str. 2, 44227 Dortmund

Ultra thin iron oxide films were grown on Ag(001) via reactive molecular beam epitaxy (metal deposition in oxygen atmosphere). The first monolayer shows FeO stoichiometry as concluded from x-ray photoemission spectra. Both low energy electron diffraction and scanning tunneling microscopy demonstrate that the FeO layer has quasi-hexagonal symmetry. This points to the growth of FeO(111) although the films is deposited on a surface with square symmetry. The periodicity as well as the height of the undulated FeO(111) film was analyzed by STM and SPA-LEED. The FeO(111) lattice is slightly rotated with respect to the Ag(001) substrate surface. This rotation causes an undulation of the oxide layer in two different directions with different undulation heights.

DS 28.8 Wed 19:30 H 2032

Lattice dynamics and magnetism of metallic Samarium in Sm-type and dhcp structured films — •Olga Bauder[1], Alessando Barla[2], Ilia Sergueev[3], Rudolf Rüffer[3], and Svetoslav Stankov[1] — [1]KIT, Karlsruhe, Germany — [2]ALBA, Barcelona, Sapin — [3]ESRF, Grenoble, France

The lattice dynamics of metallic samarium was unknown until recently. The high reactivity of Sm along with its large absorption cross section for thermal neutrons prohibited the application of inelastic neutron scattering, the standardly used method for determination of lattice dynamics. We determined the phonon density of states (DOS) of samarium by nuclear inelastic scattering on 149Sm. The experiments were performed at the end-station ID22N of the ESRF in Grenoble in a dedicated ultrahigh vacuum (UHV) system. 500 nm thick epitaxial Sm films exhibiting either the native for this metal Sm-type structure or the characteristic for the light lanthanides dhcp one were grown by molecular beam epitaxy following an elaborated procedure. In order to avoid oxidation and to reduce the multiphonon excitations the samples were investigated under UHV conditions and at 100 K. The magnetic properties of both structures were investigated by nuclear forward scattering in the temperature range 10 K - 300 K. From the phonon DOS a number of thermodynamic properties for this metal were determined. *S.S. acknowledges the support by the Helmholtz Association for establishing a Helmholtz-University Young Investigator Group *Interplay between structure and dynamics in epitaxial rare earth nanostructures* (VH-NG-625).*

DS 29: High-k and low-k dielectrics (joint session with DF)

Time: Wednesday 9:30–11:30 Location: EB 407

DS 29.1 Wed 9:30 EB 407

High dielectric constants due to charge order induced electrical heterogeneity — •Stephan Krohns[1], Pit Sippel[1], Holger Kirchhain[1], Stefan Riegg[1], Peter Lunkenheimer[1], Armin Reller[2], and Alois Loidl[1] — [1]Experimental Physics V, University of Augsburg — [2]Resource Strategy, University of Augsburg

One of the most imminent challenges of modern materials science is the development of new materials with less critical elements that have comparable or better functionalities than those currently used. We illustrate an interdisciplinary approach by applying it to the prototypical example of materials with extremely high dielectric constant to validate the innovative potential in a very early stage of research.[1]

Not only the validation of the economic and technical potential of high dielectric constant materials are in the focus of interest, but also the mechanisms generating this dielectric phenomena. Most of the materials exhibiting those effects, among them numerous transition-metal oxides[2], have complex ground states emerging from strong electronic correlations. $La_{15/8}Sr_{1/8}NiO_4$ for example shows a very high dielectric constant up to gigahertz frequencies at room temperature and it seems that charge order induced electrical heterogeneity can be the origin. To scrutinize that, we also thoroughly investigate the structural, magnetic and dielectric properties of various isostructural $La_{2-x}(Ba,Ca,Sr)_xNiO_4$ compounds especially emphasizing the contribution of electronic phase separation to the permittivity.

[1] S. Krohns *et al.*, Nat. Mat. **10**, 899 (2011). [2] P. Lunkenheimer *et al.*, Eur. Phys. J. Special Topics **180**, 61 (2010).

DS 29.2 Wed 9:50 EB 407

Bilayer gate dielectric stacks of cerium oxide and titanium oxide for nanoelectronics — •Meng Meng Vanessa Chong[1,2], Kam Chew Leong[2], Pooi See Lee[1], and Iing Yoong Alfred Tok[1] — [1]School of Materials Science and Engineering, Nanyang Technological University, Block N4.1, Nanyang Avenue, Singapore 639798 — [2]Global Foundries Singapore Pte. Ltd., Singapore 528830

Numerous materials systems are under consideration as potential replacements for SiO2 as the gate oxide material for sub-0.1 micron CMOS technology. Many properties have to be considered in selecting a suitable material because of emerging issues with high-k technology development. Though, many dielectrics appear favorable in some of these areas, but very few materials are promising with respect to all the required properties.

This work focuses on the rare earth oxide - CeO2 as alternative dielectric as it has small lattice mismatch with Si and high k-values. This study also shows the integration of a high-k passivation layer (TiO2) to suppress the formation of undesirable interfacial layer. Physical characterizations are done to determine the stoichiometry, surface roughness and interface quality.

In addition, temperature dependent measurements are done to identify the different conduction mechanisms such as Poole-Frenkel emission. Identification of various leakage constituent is important for estimation and reduction of leakage power. Furthermore, in-depth electrical analysis helps to determine the quality of the film and dielectric interface.

DS 29.3 Wed 10:10 EB 407

High quality REO thin films from wet chemical deposition — •Maraike Ahlf[1,2], Meng Meng Vanessa Chong[2,3], Mathias Wickleder[1], Alfred Ing Yoong Tok[2], Pooi See Lee[2], and Katharina Al-Shamery[1] — [1]University of Oldenburg, IRAC, Germany — [2]Nanyang Technological University, MSE, Singapore, Singapore — [3]Global Foundries Ltd., Singapore

The aggressive scaling in microelectronics leads to the need of new high performance thin film materials as gate oxides in MOS devices. High leakage currents suffered for conventionally used SiO_2 when scaling down to sub 22 nm requires alternative high κ dielectrics. REOs are potential candidates to replace SiO_2 due to their ecellent electrical properties. This necessitates the synthesis of new RE precursors and deposition methods to achieve impurity free films, since conventionally used techniques suffer from problems such as C impurities from the organic precursors used and formation of interfacial layers or byproducts due to high process temperatures. Results of an unconventional, low temperature, patented, wet chemical approach which is easy to realize and integrate into device production to deposit Nd_2O_3 ultra thin, high quality gate stacks will be presented. The constitution and annealing dependent crystallization behavior on Si and the deposition mechanism of inorganic designer RE-precursors has been investigated with XPS, XRD, AFM and HRTEM. CV and IV measurements show κ values as twice as high and leakage currents down to 10 orders of magnitude lower than conventionally SiO_2. Various current conduction mechanisms can be understood from varying temperature measurements.

DS 29.4 Wed 10:30 EB 407

Epitaxial growth of $\mathbf{Ba_{0.6}Sr_{0.4}TiO_3}$ on highly conductive $\mathbf{SrMoO_3}$ thin films by Pulsed Laser Deposition — •Aldin Radetinac, Philipp Komissinskiy, and Lambert Alff — Institut für Materialwissenschaften, Technische Universität Darmstadt, Petersenstraße 23, 64287 Darmstadt, Germany

High-quality thin films and heterostructures of dielectric and conducting oxides are necessary for realization of all-oxide tunable capacitors. Here we present epitaxial $Ba_{0.6}Sr_{0.4}TiO_3/SrMoO_3$ (BST/SMO) heterostructures grown by Pulsed Laser Deposition (PLD) on single crystal $SrTiO_3$ (100) and $GdScO_3$ (110) substrates. 80 nm thick highly conducting (001) SMO films with a resistivity below 100 $\mu\Omega$cm are deposited in argon atmosphere at 5x10^{-4} Torr [1]. A 5 nm thick initial epitaxial BST buffer layer is grown at low oxygen pressure of 10^{-5} Torr and flow of 0.7 sccm. The buffer layer prevents oxidation of the SMO film to $SrMoO_4$ and allows further deposition of the fully oxidized paraelectric BST at oxygen pressure of 5x10^{-4} Torr and 0.9 sccm flow. To our knowledge this study shows for the first time how metastable materials like SMO can be incorporated in oxide electronic devices. The work is supported by the GRK 1037 (TICMO) project of the DFG.

[1] A. Radetinac, K. S. Takahashi, L. Alff, M. Kawasaki and Y. Tokura, Appl Phys Express 3 (7) (2010)

DS 29.5 Wed 10:50 EB 407

***P*-type conductivity in oxygen deficient $\mathbf{HfO_{2-x}}$ thin films grown by Reactive Molecular Beam Epitaxy** — •Erwin Hildebrandt[1], Jose Kurian[1], Mathis Müller[1], Thomas Schroeder[2], Hans-Joachim Kleebe[1], and Lambert Alff[1] — [1]Institute of Materials Science, Technische Universität Darmstadt, Germany — [2]IHP, Frankfurt(Oder), Germany

Highly oxygen deficient thin films of hafnium oxide HfO_{2-x} were grown using reactive molecular beam epitaxy on *c*-cut sapphire substrates. The oxygen content and, thus, oxygen vacancy concentration was engineered by controlled oxidation using RF-activated oxygen during growth. Hafnium oxide, a high-*k* dielectric insulator in its stoichiometric form, turns into a *p*-type semiconductor above a threshold of oxygen vacancies with up to 6 times 10^{21} charge carriers per cm^3. The introduction of oxygen vacancies reduces the optical band gap from 5.7 eV for stoichiometric HfO_2 by more than 1 eV. The absence of crystalline and/or amorphous metallic hafnium phases was proven by X-ray diffraction and a tilting series using High-Resolution Transmission Electron Microscopy. We suggest the formation of an oxygen vacancy induced *p*-type defect band within the energy gap as the origin of the observed *p*-type conductivity [1].

[1] E. Hildebrandt, J. Kurian, M. M. Müller, T. Schroeder, H.-J. Kleebe, and L. Alff, Appl. Phys. Lett. **99**, 112902 (2011).

DS 29.6 Wed 11:10 EB 407

Hydrogen Impurity in $\mathbf{Y_2O_3}$: an *Ab − Initio* and a μSR perspective — •Estelina L. Silva, Apostolos Marinopoulos, Rui Vilão, and Ricardo Vieira — CEMDRX and CFC, Physics Department, University of Coimbra, P-3004-516 Coimbra, Portugal

Density functional calculations were performed for interstitial hydrogen in Y_2O_3, by employing the semi-local GGA-PBE and the hybrid HSE06 exchange-correlation functionals. It was observed that the lowest energy H^0 and H^- configurations prefer to relax in the interstitial, vacant O, sites. For these charge systems, two different geometrical configurations (interstitial vacant Y and bond O-H type) also occur as higher-energy metastable sites. In contrast, the H^+ equilibrium state was found only when a O-H bond is formed. The overall results for the formation energies, obtained by employing the two functionals are consistent, for which amphoteric behavior was found for hydrogen after considering the lowest-energy structures for each charge state. To compare results with μSR measurements, the formation energies of the metastable configurations were also evaluated. The results are consistent with the μSR data, where the co-existence of the observed diamagnetic signal is attributed to a shallow donor-like muonium and the paramagnetic signal to an acceptor-like deep muonium configuration.

For the interstitial configurations, of the neutral and negative charge systems, a defect level was found in the gap and positioned slightly above the valence band maximum, whereas for the bond O-H site, the defect level is located above the middle of the band gap, closer to the conduction band.

DS 30: Thin film characterization: structure analysis and composition (TEM, LEED, PAS)

Time: Thursday 9:30–11:00 Location: H 0111

DS 30.1 Thu 9:30 H 0111

TEM investigation of magnetically exchange coupled FeTb/[Co/Pt]$_n$ films — •Herbert Schletter, Christian Schubert, Birgit Hebler, Manfred Albrecht, and Michael Hietschold — Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz

The coupling phenomena between different magnetic materials are of interest for fundamental research as well as for applications. Interesting magnetic behaviour is reported for the coupling of a ferrimagnetic (FI) amorphous FeTb layer to ferromagnetic (FM) $[Co/Pt]_n$ multilayers [1]. For our studies, such two-component systems were deposited by room temperature sputtering onto SiO_2/Si substrates. In contrast to [1], magnetic characterization by means of SQUID revealed an unexpectedly strong exchange coupling even when a 3 nm thick Pt spacer layer was introduced between FM and FI.

Since the exchange coupling strongly depends on the interface morphology, TEM was used to gather structural information of the sample. The investigation showed, that parts of the FM layer possess high roughness caused by deep trenches between the crystallites. As a result, the spacer layer might be discontinuous and therefore its decoupling effect would be hindered.

As a further step, FeTb layers (identical to the ones in the two-component systems) were deposited onto prepatterned substrates. The structural changes caused by the substrate patterns were studied by TEM and correlated with changes in the magnetic properties.

[1] S. Manging et al., Phys. Rev. B **78**, 024424 (2008)

DS 30.2 Thu 9:45 H 0111

Structural investigations of ferecrystals $[(\mathrm{SnSe})_{1+x}]_m[\mathrm{TaSe}_2]_1$ by transmission electron microscopy — •Corinna Grosse[1], Ryan Atkins[2], Holm Kirmse[1], Wolfgang Neumann[2], and David C. Johnson[2] — [1]AG TEM, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Department of Chemistry, University of Oregon, Eugene OR 97401-3753, USA

Ferecrystals are a new kind of layered materials with an unusual, turbostratically disordered structure. Layered materials can have structural and physical properties which differ from those of bulk compounds. Structural investigations of the materials are necessary to gain an insight into the mechanisms which can influence their physical properties. The new family of ferecrystals $[(\mathrm{SnSe})_{1+x}]_m[\mathrm{TaSe}_2]_1$ with $m = 1$, 3, and 6 was investigated by various methods of transmission and scanning transmission electron microscopy (TEM/STEM), including selected area electron diffraction (SAED) and energy-dispersive X-ray spectroscopy (EDXS). The high-resolution TEM and STEM images show in-plane crystallinity, atomically abrupt interfaces and turbostratic disorder in the $[(\mathrm{SnSe})_{1+x}]_m[\mathrm{TaSe}_2]_1$ ferecrystals. Certain layer-to-layer orientations appear prevalently, suggesting local ordering between the different types of layers in parts of the ferecrystals. The SAED patterns show an increase in ordering with increasing index m. The chemical composition of the layers was determined by means of EDXS.

DS 30.3 Thu 10:00 H 0111

Quantification of LEED measurements. I. Systematic Errors — •Falko Sojka, Matthias Meissner, Marco Gruenewald, Roman Forker, and Torsten Fritz — University of Jena, Institute of Solid State Physics, Max-Wien-Platz 1, 07743 Jena, Germany

Low energy electron diffraction (LEED) on epitaxial layers is a powerful tool to examine long-range ordering at the interface. However, due to limitations like distortion of the LEED images, often additional efforts have to be made in order to derive precise epitaxial relations.

We developed and implemented an algorithm to determine and correct systematic distortions in LEED-images. The procedure is independent of the design of the device (MCP-LEED vs. conventional LEED). Therefore, only a calibration sample with a well-known structure and a suitably high number of diffraction spots, i.e. Si(111)-7x7, is required. The algorithm provides a correction matrix which can be used to rectify all further measurements generated with the same device. In detail, we distinguish between a radial and an asymmetric distortion. Additionally, we found an axial distortion which occurs due to a tilted sample surface during the measurement. We will show that this axial distortion can be described theoretically with the Ewald Construction, and that it is thus possible to correct those measurements, too. After all, a relative accuracy of the lattice parameter determination better than 1 % can be achieved.

DS 30.4 Thu 10:15 H 0111

Quantification of LEED measurements. II. Application to epitaxial organic films — •Matthias Meissner, Falko Sojka, Marco Gruenewald, Roman Forker, and Torsten Fritz — University of Jena, Institute of Solid State Physics, Max-Wien-Platz 1, 07743 Jena, Germany

Low energy electron diffraction (LEED) on epitaxial layers is a powerful tool to examine long-range ordering at the interface. However, due to limitations like distortion of the LEED images, often additional efforts have to be made in order to derive precise epitaxial relations.

Based on LEED images corrected for their distortion and calibrated by means of a Si(111)-7x7 diffraction pattern (cf. talk by Falko Sojka), a home-made algorithm finds the LEED spots belonging to a certain structure and fits a lattice to all those spots simultaneously. This provides us with absolute lattice parameters within a small error margin. Additionally, in the case of organic-inorganic epitaxy, measurements at higher energies can be used to relate the adsorbate lattice to the substrate lattice and derive the epitaxy matrix. The precision of this procedure will be evaluated on the basis of two systems: (a) 3,4,9,10-perylenetetracarboxylic dianhydride (PTCDA) on epitaxial graphene, featuring two different PTCDA phases, one known, the other not; (b) Tin-phthalocyanine (SnPc) on Au(111), not being described in literature yet.

DS 30.5 Thu 10:30 H 0111

Interdiffusion in Au/Cu thin films studied by depth dependent CDBS — •Markus Reiner[1], Philip Pikart[1,2], and Christoph Hugenschmidt[1,2] — [1]TU München, Physik-Department, Lehrstuhl E21 — [2]TU München, ZWE FRM II

The non-destructive positron annihilation spectroscopy (PAS) with the monoenergetic positron beam at NEPOMUC allows the investigation of thin film samples. As model system, a couple of a vapor deposited Au film (180 nm) on top of a Cu film (480 nm) on a Si substrate was studied by coincident Doppler broadening spectroscopy (CDBS), which is sensitive to the chemical vicinity of the annihilation site on an atomic scale. Depth dependent and time-resolved measurements showed that the experimentally observed signature of the gold film completely vanished after a heating cycle of several hours (maximum temperature of 415 °C). Ab-initio calculations of various AuCu-alloys confirmed the interpretation that a homogeneous AuCu layer was formed on top of the Cu film.

DS 30.6 Thu 10:45 H 0111

Structural characterization of lead sheets for organ pipes by Positron Annihilation Spectroscopy — •Maik Butterling — Helmholtz-Zentrum Dresden-Rossendorf

An important issue when restaurating organ pipes made from lead alloys is the engineering of such material by mechanical hammering to increase the density. Microscopic effects of work-hardening on the surface near layers of lead sheets were investigated by depth resolving Doppler Broadening Spectroscopy measurements using the slow positron beam SPONSOR [1] of the Helmholtz-Zentrum Dresden-Rossendorf. The influence of small differences in the chemical composition of the samples is also discussed.

[1] W. Anwand, H.-R. Kissener, G. Brauer, Acta Phys. Polonica A 88, 7-11 (1995).

DS 31: Organic thin films I

Time: Thursday 11:15–13:00 Location: H 0111

DS 31.1 Thu 11:15 H 0111

Development of a MOKE Spectrometer with Sensitivity in the Infrared Spectral Range — •Alexander Kopylov, Michael Fronk, Dietrich R.T. Zahn, and Georgeta Salvan — Chemnitz University of Technology, 09107 Chemnitz, Germany

Magneto-optical spectroscopy can be used to assign the character and the symmetry of molecular states in molecules. This approach has been successfully applied using magnetic circular dichroism along the years. We previously showed that magneto-optical Kerr effect (MOKE) spectroscopy is a complementary tool which can be applied for paramagnetic or diamagnetic films on opaque substrates. In this work we present the development of a MOKE spectrometer for the IR to UV spectral range from 0.3 eV to 5.5 eV. This allows low energetic magneto-optical transitions to be probed as demonstrated by the example of manganese phthalocyanine, which has a gap between the lowest unoccupied molecular orbital and the highest unoccupied molecular orbital of only ~0.5 eV [1].

[1] M. Grobosch, B. Mahns, C. Loose, R. Friedrich, C. Schmidt, J. Kortus, and M. Knupfer, Chemical Physics Letters 505, 122 (2011).

DS 31.2 Thu 11:30 H 0111

Spectroscopic Ellipsometry and Magneto-optical Kerr Effect Spectroscopy Characterization of Phthalocyanine Thin Films on Ferromagnetic Substrates — •Michael Fronk, Francisc Haidu, Michael Ludemann, Alexander Kopylov, Christian Schubert, Manfred Albrecht, Dietrich R.T. Zahn, and Georgeta Salvan — Chemnitz University of Technology, Germany

Since many years organic complexes like phthalocyanines attract research interest due to their applicability in organic electronic devices such as OLEDs and OFETs. Already in the 1970s phthalocyanines were magneto-optically studied by means of magnetic circular dichroism (MCD) for the clarification of the electronic structure of the molecules in solution and in form of films on transparent substrates. Recently our group successfully applied the magneto-optical Kerr effect (MOKE) to measure organic films on opaque substrates [1]. However, in order to perform basic research with an eye on the application of organic complexes in spintronic devices, the challenge is to measure the magneto-optical response of dia- or paramagnetic molecules on ferromagnetic substrates with dominating signal contributions. In the present work ellipsometry is used to characterize the bare ferromagnetic substrates (LSMO and Co-Pt layered systems) as well as samples with films of CoPc and CuPc in terms of their dielectric functions. MOKE is measured at different magnetic field strengths in order to access the signal of the organic films which is the only field dependent contribution above the saturation field of the substrate.

[1] M. Fronk, et. al., Phys. Rev. B 79 (2009) 235305

DS 31.3 Thu 11:45 H 0111

Charge transfer at phthalocyanine heterojunctions — •Susi Lindner, Benjamin Mahns, and Martin Knupfer — IFW Dresden, P.O. Box 270116, 01171 Dresden

Motivated by interesting electronic and magnetic properties of organic semiconductors like transition metal phthalocyanines we studied the organic-organic interfaces of CoPc, F$_{16}$CoPc and MnPc on various metal substrates (Au and Ag) by means of x-ray and ultra violet photoemission spectroscopy. We show that a charge transfer can be achieved at the interface between this well known molecules. Additionally, in this effect the transition metal center is mainly involved resulting in oxidized Mn$^{\delta+}$Pc and reduced F$_{16}$Co$^{\delta-}$Pc, as well as Co$^{\delta-}$Pc species.

This project is supported by the DFG (KN 393/14).

DS 31.4 Thu 12:00 H 0111

Hybrid solution/vacuum-processed bilayer heterojunction organic solar cells: Nucleation and growth of copper phthalocyanine from solution — •Fatemeh Ghani[1], Ivelin Bochukov[2], Konstantinos Fostiropoulos[2], and Hans Riegler[1] — [1]Max Planck Institute f. Colloid & Interfaces, Potsdam-Golm, Germany — [2]Helmholtz-Zentrum, Berlin, Germany

Unsubstituted metal phthalocyanines(M-Pc) are used as electron donor in vacuum-processed organic solar cell(OSC). However, low cost wet-deposition techniques like spin coating provide several parameters to produce appropriate structures concerning nucleation and growth from solution. But unfortunately fewer solvents for M-Pcs are known. Based on a detailed solubility study[1], we prepare solution-processed M-Pc films. Structures of particular interest are thin films of unsubstituted copper phthalocyanine(CuPc) deposited by spin coating or dip coating of the trifluoroacetic acid solution. By evaporation of the solvent, the molecules aggregate into bundles of fibers of 1-2 nm thickness and μm length on the substrate. We show that the size and form of the structures can be controlled systematically by varying nucleation and growth parameter such as temperature, solution concentration and solvent mixture. We used the solution-processed CuPc film in a hybrid solution/vacuum-processed OSC and studied the power efficiency as a function of CuPc film-thickness.

[1] Ghani, F.; Kristen, J.; Riegler, H., Solubility properties of unsubstituted metal phthalocyanines in different types of solvents, J. Chem. Eng. Data(in press).

DS 31.5 Thu 12:15 H 0111

Characterization of inorganic Surfaces modified by thiol-ene Polymer Grafting — •Christian Kuttner[1], Moritz Tebbe[1], Michaela Eder[2], Helmut Schlaad[2], Ingo Burgert[2,3], and Andreas Fery[1] — [1]Physical Chemistry II, Bayreuth University, 95447 Bayreuth, Germany — [2]Max-Planck Institute of Colloids and Interfaces, 14424 Potsdam, Germany — [3]ETH Zurich, Institute for Building Materials & Empa, Wood Lab, 8093 Zurich, Switzerland

Control of the interfacial properties is crucial for inorganic-organic composites. We studied interactions between inorganic surfaces grafted with macromolecules and a given epoxy matrix. The aim was to develop a better understanding of adhesion principles in (fiber-reinforced) composites and thus optimizing composites.

Thiol-ene grafting was utilized to introduce a polymeric gradient on silica-like surfaces following a two-step approach by Schlaad et al. [1], which allows initiator-free grafting of macromolecules. Different grafting-techniques were tested for applicability and adapted to modify fiberglass. The resulting coatings were nano-structurally and nano-mechanically characterized. Layer morphology (AFM, SEM, SE) and swelling behavior (SE) were investigated. After embedding the modified fibers in an epoxy matrix, cross-sections were prepared for force-volume analysis. The stiffness distribution at the fiber-matrix interface was investigated. The interfacial shear strength between modified fibers and the epoxy matrix was measured by a pull-out experiment to benchmark the non-covalent fiber-matrix construction.

[1] Bertin A, Schlaad H; Chem. Mater. 2009, 21 (24), 5698

DS 31.6 Thu 12:30 H 0111

Structures of Chlorosilanes Self-Assembled on Oxide Surfaces — •Hans-Georg Steinrück, Michael Klimczak, Stefan Gerth, and Andreas Magerl — Lehrstuhl für Kristallographie und Strukturphysik, Staudtstr. 3, D-91058 Erlangen

The topic of our recent research was to further investigate the bonding process of trichlorosilanes to oxide surfaces.

As a starting point octadecyltrichlorosilane (OTS, C$_{17}$H$_{37}$Cl$_3$Si) adsorbed on the amorphous native oxide of a silicon wafer was chosen. Using X-ray reflectivity measurements a densely packed uniform OTS self-assembled monolayer with thickness of $\approx 26\,\text{Å}$ was found. This agrees well with several publications.

Starting from this observation, the substrate was systematically varied, by choosing (100) oriented single crystalline quartz (SiO$_2$) and (100) oriented single crystalline (Al$_2$O$_3$). Due to their crystal specific lattice parameters, a different surface coverage was expected.

To gather further insight, especially on the surface coverage and on the thickness of the monolayer, X-ray reflectivity measurements were performed for these two systems. It was found that the surface coverage on quartz is about 24% and on sapphire about 40% smaller than on the amorphous silicon dioxide. This leads to a tilt of the molecules of 30° and 45° respectively, away from the surface normal. This result can be attributed to the different distances of the bonding sites on the three substrates, which lead to unfavorable conditions for a densely packed monolayer on the crystalline substrates. Note that compared to the amorphous oxide possible bonding sites rectangular lattice of $5.17\,\text{Å} \times 4.54\,\text{Å}$ (SiO$_2$) and $4.76\,\text{Å} \times 12.99\,\text{Å}$ (Al$_2$O$_3$).

DS 31.7 Thu 12:45 H 0111

Depletion of Water on Self-assembled-Monolayers — •Bastian Rückert, Hans-Georg Steinrück, Michael Klimczak, Stefan Gerth, and Andreas Magerl — Chair of Christallography and Structural Physics

Octadecyltrichlorosilane (C18H37Cl3Si, chain length 25 Å) selfassembled on the native oxide of a silicon wafer was chosen as a model system to investigate slip parameters and the influence of shear on hydrophobic surfaces. To gather insight on the structure of this monolayer, X-ray reflectivity (XRR) measurements were performed.

In contact to water a depletion layer of 3 Å with a reduced water density of 60% was observed at the solid-liquid interface. Further it is shown that this depletion zone is independent on shear.

To investigate the impact of the chain length to the monolayer thickness and the depletion layer as a function of the applied shear the chain length of the molecules were systematically varied up to Triacontyltrichlorosilane (C30H61Cl3Si, chain length 35 Å). Again a depletion layer had to be taken into account in order to describe the data.

Searching for any changes in the existing depletion layer or the layer system of Triacontyltrichlorosilane none were found. Even varying the shear rates neither of both showed changes in the interpreted data.

DS 32: Thermoelectric materials I (Focused session – Organizers: Meyer, Heiliger)

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

Invited Talk DS 32.1 Thu 9:30 H 2032

Tuning thermoelectric properties of oxides by the interplay between spin/charge/lattice — •Sylvie Hebert — Laboratoire CRISMAT UMR6508 CNRS et ENSICAEN

Following the discovery of a large thermopower in NaxCoO2 with x ~ 0.7 [I. Terasaki et al., PRB56, R12685 (1997)], the thermoelectric properties of oxides have been intensively investigated in the last 10 years. The presence of strong correlations in these materials could be a way to enhance the thermopower, and low dimensional structures could also be beneficial. Moreover, these materials present fascinating properties beyond thermoelectricity, as superconducting properties appearing in the hydrated phase with x ~ 0.3, showing the richness of their phase diagram.

For p type oxides, the most interesting materials are layered compounds deriving from NaxCoO2, with layers of edge shared CoO6 octahedra, with a mixed valency of Co3+ and Co4+ in low spin states located on a triangular lattice. Following these results, we have been investigating several families of oxides, p or n type, to better understand the interplay between the crystallographic structure, the different spin and valence states, and the thermopower. In this presentation, several examples will be presented emphasizing the relative influence of electronic correlations, and spin and orbital degeneracies in these oxides.

Invited Talk DS 32.2 Thu 10:00 H 2032

Oxide materials for high-temperature thermoelectrics — •Michitaka Ohtaki — Kyushu University, Fukuoka, Japan

Increasing energy demand in worldwide obviously requires more energy security options. Thermoelectric (TE) conversion is becoming more and more of vital importance for higher overall energy efficiency. However, conventional TE materials such as Bi2Te3 and PbTe based on Bi, Te, and Pb are unlikely to prevail for wide commercialization because of the toxicity, poor heat durability, and low abundance of the comprising elements, particularly for those containing Te. In terms of durability at high temperature in air, metal oxides are most attractive. Although strongly ionic characters and the light constituent element, oxygen, of metal oxides are obviously against the conventional guiding principles for higher ZT and hence metal oxides have been totally disregarded in the history of thermoelectrics until the early 1990s, several oxide materials such as CaMnO3, ZnO, SrTiO3, NaCoO2, and Ca3Co4O9 have been reported to actually show a promising thermoelectric performance [1,2]. In this paper, a landscape of oxide thermoelectric materials will be given with respect to the recent materials development based on analyses of the carrier mobility and the lattice thermal conductivity. Some strategies for selective phonon scattering for higher ZT in oxides will be given.

References [1] M. Ohtaki, K. Araki, K. Yamamoto, J. Electron. Mater., 38 1234 (2009). [2] N. V. Nong, N. Pryds, S. Linderoth, M. Ohtaki, Adv. Mater., 23, 2484 (2011).

Topical Talk DS 32.3 Thu 10:30 H 2032

Investigations of the thermal conductivity of thermoelectric thin films and nanostructures — •Friedemann Voelklein, Heiko Reith, Matthias Schmitt, and Daniel Huzel — RheinMain University of Applied Sciences Wiesbaden, Germany

The characterization of the thermal transport properties of thin films and nanostructures is important both for understanding of their transport mechanisms and for their technical applications. Thermal conductivity and diffusivity are crucial material parameters for the design of integrated devices, MEMS, sensors and actuators. The coefficient of performance of thermoelectric devices such as generators, coolers and sensors can be improved by an increase of thermoelectric efficiency z. Considerable decreases of thermal conductivity (and increases of z) can be observed in nanostructured thermoelectric materials due to finite size effects. Thus, nanowires and nanoscale materials are promising candidates for new thermoelectric devices with significantly increased thermoelectric coefficients of performance. Measurements of thermal conductivities of thin films and nanostructures are associated with various experimental problems. We report on methods for the characterization of thermal conductivity by using diagnostic microchips with suspended thin films and nanowires. Results of thermal conductivity measurements on thermoelectric thin films and nanostructures are discussed using finite size effects models.

DS 33: Thermoelectric materials II: Reduced dimensionality (Focused session – Organizers: Meyer, Heiliger)

Time: Thursday 11:15–12:45 Location: H 2032

Topical Talk DS 33.1 Thu 11:15 H 2032

Calculation of thermoelectric properties of nanostructured semiconductors — •Peter Kratzer and Gregor Fiedler — Fakultät für Physik and Center for Nanointegration (CeNIDE), Universität Duisburg-Essen, Duisburg, Germany

Epitaxial nanostructuring, e.g. in the form of superlattices, enables high figure of merit ZT even with perfectly crystalline samples of standard semiconductors. One decisive factor is the reduction of thermal conductivity, as demonstrated e.g. for an array of self-assembled SiGe quantum dots (QDs) in Si [Nature Materials **9**, 491 (2010)]. Complementing these efforts, our work uses electronic structure + Boltzmann transport theory to explore the chances for increasing σS^2 in ZT.

We employ the tight-binding method to calculate the conduction-band states in an array of Ge QDs in Si. It is found that the strained Si between the QDs supports low-lying dispersive states, while the strongly compressed region between two vertically stacked QDs leads to a resonance in the conduction band. The consequences of the modified electronic structure for thermoelectric properties will be discussed.

In a more general framework, the role of transitions between bound and free states in a superlattice for the cross-plane transport relaxation time is investigated. If the mean free path of the phonons mediating these transitions exceeds the superlattice period, combined non-equilibrium effects of the electron and phonon system need to be considered. We predict an additional contribution to the thermopower that is similar to the phonon drag, but scales linearly with the number of superlattice periods and extends to higher temperatures.

DS 33.2 Thu 11:45 H 2032

Giant thermoelectric efficiency in single electron transistors with superconducting island — •Christopher Eltschka[1] and Jens Siewert[2,3] — [1]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany — [2]Departamento de Química Física, Universidad del País Vasco, 48080 Bilbao, Spain — [3]Ikerbasque, Basque Foundation for Science, 48011 Bilbao, Spain

It is well known that dimensional reduction of the electron dynamics may enhance the thermodynamic efficiency [1,2]. A special case of such reduced dimensionality is the single-electron transistor (SET) where at low temperatures electron transport is governed by Coulomb blockade effects. We specifically consider an SET with superconducting island (NSN SET) in the parity regime. We find a dramatically enhanced value for the figure of merit ZT. By extending the statistical interpretation of the thermopower by Matveev [3] to the figure of merit, we are able to explain this high value purely from the statistical distribution of transport. This statistical interpretation of ZT indicates a general strategy to increase ZT which might be useful also in the analysis of other systems.

[1] L. D. Hicks, M. S. Dresselhaus, Phys. Rev. B 47, 12727 (1993)

[2] G. D. Mahan, J. O. Sofo, Proc. Natl. Acad. Sci. 93, 7436 (1996)

[3] K. A. Matveev, Statistical and Dynamical Aspects of Mesoscopic Systems. Proceedings of the XVI Sitges Conference on Statistical Mechanics (2000)

DS 33.3 Thu 12:00 H 2032

Nano-sized semiconductor pillars for thermoelectric applications — •Thorben Bartsch, Matthias Schmidt, Christian Heyn, and Wolfgang Hansen — Institut für Angewandte Physik, Jungiusstr. 11, D-20355 Hamburg,Germany

Nanostructures are an attempt to enlarge the efficiency of thermoelectric devices by drastic reduction of the thermal conductivity and enhancement of the electrical properties [1]. We fabricate novel, epitaxially grown air-gap heterostructures that contain a nanometer sized air gap stabilized by epitaxial semiconductor pillars with length of only few nanometers. Caused by the small dimension and the low density of the pillars, the thermal conductance is several orders of magnitude smaller than in comparable bulk structures. The measured conductance can be described with a simple model of ballistic phonon transport through the pillars [2]. Here, first experimental results will be discussed that probe the thermoelectric properties of the semiconductor nanopillars in the air-gap heterostructures.

[1] K. Nielsch et al. Adv. Energy Mater. 1, 713 (2011)

[2] Th. Bartsch et al. submitted , published on arXive:http://arxiv.org/abs/1111.1164

DS 33.4 Thu 12:15 H 2032

Suppression of phonon heat conduction in undulated nanowires — Denis L. Nika[1], Alexandr I. Cocemasov[1], Calina I. Isacova[1], Dmitrii V. Crismari[1], Alexander A. Balandin[2], •Vladimir M. Fomin[3], and Oliver G. Schmidt[3,4] — [1]Lab. PIN "E. Pokatilov", Dep. Theor. Physics, Moldova State U., MD-2009 Chisinau, Republic of Moldova — [2]Nano-Device Lab., Dep. Electrical Engineering, U. California-Riverside, CA 92521 Riverside, U.S.A. — [3]Institute for Integrative Nanosciences, IFW-Dresden, D-01069 Dresden, Germany — [4]Material Systems for Nanoelectronics, Chemnitz University of Technology, D-09107 Chemnitz, Germany

We have theoretically demonstrated that the phonon heat flux can be significantly suppressed in Si, Si/SiO$_2$ and Si/Ge nanowires with periodical modulation of their cross-section [undulated nanowires (UNWs)] in comparison with generic Si nanowires in a temperature range from 50 K to 400 K. The phonon energy spectra in UNWs are calculated in the framework of five-parameter Born – von Karman-type and six-parameter Valence Force Field models of lattice dynamics. A 4- to 10-fold reduction of the heat flux in UNWs is explained by the exclusion of phonon modes trapped in UNWs segments from the heat flow. Discussions with A. Rastelli and X. Zianni are gratefully acknowledged. The work was supported by the IB BMBF under Project MDA 09/007, the DFG SPP 1386 under Project RA1634/5-1 and Moldova State Project 11.817.05.10F. The work at UCR was supported by FENA.

DS 33.5 Thu 12:30 H 2032

Thermoelectric power factor of a 70 nm Ni-nanowire in a magnetic field — •Rüdiger Mitdank[1], Martin Handwerg[1], Corinna Steinweg[2], William Töllner[3], Mihaela Daub[4], Kornelius Nielsch[3], and Saskia F. Fischer[1] — [1]Novel Materials, Institut für Physik, Humboldt Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany — [2]Werkstoffe und Nanoelektronik, Ruhr-Universität Bochum, 44780 Bochum, Germany — [3]Institute of Applied Physics, Universität Hamburg, Jungiusstr. 11, 20355 Hamburg, Germany — [4]Max Planck Institute of Microstructure Physics, Weinberg 2, 06120, Germany.

Thermoelectric (TE) properties of a single nanowire (NW) are investigated in a microlab which allows the determination of the Seebeck coefficient S and the conductivity σ [1]. A significiant influence of the magnetization of a 70 nm ferromagnetic Ni-NW on its power factor S*σ is observed. Mainly, an evident relationship between magnetoresistance and magneto-thermopower was found, confirming Mott's relation. We detected a strong magneto-thermopower effect of about 10% and an anisotropic magneto resistance as a function of an external magnetic field B in the order of 1%. At B = 0 T we determined the absolute value of S = - (19 +- 2) μV/K. At zero field the figure of merit ZT = 0.02 was calculated using the Wiedemann-Franz- law for the thermal conductivity. The TE efficiency increases in a transversal magnetic field (B =0.5 T) due to an enhanced power factor by nearly 20%.

[1] http://arxiv.org/abs/1111.1873

DS 34: Organic thin films II: Interface spectroscopy

Time: Thursday 15:00–17:30 Location: H 2032

DS 34.1 Thu 15:00 H 2032

Nature of interactions at interfaces between transition metal phthalocyanines and metals — •Heiko Peisert, Fotini Petraki, Umut Aygül, Florian Latteyer, Johannes Uihlein, and Thomas Chassé — University of Tuebingen, Institute of Physical Chemistry, Auf der Morgenstelle 18, 72076 Tuebingen, Germany

Transition metal Pcs (TMPcs) are potential candidates for various applications, most recently they are considered as a promising material for the development of low dimensional molecular magnets or organic spintronic devices. Although electronic properties of TMPcs have been extensively investigated, results are controversial discussed. Moreover, the nature of the interaction at several interfaces is still unclear. In particular, the involvement of the central metal atoms seems to be a key issue for the electronic interface properties. The contribution gives an overview about our recent studies on the interaction of TMPcs (TM: Mn [1], Fe, Co [2,3], Ni) at metal interfaces (Au, Ag) using mainly photoexcited electron spectroscopies (photoemission, resonant photoemission, X-ray absorption). In all cases, charge transfer processes from metallic substrates to the metal 3d levels of the phthalocyanine molecule occur. However, the detailed electronic situation depends clearly on the system under consideration.

[1] F. Petraki, H. Peisert et al., J. Phys. Chem. C 115 (2011) 21334.

[2] H. Peisert, I. Biswas, U. Aygül, A. Vollmer, T. Chassé, Chem. Phys. Lett. 493 (2010) 126.

[3] F. Petraki, H. Peisert et al., J. Phys. Chem. Lett. 1 (2010) 3380.

DS 34.2 Thu 15:15 H 2032

Origin of pinning-levels at molecularly modified electrodes — •Stefanie Winkler[1], Ralf-Peter Blum[2], Ralph Rieger[3], Joachim Räder[3], Jürgen P. Rabe[2], Klaus Müllen[3], and Norbert Koch[1,2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Albert-Einstein-Str.15. 12489 Berlin — [2]Humboldt-Universität zu Berlin, Institut für Physik, 12489 Berlin — [3]Max Planck Institute für Polymerforschung, Ackermannweg 10, 55128 Mainz

Our photoemission study reveals pronounced work function (ϕ) increases by up to 2.0 eV when a strong electron acceptor monolayer comprising tetrafluoro-tetracyanoquinodimethane or hexaazatriphenylene-hexacarbonitrile is deposited on indium tin oxide (ITO) surfaces (pristine ITO ϕ: 4.2 eV). This increase is attributed to a charge-transfer type interaction between ITO and the acceptors, involving partial filling of the LUMO of pristine acceptors. The evolution of sample ϕ and hole injection barrier upon incremental deposition of the hole transport material N,N'-bis(1-naphthyl)-N,N'-diphenyl- 1,1'-biphenyl-4,4'-diamine (α-NPD) is reported, for both type of acceptor modified ITO electrodes. We find that the onset of the highest molecular level of multilayer α-NPD is pinned 0.5 eV below the Fermi-level. Surprisingly, pinning is achieved at about 0.4 eV higher initial electrode ϕ (5.2 eV) than would be expected according to the ionization energy of α-NPD (5.3 eV). ϕ inhomogeneities at sub-monolayer acceptor coverages, resulting in laterally adjacent pinned and unpinned α-NPD on top, can explain this unexpected behaviour, which highlights the importance of knowing sample inhomogeneities on the molecular scale.

DS 34.3 Thu 15:30 H 2032

Tuning the work function of ZnO with a molecular electron acceptor — •Raphael Schlesinger[1], Yong Xu[3], Stefanie Winkler[2], Antje Vollmer[2], Patrick Rinke[3], Matthias Scheffler[3], Sylke Blumstengel[1], Fritz Henneberger[1], and Norbert Koch[1,2] — [1]Humboldt-Universität zu Berlin — [2]Helmholtz-zentrum Berlin, BESSY II — [3]Fritz-Haber-Institut Berlin

Combining conjugated organic with inorganic semiconductors opens up new possibilities for tailoring the properties and efficiency of optoelectronic devices by utilizing the advantages of each material class. Being able to tune the alignment of the frontier energy levels of hybrid inorganic/organic systems is essential to control their function. Employing molecular acceptor interlayers to tune the work function (ϕ)

of a metal and thus the energy level alignment between the metal and an organic semiconductor was demonstrated previously.

We now extend this concept to the polar surfaces of ZnO by using the strong molecular acceptor F4TCNQ. ϕ of bare ZnO surfaces was strongly increased by up to 3eV upon adsorption of a monolayer of the acceptor, as evidenced by photoelectron spectroscopy. In contrast to the strong inorganic-to-organic electron transfer found for F4TCNQ on metal surfaces, no peak associated with the LUMO below E_F, that would be expected for electron transfer from ZnO, is found in our experiments. DFT calculations suggest strong intramolecular charge rearrangement of F4TCNQ as mechanism for the ϕ increase on ZnO. The energy level alignment of sexiphenyl (6P) adsorbed on top of acceptor interlayers on ZnO is shown to be controlled via the ϕ changes.

DS 34.4 Thu 15:45 H 2032

Charge Generation and Recombination in Perylene Solid State Dye-sensitized Solar Cells — •Michael Meister, Ian A. Howard, Yoojin Kim, Henrike Wonneberger, Chen Li, Denis Andrienko, Klaus Müllen, and Frédéric Laquai — MPI für Polymerforschung Mainz

Perylene derivatives have attracted strong interest in replacing the commonly used Ru complexes as all organic sensitizers in solid state dye-sensitized solar cells (sDSCs), since they combine a strong absorption with reasonably good device efficiencies if used with Spiro-MeOTAD as solid state hole transporter. Here we present a photophysical study of promising perylene monoimide dyes (PMI) for sDSCs. By employing time resolved photoluminescence, quasi steady-state photoinduced absorption (PIA) and transient absorption (TA) spectroscopy in a broad visible and near-infrared spectral region on device-like structures, we gain insight into the mechanisms of charge generation and recombination. The results show that Li-TFSI, a commonly used additive, facilitates charge generation. As it turns out, reductive quenching, where hole transfer occurs prior to electron injection, plays a major role in charge generation for these dyes. However, we have evidence that initially separated charges are attracted back to the interface, likely due to the low dielectric constants, leading to increased recombination. This would be a major drawback of sDSCs. We suggest that to overcome this problem within the existing device configuration, exciton quenching must lead to a charge pair that is further spatially separated.

DS 34.5 Thu 16:00 H 2032

Influence of interface dipoles on the open circuit voltage of polymer/PCBM based photovoltaic cells — •Johannes Frisch[1], Stefanie Winkler[1], Jens Niederhausen[1], Patrick Amsalem[1], Antje Vollmer[2], Marcel Schubert[3], Dieter Neher[3], Eduard Preis[4], Ullrich Scherf[4], and Norbert Koch[1,2] — [1]Humboldt-Universität zu Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany — [3]Universität Potsdam, Germany — [4]Bergische Universität Wuppertal, Germany

In heterojunction organic photovoltaic cells (OPVCs) the offset between the highest occupied molecular level of the donor and the lowest unoccupied molecular level of the acceptor (i.e., the photovoltaic gap) sets an upper limit for the open circuit voltage (Voc). Commonly, vacuum level alignment (VLA) at the donor/acceptor interface is assumed. In contrast, we found interface dipoles (ID) at such interfaces that affect the photovoltaic gap and therefore Voc. We report ultraviolet photoelectron spectroscopy measurements for three different polymer-PCBM heterojunctions, comprising the donors P3HT, poly(9,9'dioctylfluorene-alt-4,7-bis(2,5-thiendiyl)-2,1,3-benzothiadiazole) (PFTBTT) and poly[2,6-(4,4-bis-(2-ethylhexyl)-4H-cyclopenta[2,1-b;3,4-b']dithiophene)-alt-4,7(2,1,3-benzothiadiazole)] (PCPDTBT). The energy level alignment found experimentally for these heterojunctions are discussed in relation to the Voc achieved in corresponding OPVCs. In contrast to assumed VLA, the photovoltaic gap for the P3HT/PCBM junction is 0.15 eV wider due to the ID, and for PFTBTT/PCBM the photovoltaic gap is narrower by 0.15 eV.

DS 34.6 Thu 16:15 H 2032

Effect of ionic strength on self-assembly and surface properties of oligoelectrolyte multilayers — •Samantha Micciulla, Chloé Chevigny, and Regine v.Klitzing — Technische Universität Berlin, Deutschland

Polyelectrolyte multilayers are self-assembled systems which have found many applications since their introduction in the early nineties. Easiness of preparation and properties tunability have induced an increasing interest in the field of surface modification. This requires a deep understanding of their structural features and of the tools to control their response to different surrounding environments.

The effect of key parameters (pH, dipping time, concentration, functionality, charge density) has been largely studied. Our interest is now focused on the effect of chain length. Namely, we decided to go down to the oligomeric limit (30 monomers/chain) to test the achievement of layer-by-layer multilayer growth and understand how the molecular weight influences the resulting system.

The combination of optical (Ellipsometry) and acoustic (Atomic Force Microscopy (AFM) and Quarzt Crystal Microbalance with Dissipation (QCM-D)) techniques offers an overall description of surface and rheological properties, pointing out the effect of ionic strength in solution on OEM self-assembly, as well as analogies and differences with their high molecular weight equivalents.

DS 34.7 Thu 16:30 H 2032

Orientation of Non–Planar Molecules in thin Polycrystalline Layers from Infrared Ellipsometry Spectra – OFET and OPV materials — •Jens Trollmann, Robert Lovrinčić, Carl Pölking, and Annemarie Pucci — Kirchhoff–Institut für Physik der Universität Heidelberg

The determination and control of molecular ordering in organic thin films is of particular interest for designing and improving production processes for organic field effect transistors (OFET) and organic photovoltaic (OPV) devices. By enhancing the molecular ordering in the conducting film performance of OFETs can be significantly improved. Furthermore the fill factor in organic solar cells can be increased by reorienting molecules. In this talk we show how to reliably conclude on the predominant molecular orientation in a thin film by a computation based comparison of infrared (IR) ellipsometric measurements with density functional theory calculations of vibrational eigenvalues and eigenvectors for a single molecule. To proof this concept we determined the anisotropic dielectric functions of two organic semiconductor thin films, ID583 and NDI-F, in the spectral range of 350 to 5000cm^{-1}. The approach is especially advantageous if applied to molecules with an anisotropic and non-planar structure forming X-ray amorphous layers with a preferred molecular orientation but an insufficient degree of long-range order for diffraction based methods. In such cases our analysis yields more accurate and significant results than achievable by only comparing ordinary and extraordinary refractive indices in the visible range. Funding by BMBF (Polytos) is gratefully acknowledged.

DS 34.8 Thu 16:45 H 2032

Quantitative blend analysis of polymer/fullerene films via spectroscopic ellipsometry — •Sebastian Engmann, Vida Turkovic, Harald Hoppe, and Gerhard Gobsch — Technische Universität Ilmenau, Institut für Physik, Experimentalphysik 1, Weimarer Straße 32, 98693 Ilmenau

Spectroscopic ellipsometry (SE) was used to determine the shape of fullerene inclusions in polymer/fullerene blends. The spatial distribution of the fullerene phase over the film depth is investigated, and we found evidence for spinodal de-mixing. The time development of the phase separations are investigated. Furthermore, ellipsometric measurements, in combination with refined optical modeling, are used to quantitatively describe the degree of spatial order of the polymer phase within polymer/fullerene blends.

DS 34.9 Thu 17:00 H 2032

Temperature-sensitive swelling behavior of poly(N-isopropylacrylamide) brushes characterized by in-situ infrared spectroscopic ellipsometry — •Andreas Furchner[1], Dennis Aulich[1], Eva Bittrich[2], Sebastian Rauch[2], Petra Uhlmann[2], and Karsten Hinrichs[1] — [1]Leibniz-Institut für Analytische Wissenschaften – ISAS – e. V. — [2]Leibniz-Institut für Polymerforschung Dresden e. V.

Polymer brushes are very attractive material systems for biophysics and biochemistry. In aqueous environment, their surface properties show stimuli-responsive behavior on changes in, for example, temperature, pH, or solvent. This makes polymer brushes useful functionalized surfaces for applications like controlled protein and cell adsorption.

A suitable method for studying the film properties at the solid-liquid interface is infrared spectroscopic ellipsometry (IR-SE) in combination with a special in-situ cell. This allows to investigate the structural and chemical properties of polymer brushes in situ.

An important representative for temperature-sensitive polymer brushes is poly(N-isopropylacrylamide) [PNIPAAm], which is of great technological interest owing to the phase transition at its lower critical solution temperature of 32°C. After an ex-situ characterization using an appropriate optical layer model, the swelling behavior of PNIPAAm brushes was investigated in neutral water at different temperatures around 32°C using in-situ IR-SE.

DS 34.10 Thu 17:15 H 2032

Near-field Optical Imaging of Phase Separations in Organic Bulk Heterojunction Solar-cell Blends — •Dai Zhang, Xiao Wang, and Alfred Meixner — IPTC, Uni Tübingen, Auf der Morgenstelle 15,Tübingen, Germany

Semiconductor Polymers and fullerenes are widely employed in organic solar cell as electronic donors and acceptors. To achieve high performance of the solar cell, the formation of bulk heterojunction (BHJ) morphology in the polymer and fullerenes blends at nm scale is critical [1].

We have recently demonstrated high resolution near-field spectroscopic mappings of organic semiconductor thin film and polymer:fullerene blend films [2-4]. From the simultaneously recorded morphology and spectroscopic information, the interplay among the blend film BHJ morphology, the local donor and acceptor distributions, and their photoluminescence (PL) quenching were discussed. The PL and Raman signals of the donor and acceptor have been probed at optical resolution of approximately 15 nm. In addition, the local degradation behaviours of the semiconductor donor molecule and the acceptor molecule were investigated.

[1] J. Peet, A. J. Heeger, G. C. Bazan, Acc. Chem. Res., 42, 1700 (2009). [2] X. Wang, D. Zhang, K. Braun, H-J. Egelhaaf, C. J. Brabec, A. J. Meixner, Adv. Func. Mater. 20, 492 (2010). [3] D. Zhang, U. Heinemeyer, C. Stanciu, et al, Phys. Rev. Lett., 104, 056601 (2010). [4] X. Wang, H. Azimi, M. Morana, H.-J. Egelhaaf, A. J. Meixner, D. Zhang, Small, 7, 2793 (2011).

DS 35: Organic thin films III: Monolayers and crystals

Time: Thursday 17:45–19:30 Location: H 2032

DS 35.1 Thu 17:45 H 2032

Dithiocarbamate Monolayers for Noble Metal Surface Functionalization — •Tobias Schäfer[1], Philip Schulz[1], Christian Effertz[1], Daniel Gebauer[1], Dominik Meyer[1], Riccardo Mazzarello[2], and Matthias Wuttig[1] — [1]I. Institute of Physics (IA), RWTH Aachen University — [2]Institute for Theoretical Solid State Physics, RWTH Aachen University

Organic electronic devices like organic light emitting diodes (OLED), photovoltaics (OPV) and thin-film transistors (OTFT) are well-known for their potential in the field of optoelectronics. Yet a significant improvement in device functionality is expected by tailoring the interface between metal electrode and the functional organic film. One approach is to modify the electrodes by self-assembled monolayers (SAMs).

Here, we present a combined experimental and theoretical investigation of dithiocarbamate (DTC) monolayers on noble metal surfaces. The monolayer systems were investigated by photoelectron (PES) and infrared spectroscopy (FT-IR) which show densely packed DTC films heading to very low work functions. The pronounced alignment of the electronic structure can be reproduced well by density functional theory (DFT). Thereby the low work function is explained by the formation of strong bond dipoles, intrinsic molecular dipoles and the high packaging density of the molecules. The superior electronic coupling between metal electrode and active organic layers was shown in an OTFT geometry. Thus, we present a promising and reliable route towards low work function metal contact interfaces to n-type and ambipolar organic transport layers.

DS 35.2 Thu 18:00 H 2032

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

Here we report on the interaction mechanisms at metal-organic and organic-organic interfaces in heterostructures of highly-ordered ultrathin layers of the dye molecules 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) and tin(II)-phthalocyanine (SnPc) on Ag(111). The thin films were characterized optically by in situ Differential Reflectance Spectroscopy (DRS), followed by an extraction of the related optical constants.

For the first monolayer PTCDA and the first monolayer SnPc the well-known covalent interaction [1] between adsorbate and substrate is manifested in broad and structureless absorption spectra. Further layers of PTCDA and SnPc, however, are efficiently optically decoupled from the first monolayer. Hence, a monomer signature for the respective molecules is observed until aggregation occurs. In the first monolayer of PTCDA on top of a SnPc monolayer film the coexistence of neutral and anionic PTCDA is concluded. Furthermore, SnPc on top of a PTCDA and on top of a SnPc monolayer was investigated optically. Accordingly, the existence of a PTCDA interlayer induces a highly-ordered growth of SnPc up to several monolayers.

REFERENCES

[1] M. Häming et al., Phys. Rev. B 82, 235432 (2010).

DS 35.3 Thu 18:15 H 2032

A systematic study on fluorination: Rubrene and its fluorinated derivates — •Falk Anger[1], Evelyn Adamski[1], Katharina Broch[1], Alexander Gerlach[1], Toshiyasu Suzuki[2], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen — [2]Institute for Molecular Science, Myodaiji, Okazaki 444-8787, Japan

A promising way to modify the electronic levels of organic semiconductors is partial or complete fluorination. Rubrene ($C_{42}H_{28}$) has been shown to be a suitable semiconductor for applications, for which numerous experimental efforts have been done. In this study, we present thin films of partly ($C_{42}H_{14}F_{14}$) and completely ($C_{42}F_{28}$) fluorinated rubrene. For the first time we investigated thin films of these materials grown on a native SiO_2 substrate using optical spectroscopy, complementary X-ray reflectivity and AFM. The materials grow to a large extent amorphously and exhibit a smooth surface. However, depending on the growth parameters the molecules can form ordered, dendritic structures that extend on a micrometer scale. The variation of the HOMO-LUMO transition with fluorination is discussed.

[1] M. Kytka *et al.*, J. Chem. Phys. **130**, 214507 (2009)

[2] S. Kowarik *et al.*, Phys. Chem. Chem. Phys. **8**, 1834-1836 (2006)

DS 35.4 Thu 18:30 H 2032

3h-Auger decay in the π-band of HOPG — •Matthias Richter, Daniel Friedrich, and Dieter Schmeisser — Brandenburg University of Technology Cottbus, Applied Physics and Sensors, K.-Wachsmann-Allee 17, 03046 Cottbus, Germany

In this contribution we report on the electronic structure of highly oriented pyrolitic graphite (HOPG). HOPG is a model system because of the clear separation between π- and σ-bands in the valence band regime. X-ray based measurements were done at the U49/2-PGM2 beam line at BESSYII in Berlin. The resonant photoemission spectra (resPES) at the carbon K-edge give a complete picture of the occupied and unoccupied states in these sp^2 hybridized system. Above the K-edge the resPES data are dominated by the Auger process causing a C2p4 final state. The Auger lines appear at constant kinetic energy (spectator, 2h) or constant binding energy (participator, 1h). For the features right at the resonance we observe a different Auger decay mechanism. We attribute it to the decay out of an excitonic intermediate state with a long lifetime. It involves three valence hole states. The original primary core hole is filled by a normal KLL Auger decay. The excited electron rests in the excitonic intermediate state and decays later. We discuss the spectral features of such combined spectator-participator decays in detail which are found only close to resonance and only in the localized valence states of excitonic excitation i.e.C1s - $1\pi^*$ transitions [1, 2, 3]. [1] Richter et al. (2011) BioNanoScience, submitted. [2] Michling et al. (2011) IOP C Ser Mater Sci Eng, submitted. [3] Schmidt et al. (2011) Solid State Ionics, submitted.

DS 35.5 Thu 18:45 H 2032

Nanoscale assembly, morphology and screening effects in nanorods of newly synthesized substituted pentacenes — •Maria Benedetta Casu[1], Sabine-Antonia Savu[1], Simon

Schundelmeier[1], Sabine Abb[1], Christina Tönshoff[2], Holger F. Bettinger[2], and Thomas Chassé[1] — [1]Institute of Physical and Theoretical Chemistry, University of Tübingen, Tübingen, Germany — [2]Institute of Organic Chemistry, University of Tübingen, Tübingen, Germany

We have investigated nanorods of two newly synthesized substituted pentacenes deposited on Au(111): δ4-substituted (2,3-X2-9,10-Y2) pentacene with X = Y = methoxy group and X = Fluorine, Y = methoxy, by using X-ray photoemission spectroscopy (XPS) and atomic force microscopy (AFM). Energy dependent photoemission spectra show complex features that we have analyzed in detail by using a fitting procedure. Our analysis reveals the unusual presence of surface core level shifts due to the high electronegativity of the fluorine atoms and the structure of the nanorods. In addition, the distinctive features of growth and morphology of the nanorods are subjected to a template effect by the substrate lattice geometry, leading to a systematic organization of the nanorod assemblies.

DS 35.6 Thu 19:00 H 2032

Organic Field-Effect Transistor Operation With Different Gatings — •Nis Hauke Hansen[1], Carina Wunderlich[1], and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — [2]ZAE Bayern e.V., D-97074 Würzburg

To enable superior insulation characteristics together with low-voltage operation, e.g. for portable electronic devices, organic thin film transistors (TFT) can be gated by ultrathin self-assembled monolayer (SAM) dielectrics [1]. Alternatively, the choice of ionic liquids (IL) as gate dielectric allows for accumulation of high charge carrier densities in the order of $10^{13} cm^{-2}$, corresponding to a charge carrier doping of up to 0.3 holes per molecule. In this contribution we employed both approaches to gate TFTs based on vacuum sublimed Pentacene (PEN) and Diindenoperylene (DIP) films as semiconducting channel. The observed current-voltage (IV) characteristics show low threshold voltages between -3 and -1 V for all devices under investigation and hole mobilities up to $10^{-1}\frac{cm^2}{Vs}$ for SAM gate dielectrics in combination with PEN as well as DIP. Utilizing an IL as gate dielectric high charge carrier densities in the order of $10^{13}cm^{-2}$ have been confirmed. In order to correlate the electronic performance with thin film morphology, atomic force microscopy (AFM) and x-ray diffraction (XRD) measurements have been performed indicating the influence of the respective gating on the structural properties of the molecular semiconductors.

[1] H. Klauk, et al., Nature 445 (2007) 745

DS 35.7 Thu 19:15 H 2032

A comparative study of the absorption spectra of binary mixtures of organic semiconductors — •Katharina Broch[1], Antje Aufderheide[1], Jens Reinhardt[1], Alexander Hinderhofer[1], Christian Frank[1], Falk Anger[1], Reinhard Scholz[2], Alexander Gerlach[1], and Frank Schreiber[1] — [1]Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen — [2]Technische Universität Dresden, Institut für Angewandte Photophysik, George-Bähr-Straße 1, 01069 Dresden

Mixtures of organic semiconductors can be used to increase the donor-acceptor interface in organic optoelectronic devices. However, the influence of molecular geometry and chemical structure on the mixing behaviour as well as on the optical properties is still not completely understood. We present a comparative study of binary mixtures of three organic semiconductors, i.e. pentacene (PEN), perfluoropentacene (PFP) and diindenoperylene (DIP), in different combinations [1,2]. Using spectroscopic ellipsometry we study the optical properties of the mixed films including possible intermolecular interactions. By comparing the spectroscopic results with detailed x-ray data [3,4], we discuss the influence of the mixing behaviour and structural properties on the absorption spectra of the intermixed films.

[1] K. Broch et al., Phys. Rev B, **83**, 245307 (2011). [2] J. P. Reinhardt et al., in preparation [3] A. Hinderhofer et al., J. Chem. Phys., **134**, 104702 (2011). [4] A. Aufderheide et al., in preparation

DS 36: Spins in Organic Materials (jointly with MA)

Time: Thursday 16:45–19:00 Location: H 1012

DS 36.1 Thu 16:45 H 1012

Tunneling anisotropic magnetoresistance in organic spin valves — •M. Grünewald[1,3], M. Wahler[1,3], F. Schumann[3], C. Gould[1], R. Schmidt[2], F. Würthner[2], L.W. Molenkamp[1], and G. Schmidt[1,3] — [1]Physikalisches Institut (EP3) Universität Würzburg, Am Hubland, 97074 Würzburg — [2]Institut für Organische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg — [3]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, von-Danckelmann-Platz 3, 06120 Halle

Over the past years a number of spin valves (SV) based on various organic semiconductors (OSCs) and contact materials have been demonstrated. Although some experiments indicate injection of spinpolarized carriers and some clearly show tunneling, it is still unclear for a number of other results whether their data show tunneling magnetoresistance (TMR) or actual spin injection and consequently giant magnetoresistance (GMR). We report the observation of tunneling anisotropic magnetoresistance (TAMR) in an organic SV-like structure with only one ferromagnetic electrode. The device is based on a new perylene diimide-based n-type OSC. The effect originates from the tunneling injection from the bottom contact ($La_{0.7}Sr_{0.3}MnO_3$). Magnetoresistance measurements show a clear SV signal, with the typical two-step switching pattern caused by the magnetocrystalline anisotropy of the epitaxial magnetic electrode. TAMR so far has not been considered when interpreting the results of organic SVs. Our results imply that careful measurements on any organic SV are necessary in order to distinguish between TAMR and true SV-operation (TMR/GMR).

DS 36.2 Thu 17:00 H 1012

Spin properties of the Alq_3-cobalt oxide (CoO) interface — •Norman Haag, Sabine Steil, Nicolas Grossmann, Mirko Cinchetti, and Martin Aeschlimann — Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, Erwin-Schrödinger-Stra. 46, D-67663 Kaiserslautern

The effect of cobalt oxidation is crucial for the understanding of the performance of organic spin valves with Co electrodes [1], as it is expected that cobalt will partly oxidize during sample production. For this reason, we analyzed the spin properties of the interface formed between tris(8-hydroxyquinoline)aluminium (III) (Alq_3) and cobalt oxide. We deposited 30 ML of Co(100) and exposed the sample to an oxygen atmosphere with varying pressure. The degree of oxidation is extracted by evaluating the changes in the work function according to *Wang et al* [2]. Subsequently, Alq_3 was grown on the oxidized cobalt. The resulting interface was characterized by means of spin-resolved ultraviolet photoemission spectroscopy. We detected the energy level alignment and the spin polarization in the region of a few eV below E_F, both as a function of degree of oxidation. The most striking result is the shift of the Alq3 molecular orbitals of up to 1 eV (for strong oxidation) away from the Fermi level. This behavior could change the character of spin and carrier conduction (from holes to electrons) in spintronics devices.

[1] Dediu *et al.*, Nature Materials **8**, 707 (2009)

[2] Wang *et al.*, Surface Science **124**, 51 (1983)

DS 36.3 Thu 17:15 H 1012

Spin-filtering at hybrid organic-inorganic interfaces — •Sabine Steil, Nicolas Grossmann, Norman Haag, Mirko Cinchetti, and Martin Aeschlimann — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany.

Organic semiconductors have demonstrated their potential as a new class of materials for spintronics applications [1]. They are expected to constitute a new building block for advanced spintronics devices. One of their most intriguing properties is that they form hybrid interfaces with ferromagnetic metals [2]. As an example, we have recently shown that the spin-injection efficiency at the cobalt-copper phthalocyanine interface can be tailored by electron doping [3]. Here, we will show our recent experiments on the interface between cobalt(001) and tris(8-hydroxyquinoline)aluminium(III) (Alq3). Interface formation was studied by means of spin-resolved ultraviolet photoemission spectroscopy, while the spin- and time-resolved two-photon photoemission spectroscopy was used to measure the spin-dependent lifetime of hot charge carriers excited in an unoccupied hybrid interface state. The magnitude of the lifetime, gives information about the degree of hybridization of the considered state. More importantly, we found that the lifetime in such state is spin-dependent, providing direct evidence that hybrid organic-inorganic interfaces can be employed as a novel kind of spin-filter.

[1] V. A. Dediu, et al., Nat. Mater. 8, 707(2009) [2] S. Sanvito, Nat. Phys. 6, 562-564(2010) [3] M. Cinchetti et al., PRL 104, 217602(2010)

DS 36.4 Thu 17:30 H 1012

Theoretical study of dynamical switching of a single spin by exchange forces — •Robert Wieser[1], Vasile Caciuc[2], Cesar Lazo[3], Hendrik Hölscher[4], Elena Y. Vedmedenko[1], Roland Wiesendanger[1], and Stefan Heinze[3] — [1]Institut für Angewandte Physik, Universität Hamburg, D-20355 Hamburg, Germany — [2]Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [3]Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [4]Institut für Mikrostrukturtechnik, Forschungszentrum Karlsruhe, P.O. Box 36 70, D-76021 Karlsruhe, Germany

We demonstrate the possibility to dynamically switch the spin of a single atom or molecule with the magnetic tip of an atomic force microscope due to the acting exchange forces. We choose a single transition metal benzene molecule as model system and calculate the exchange interaction with an Fe tip using density functional theory. The exchange energy displays a Bethe-Slater type behavior with ferromagnetic coupling at large tip-sample distance and antiferromagnetic coupling at closer proximity. The exchange energies reach maximum values of a few 10 meV which allows to switch single spins by overcoming the energy barrier due to the magneto-crystalline anisotropy. The spin dynamics of the system was explored by solving the time dependent Schrödinger equation with additional relaxation term. We discuss six possible scenarios, defined by the occurrence of quantum tunneling, relaxation, and tip-sample distance.

DS 36.5 Thu 17:45 H 1012

Nanoscale assembly and order of paramagnetic organic radicals — Sabine-Antonia Savu[1], Indro Biswas[1], Mathias Glaser[1], Lorenzo Sorace[2], Matteo Mannini[2], Andrea Caneschi[2], Thomas Chassé[1], and •Maria Benedetta Casu[1] — [1]IPTC, University of Tübingen, Tübingen, Germany — [2]LAMM, University of Florence, Florence, Italy

Nitronyl nitroxide radicals are a class of paramagnetic compounds that are of interest not only because of their magnetic properties but also because of their use as a building block in more complex magnetic structures. A crucial aspect is the possibility to grow thin films, down to the submonolayer regime, investigating their chemical, physical, and morphological properties. In this work we present X-ray photoelectron spectroscopy (XPS), near edge X-ray absorption fine structure (NEXAFS), atomic force microscopy (AFM), and electron paramagnetic resonance (EPR) investigations of thin films of a pyrene derivative of the nitronyl nitroxide radical (nitpyrene). Nitpyrene was deposited on Au(111) single crystals, using strictly controlled evaporation conditions. The electronic structure and the interaction with the surface are discussed, as well as the growth mode. The persistence of the paramagnetic character of the molecules has been proved by EPR measurements.

DS 36.6 Thu 18:00 H 1012

Electronic structure and magnetic properties of metallocene multiple-decker sandwich nanowires — Cristian Morari[1], Florian Beiuseanu[2], and •Liviu Chioncel[3] — [1]National Institute for Research and Development of Isotopic and Molecular Technologies, 65-103 Donath, RO-400293 Cluj Napoca, Romania — [2]Department of Physics, University of Oradea, RO-410087 Oradea, Romania — [3]Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany

We present a study of the electronic and magnetic properties of the multiple-decker sandwich nanowires (CP-M) composed of cyclopentadienyl (CP) rings and 3d transition metal atoms (M=Ti to Ni) using Density Functional Theory first-principles techniques. We demonstrate that structural relaxation is an important effect in determining the magnetic ground-state of the system. Notably, the computed magnetic moment is zero in CP-Mn, while in CP-V a significant turnup in magnetic moment is evidenced. CP-Fe/Cr show a half-metallic ferromagnetic ground state with a gap within minority/majority spin channel. In order to study the effect of electronic correlations upon the half-metallic ground states in CP-Cr, we introduce a simplified three-bands Hubbard model which is solved within the Variational Cluster Approach. We discuss the results as a function of size of the reference cluster and the strength of average Coulomb U and J exchange parameters. For range of studied parameters U=2-4eV and J=0.6-1.2eV the half-metallic character is not maintained in the presence of local Coulomb interactions.

DS 36.7 Thu 18:15 H 1012

Metal-organic hybrid interface states of a ferromagnet/organic semiconductor hybrid junction as basis for engineering spin injection in organic spintronics — Stefan Lach[1], •Anna Altenhof[1], Kartik Tarafder[2], Felix Schmitt[1], Md. Ehesan Ali[2,3], Michael Vogel[1], Jens Sauther[1], Peter Oppeneer[2], and Christiane Ziegler[1] — [1]Dep. of Physics and Research Center OPTIMAS, University of Kaiserslautern, D-67663 Kaiserslautern — [2]Dep. of Physics and Astronomy, Uppsala University, S-75120 Uppsala — [3]Center for Theoretical Chemistry, Ruhr-University Bochum, D-44801 Bochum

Hybrid spintronic devices that combine organic semiconductors (OSC) with ferromagnetic (FM) substrates are expected to provide a route to devices with improved and new functionalities. A crucial role is played by the FM-OSC interface. State-of-the-art DFT+U calculations in combination with UPS and XPS as well as spin-resolved UPS directly demonstrate the formation of new hybrid interface states (HIS), induced by chemisorption of CuPc, CoPc, and FePc at Co [1]. Whereas FePc and CoPc have only weakly spin-polarized levels at the Fermi level, CuPc shows strong spin-polarization directly at EF. On the other hand, the interaction leads to a vanishing magnetic moment in case of CuPc and a strong ferromagnetic coupling in case of CoPc and FePc. The difference is explained by the symmetry of the d-orbitals which are massively involved in the hybridization. [1] S. Lach, A. Altenhof, K. Tarafder, F. Schmitt, Md. E. Ali, M. Vogel, J. Sauther, P. M. Oppeneer, Ch. Ziegler, Adv. Funct. Mat., in press

DS 36.8 Thu 18:30 H 1012

Theoretical modelling of electronic structure and exchange interactions for metal-phthalocyanines — •Wei Wu[1,2], Andrew Fisher[2], Nic Harrison[3], Sandrine Heutz[1], Tim Jones[4], and Gabriel Aeppli[2] — [1]Department of Materials and London Centre for Nanotechnology, Imperial College London — [2]UCL Department of Physics and Astronomy and London Centre for Nanotechnology, University College London — [3]Department of Chemistry, Imperial College — [4]Department of Chemistry, Warwick University

The theoretical understanding of exchange interactions in organics provides a key foundation for quantum molecular magnetism. Recent SQUID magnetometry of a well know organic semiconductor, copper-phthalocyanine [1,2] (CuPc) shows that it forms quasi-one-dimensional spin chains. Green's function perturbation theory and density functional theory simulations [3,4] are used to calculate exchange interactions and electronic structure for CuPc, CobaltPc, LithiumPc, and ChromiumPc. The exchange interactions depend strongly on stacking angles, but weakly on sliding angles. Our results qualitatively agree with the experiments and can guide experimentalists to synthesis novel materials.

[1] S. Heutz, et. al., Adv. Mat., 19, 3618 (2007) [2] Hai Wang, et. al., ACS Nano, 4, 3921 (2010) [3] Wei Wu, et. al., Phys. Rev. B 77, 184403 (2008) [4] Wei Wu, et. al., Phys. Rev. B 84, 024427 (2011)

DS 36.9 Thu 18:45 H 1012

Uncovering the electronic structure of manganese phthalocyanine — •Rico Friedrich[1], Torsten Hahn[1], Jens Kortus[1], Francisc Haidu[2], Michael Fronk[2], Georgeta Salvan[2], Benjamin Mahns[3], and Martin Knupfer[3] — [1]Institut für Theoretische Physik, TU Bergakademie Freiberg, 09596 Freiberg — [2]Institut für Physik, TU Chemnitz, 09107 Chemnitz — [3]Institut für Festkörper- und Werkstoffforschung, IFW Dresden, 01171 Dresden

Manganese phthalocyanine is a magnetic transition metal complex, that exhibits organic semiconducting behavior in the bulk. Because of its high thermal and chemical stability it is a promising candidate for molecular spintronics applications. However this compound shows extraordinary electronic structure properties which can be investigated by various spectroscopic techniques as for instance EELS, PES and Ellipsometry. Here we want to present the results of our ab initio density functional calculations on this system and show how they can help to understand the significant influences on the experimentally observed electronic properties. For this purpose also environmental influences as air exposure need to be considered since they will be of decisive character in view of real applications. In particular the change of magnetic properties is crucial as this directly affects spin transport phenomena.

DS 37: Poster II: Focused electron beam induced processing for the fabrication of nanostructures (focused session, jointly with O); Nanoengineered thin films; Layer properties: electrical, optical, and mechanical properties; Thin film characterization: structure analysis and composition (XRD, TEM, XPS, SIMS, RBS,..); Application of thin films

Time: Thursday 15:00–17:00 Location: Poster E

DS 37.1 Thu 15:00 Poster E

FEBIP on organic layer modified Ag(111) — •Patrick Wintrich, Florian Vollnhals, Johannes Zirzlmeier, Hans-Peter Steinrück, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II and Interdisciplinary Center for Molecular Materials (ICMM), Friedrich-Alexander- University Erlangen-Nuremberg, Egerlandstr. 3, 91058 Erlangen

Electron Beam Induced Deposition (EBID) has attracted increasing interest in the last few decades for the fabrication of nanosized structures. In our investigation of EBID with $Fe(CO)_5$ on an Ag(111) surface, we observed autocatalytic growth of iron structures on the whole surface, even without electron irradiation. Herein, we show that the initial decomposition can be inhibited by preadsorbing a layer of porphyrin molecules on the Ag(111); consequently, on this surface well-defined Fe nanostructures can be produced via EBID with $Fe(CO)_5$.

In analogy to the recently introduced EBISA process [1], we also can use the electron beam to locally decompose the porphyrin layer with the electron beam and thereby activate selected areas on the surface for the autocatalytic growth of $Fe(CO)_5$. We therefore can apply two different fabrication routes for iron deposits on Ag(111). In both, the first step is the deposition of the porphyrin layer. Thereafter, we can either perform the conventional EBID process or we can use the electron beam for the local decomposition of the porphyrin layer followed by the autocatalytic growth of $Fe(CO)_5$ at the activated areas.

This work was supported by the DFG through grant MA 4246/1-1.

[1] M.-M. Walz et al., Angew. Chem. Int. Ed. 49 (2010), 4669

DS 37.2 Thu 15:00 Poster E

Fabrication of Titanium Oxide Nanostructures by Electron Beam Induced Deposition — •Michael Schirmer, Florian Vollnhals, Marie-Madeleine Walz, Thomas Lukasczyk, Hans-Peter Steinrück, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Germany

In electron beam induced deposition (EBID) a focused electron beam is employed to locally dissociate adsorbed precursor molecules resulting in a deposit of the nonvolatile fragments. Usually, metalloorganic compounds are used as precursors for the fabrication of metalic deposits. Herein, we explore the potential of using tetraisopropoxide (TTIP) as precursor for the fabrication of TiOx nanostructures via EBID in ultra high vacuum. We demonstrate that the initially carbon contaminated deposits can be transformed to pure TiOx nanocrystalites via certain post treatment procedures [1]. Furthermore, we expanded the EBID technique towards the fabrication of layered nanostructures by the consecutive use of $Fe(CO)_5$ and TTIP. Thereby first, a clean iron line was deposited, which was then selectively covered with a thin capping layer fabricated from TTIP [2]. Interestingly, the ultra-thin capping layer prevents the oxidation of the iron structures, even under ambient conditions. From a more general point of view, the stepwise application of two or more precursors in EBID opens up a novel pathway for tailoring the fabrication of nanostructures.

This work is supported by the DFG through grant MA 4246/1-2.
[1] M. Schirmer et al., Nanotechnology, 22 (2011) 085301; [2]
M. Schirmer et al., Nanotechnology, 22 (2011) 475304.

DS 37.3 Thu 15:00 Poster E

Theoretical modelling of EBID precursors on a substrate — Kaliappan Muthukumar, Ingo Opahle, •Juan Shen, Harald O. Jeschke, and Roser Valenti — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Straße 1, 60438 Frankfurt am Main

Among the many unknowns in the microscopic processes underlying the electron beam induced deposition of nanostructures are the details of the adhesion of the precursor molecules on the substrate. The mechanism of adsorption for a single molecule will be the starting point for the simulation of the dynamical processes during the initial stages of the growth of a metallic nanodeposit. By means of density functional theory (DFT) calculations with and without inclusion of long range van der Waals (vdW) interactions, we have studied the interaction of tungsten hexacarbonyl $W(CO)_6$ and trimethyl methylcyclopentadienyl platinum ($MeCpPtMe_3$) as precursor molecules with partially hydroxylated and fully hydroxylated SiO_2 substrates corresponding to different experimental conditions.

DS 37.4 Thu 15:00 Poster E

New Developments in MAD Technique: Layer-By-Layer Growth of Thin Oxide Films and Superlattices — •Camillo Ballani[1], Sebastian Hühn[1], Markus Jungbauer[1], Markus Michelmann[1], Felix Massel[1], Oleg Shapoval[2], Alexander Belenchuk[2], and Vasily Moshnyaga[1] — [1]I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Institute of Applied Physics, Academiei str. 5, MD-2028 Chisinau, Moldova

Metalorganic aerosol deposition (MAD) technique[1] was shown to be very advantageous in preparation of thin films of complex functional oxides, like cuprates, manganites, titanites. Due to their unique bulk and interfacial electronic/structural properties these strongly correlated oxides are recently in the focus of fundamental and applied research, including large scale research cooperation within the EU FP 7 Framework. We report here further MAD developments toward the in-situ growth control via optical ellipsometry and atomic layer deposition (MAD-ALD). The results on the structure and magnetotransport of individual layer-by-layer grown thin films (LSMO, BSTO) as well as of superlattices (LCMO/PCMO, LBMO/LMO, LCMO/BTO) will be presented and discussed with the main focus on the optimization of colossal magnetoresistance and artificial multiferroic behavior by means of electronic and/or structural interface engineering. Financial support from EU FP 7 IFOX (interfacing oxides) is acknowledged. [1]Appl. Phys. Lett. 74, 1842 (1999).

DS 37.5 Thu 15:00 Poster E

Gas phase aggregation cluster source for composite material deposition — •Tilo Peter[1], Sven Bornholdt[2], Thomas Strunskus[1], Vladmir Zaporojtchenko[1], Holger Kersten[2], and Franz Faupel[1] — [1]Institute for Materials Science, Kiel, Germany — [2]Institute of Experimental and Applied Physics, Kiel, Germany

A method to create nanocomposites of Ag nanoparticles in a plasma polymer matrix with tailored optical properties is presented. A beam of Ag nanoparticles with tailored size distribution is created in a magnetron discharge gas aggregation cluster source and combined with a plasma polymerization process of Hexamethyldisiloxane in an Ar/O_2 atmosphere. This process will lead to incorporation of the Ag clusters into the plasma polymer and to formation of the desired nanocomposite material.Variation of size, distance and amount of the Ag nanoparticles allows to tune intensity and wavelength of the silver plasmonic resonance over a broad range. Thus optical properties can be engineered for a desired application. Characterization of the samples with a focus on optical properties was done by TEM, EDX and UV-Vis spectroscopy.

DS 37.6 Thu 15:00 Poster E

Work function measurements of sputtered TiO_2 in UHV ambience — •Sonja Urbahn, Rüdiger M. Schmidt, Alexandra Yatim, and Matthias Wuttig — I. Physikalisches Institut (IA) RWTH-Aachen University

Titanium Dioxide (TiO_2) is a material with unique properties which have led to various applications such as anti-reflective coatings or self-cleaning surfaces. In particular the latter is made possible by its outstanding photocatalytic activity. However, the underlying process behind this attractive feature is still sparsely investigated.

Thus it is the aim of the present work to correlate the structural features of reactively sputtered TiO_2 with its photocatalytic activity to be able to optimize future applications. Since self-cleaning implies the diffusion of photo generated charge carriers to the surface where they react with adsorbates, a change of the photocatalytic activity involves a change of the surface potential and thus of the work function. We show data measured with a Kelvin probe in UHV-ambience and link the characteristic behavior under UV illumination with structural properties and specific deposition parameters. Additionally we compare the UHV measurements with previously performed experiments in air to gain a deeper insight into the influence of different atmospheres. Our data contribute to the understanding of the photocalytic properties on a microscopic scale.

DS 37.7 Thu 15:00 Poster E

Mode Shape and Dispersion Relation of bending Waves in thin Silicon Membranes — •Reimar Waitz[1], Stephan Nössner[1], Michael Hertkorn[1], Olivier Schecker[1,2], and Elke Scheer[1] — [1]Universität Konstanz — [2]now at: Robert Bosch GmbH

We study the vibrational behavior of silicon membranes with a thickness in the range of a few hundred nanometers and macroscopic lateral size. A piezo is used to couple in transverse vibrations, which we monitor with a phase-shift interferometer using stroboscopic light.The observed wave pattern of the membrane deflection is a superposition of the mode corresponding to the excitation frequency and several higher harmonics. Using a Fourier transformation in time, we separate these contributions and image up to the 8th harmonic of the excitation frequency. With this method we determine the dispersion relation of membrane oscillations in a frequency range up to 12 MHz. We develop a simple analytical model combining stress of a membrane and bending of a thin plate that describes both the experimental data and finite-elements simulations very well. We derive correction terms to account for a finite curvature of the membrane and for the inertia of the surrounding atmosphere. A simple criterion for the transition between stressed membrane and thin plate behavior is presented.

DS 37.8 Thu 15:00 Poster E

Analysis of process parameters for a DCMS process of a rotating ceramic ITO target — •Patrick Ries and Matthias Wuttig — Institute of Physics (IA), RWTH Aachen University

ITO is the most commonly used but at the same time rather expensive Transparent Conducting Oxide. This fact is due to the high Indium to Tin ratio of 90:10 that is necessary to obtain the best electrical conductivity. If it is possible to find another ratio with similar electrical properties but higher Tin content, this would be of great industrial relevance. To accomplish this goal and to check the hypothesis an in-house developed serial co-sputtering system is employed. The tool consists of a rotating primary cathode and up to two secondary cathodes for co-sputtering processes. The process parameters of a DC-sputtered ceramic ITO target installed on the primary cathode are analyzed and correlations with the thin film properties, especially the resistance and the transmittance are shown. The resistance behavior upon changing the Tin content via a co-deposition process from a secondary cathode will be presented.

DS 37.9 Thu 15:00 Poster E

Single-crystalline $CaMoO_3$ and $SrMoO_3$ films grown by Pulsed Laser Deposition in a reductive atmosphere — •Aldin Radetinac[1], Kei S. Takahashi[2], Lambert Alff[1], Masashi Kawasaki[2,3], and Yoshinori Tokura[2,4] — [1]Inst. für Materialwissenschaften, TU Darmstadt, Petersenstraße 23, 64287 Darmstadt, Germany — [2]Cross-correlated Materials Research Group (CMRG), RIKEN, Wako, Saitama 351-0198, Japan — [3]Inst. for Materials Research, Tohoku University, Sendai 980-8577, Japan — [4]Dep. of Applied Physics, University of Tokyo, Tokyo 113-8656, Japan

Single-crystalline thin films of $CaMoO_3$ and $SrMoO_3$ with a Mo^{4+} state perovskite structure have been epitaxially grown by pulsed-laser deposition from Mo^{6+} state ceramic targets [1]. Phase-pure films were obtained on nearly lattice-matched perovskite substrates using argon gas flow during the deposition. Transport properties of the films are consistent with those of paramagnetic and metallic phases, whereas the residual resistivities are far lower than those reported previously for films and bulk polycrystals. These results indicate that this growth method can be useful for exploring the interfaces and junction properties of 4d and 5d transition metal oxides that are unstable in a conventional oxidative atmosphere. This study was partly supported by the Japan Society for the Promotion of Science (JSPS) through its FIRST Program.

[1] A. Radetinac, K. S. Takahashi, L. Alff, M. Kawasaki and Y. Tokura, Appl Phys Express 3 (7) (2010)

DS 37.10 Thu 15:00 Poster E

Photocurrent in sputtered TiO_2 thin films: Investigation of the influence of the measurement ambient on the electronic properties in view of its photocatalytic activity — •Alexandra K. Yatim, Dominik Wagner, Azza Amin, and Matthias Wuttig — I. Institute of Physics IA, RWTH Aachen University, Germany

Titanium dioxide (TiO_2) is a material used in many products of our daily life. However, one of its most attractive qualities is its photocatalytic activity. Since TiO_2 furthermore provides a large refractive index and a high transmittance in the visible spectral region, it has become the material of choice in the fabrication of self-cleaning coatings in the architectural glazing industry. Interestingly, although products already exist on the market, little is known about the underlying mechanism governing the strong photocatalysis. Furthermore, there is no scientific consensus about the functional principle of the self-cleaning and pollution-decomposing effect of TiO_2-coated surfaces. These effects are based on the generation of electron-hole pairs by UV illumination. Although photocurrent measurements are a bulk-sensitive method due to the detection of all free photo-generated charge carriers in the film, the measurements show that the atmosphere has a decisive impact on the photocurrent. This is plausible since the photocatalytic self-cleaning implies the decomposition of adsorbates on the surface, which is accomplished by the diffusion of the charge carriers to the surface. These charge carriers then do not contribute to the current any more. In order to evaluate the influence of ambient air, the electronic processes in TiO_2 at different oxygen partial pressures have been analysed.

DS 37.11 Thu 15:00 Poster E

Controlling the properties of laser deposited polymer-metal nanocomposites close to the percolation threshold — •Felix Schlenkrich, Susanne Schlenkrich, and Hans-Ulrich Krebs — Institut f. Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Polymer-metal nanocomposites consisting of metal clusters embedded in a polymer are of interest for many applications, for instance in microelectronics or sensor technology. For sensors, most interest lies especially in the region close to the percolation threshold, where the film properties drastically change. Such nanocomposites were pulsed laser deposited at $248\,nm$ at fluences of $120\,\frac{mJ}{cm^2}$ in the case of polymers (Polymethyl methacrylate and Polycarbonate) and $4\,\frac{J}{cm^2}$ for metals (Ag, Cu). Enhancing the metal amount within these samples the transition from isolated metal clusters to closed metal layers was studied by electron microscopy and resistance measurements. In this contribution we discuss, how the structural and electrical properties of the composite films depend on the amount of metal deposited on the polymer, the reactivity between metal and polymer, hardness of the polymer, and electrical properties of the components. Then we concentrate on the region close to the percolation threshold, where the electrical conductivity is strongly influenced by the microstructure, and show, how the properties of the polymer/metal composite films can be controlled by heat treatments.

DS 37.12 Thu 15:00 Poster E

IR spectroscopic studies on the influence of Fe and Mg on the Si-O stretching vibration in Fe/Mg-Si-O systems — •Martin Wunder, Steffen Wetzel, and Annemarie Pucci — Kirchhoff-Institut für Physik, INF 227, 69121 Heidelberg

Fe-Mg silicates are among the most abundant minerals in space. Their IR spectral features strongly depend on the chemical composition and formation conditions. Therefore a thorough spectral analysis of the $10\,\mu m$ feature can reveal important information on the dust formation processes. Interfacial interaction effects are generally neglected in such analysis. In order to deepen the understanding of the origin of IR spectral changes, we performed in situ IR spectroscopic transmission measurements during the condensation of layers produced by evaporation of Fe, Mg and SiO under UHV conditions. Particularly we addressed the influence of elemental metal on the 10 μm feature of silicates in our experiments. Details of the experimental setup and results from the measurements on multilayer structures and layers formed by co-evaporation will be presented. These measurements demonstrate a strong Fano-type interaction between the metal particles and the Si-O vibration. Furthermore a strong shift of the resonance frequency is observed for co-evaporation experiments.

DS 37.13 Thu 15:00 Poster E

Ink-jet printed conducting oxide nanoinks: processable at room temperature — •Falk von Seggern[1,2], Subho Dasgupta[1], Robert Kruk[1], and Horst Hahn[1,2,3] — [1]INT, KIT, Eggenstein-Leopoldshafen, Germany — [2]Joint Research Laboratory Nanomaterials, TU Darmstadt and KIT, Darmstadt, Germany — [3]CFN, KIT, Karlsruhe, Germany

A printable grade of ITO-nanoink can offer solutions to a range of practical problems and issues in various important fields of interest which are generally referred under a common platform called *printable electronics*. Printing of ITO inks offer a fast and inexpensive way of producing large area transparent conducting oxide (TCO) films for various applications in this area. Additionally, the piezo-controlled drop-on-demand (DOD) ink-jet printing provides an easy and flexible method of patterning as an alternative for conventional photolithographic processes, although with considerable lower resolution.

We have produced a nanoink based on ITO nanoparticles which is stable over several weeks. This means that no significant agglomeration occurred within this period of time which is necessary to ensure a sufficiently long storage time of such dispersion-based inks. Furthermore, the ink shows nice and stable printing behavior which includes constant drop formation and no clogging of the nozzles etc. Finally, the properties of the printed film are characterized and preliminary results will be presented. We have used piranha treated polymer substrates (PEN) to facilitate the possibility of performing mechanical tests (tensile, bending etc.) in the future.

DS 37.14 Thu 15:00 Poster E

Thermal transformations in Cs_xC_{58} fullerides — •Seyithan Ulas[1], Daniel Löffler[2], Patrick Weis[1], Artur Böttcher[1], and Manfred Kappes[1] — [1]KIT, Institut für Physikalische Chemie, Karlsruhe, Germany — [2]BASF, Intermediates Research, Ludwigshafen, Germany

Monodisperse cluster films consisting of C_{58} fullerene cages have been fabricated by soft-landing of mass-selected C_{58} cations created by electron-impact induced fragmentation/ionization of C_{60} cages [1]. The doping of the C_{58} films by alkali metals leads to the formation of fullerides, Cs_xC_{58} [2]. The temperature resolved mass spectra taken during the sublimation of Cs_xC_{58} phase reveal three well distinguishable components, C_{56}, C_{58} and C_{60}. The new components, C_{56} and C_{58}, indicate the transfer of a C_2 unit from a C_{58} cage to an adjacent one, -[C_{58}]-[C_{58}]$\rightarrow C_{56}+C_{60}$ to be a process which competes with the breakage of the intercage bonds constituted by non-IPR sites (e.g. 2AP-2AP). The Cs doping raises the $C_{58} \rightarrow C_{60}$ conversion ratio from 0.04 for pristine C_{58} films up to 3.9 for a saturated Cs_xC_{58} phase. Consequently, sublimation of the saturated Cs_xC_{58} fullerides proceeds predominantly via C_{60} emission. The Cs_xC_{58} films survive the annealing procedure (up to 1100K) as a new conducting carbon phase constituted by chains of fused cages which exhibit interesting vibronic and mechanic properties.

[1] A. Böttcher, et al., PCCP 7, 2816 (2005).

[2] D. Löffler, et al. Phys. Rev. B 77,155405 (2008).

DS 37.15 Thu 15:00 Poster E

Thin C_{58} films on Au(111) — Noelia Bajales[1], Stefan Schmaus[1], Thoshio Miyamachi[1], Wulf Wulfhekel[1], Melani Stendel[2], Alexej Bagrets[2], Christian Seiler[2], Ferdinand Evers[2], Seyithan Ulas[3], Bastian Kern[3], •Artur Böttcher[3], and Manfred Kappes[3] — [1]KIT, Physikalisches Institut, Karlsruhe, Germany — [2]KIT, Institut für Theorie der Kondensierten Materie, Karlsruhe, Germany — [3]KIT, Institut für Physikalische Chemie, Karlsruhe, Germany

C_{58} cages have been deposited on the Au(111) surface by means of low-energy cluster beam deposition technique. The properties of thin C_{58} films have been studied by means of scanning tunneling microscopy, 4K-STM, elastic tunneling spectroscopy, STS, ultraviolet photoionization spectroscopy, UPS, and thermal desorption spectroscopy, TDS. In the very initial deposition stages the individual C_{58} cages occupy the elbows of the herringbone reconstruction preferentially. In contrast to highly symmetric C_{60} cages individual C_{58} cages exhibit internal asymmetric structures. Further film growth proceeds via formation of dimers and trimers which act as nucleation centers and govern the growth of 2D and 3D islands. Individual cages can not be desorbed from the surface, i.e. their estimated binding energy overcomes 3 eV. For coverages >0.5 MLE detectable emission of C_{58} cages peaked at 820 K has been observed. This desorption band reveals the thermal decomposition of the quasi-covalent intercage bonds, C_{58}-C_{58}. STS reveals highly asymmetric distribution of the local density of HOMO and LUMO states. For thick C_{58} films a gap of 1.2 eV has been derived.

DS 37.16 Thu 15:00 Poster E

Epitaxial growth of Bismuth on Si(557) — •Saddam Banyoudeh, Daniel Lükermann, Christoph Tegenkamp, and Herbert Pfnür — Leibniz Universität Hannover, Institut für Festkörperphysik, Abteilung ATMOS, Appelstr. 2, 30167 Hannover

Bismuth is a semi-metal with unique electronic properties such as a large carrier mean free path, a small effective mass and high surface conductivity. Because of these attributes Bismuth thin films are an attractive system to study finite size effects and quantum transport phenomena. In our experiment we have investigated the growth of ultra-thin Bi films in the range of 10 to 40 monolayers on different wetting layer phases of Bismuth on vicinal Si(557) by spot profile analysis low energy electron diffraction (SPALEED). The orientation and structure of the films strongly depends on the initial interface. Starting with the Bi-$\sqrt{3}$-α-phase (1/3ML) we obtain 6 domains of Bi(110) with its pseudo-cubic structure rotated by 60° against each other. On the initial Bi-$\sqrt{3}$-β-phase (1ML) rotationally disorderd Bi(110) was formed. But most interesting is the growth of Bi on the so called mixed phase (2/3ML). Here only two domains of Bi(110) where formed which are rotated by 13.5° with respect to the step direction of Si(557). The SPALEED analysis shows that these films are stepped and contain higher index facets.

DS 37.17 Thu 15:00 Poster E

Structural study of amorphous SiCN:H hard coatings — •Andrea Sendzik, Steffen Schulze, Marcus Günther, Frank Richter, and Michael Hietschold — Institute of Physics, Chemnitz University of Technology, Reichenhainer Straße 70, 09126 Chemnitz, Germany

The thin coatings were produced by PECVD. A series of samples has been prepared, differing in terms of gas composition. The composition of the films was determined by ERDA. So it comes out that the silicon to carbon ratio remains nearly constant, but the ratio of nitrogen to silicon strongly depends on the deposition parameters. The atomic structure was investigated by TEM. From diffraction patterns and EELS-spectra findings about the short-range order of atoms, the composition, and the chemical bonding were made. Particular on the basis of the EELS spectra the bonding structure can be seen to vary with the gas rates. Core-level loss spectra indicate that there is predominantly single bonding, with the tendency to multiple bonding with rising nitrogen content. To get more information about the atomic structure, we have calculated the radial distribution functions (RDF) from diffraction patterns. With the help of Gaussian peak fitting one can assign the peaks and identify the elemental bonds occuring in the amorphous coating. With the results from the EELS and the RDF we are able to present a first schematic structure model of the amorphous SiCN hard coatings.

DS 37.18 Thu 15:00 Poster E

Structure and thermal stability of laser deposited ZrO_2/Ti multilayers — •Sarah Hoffmann, Benedikt Ernst, Tobias Liese, and Hans-Ulrich Krebs — Georg-August-Universität, Göttingen, Germany

ZrO_2/Ti thin multilayer systems have important applications in X-ray optics, especially in the 'water window' regime (wavelengths: 2.3-4.4 nm) as X-ray mirrors and multilayer Laue lenses (MLLs) [1]. To increase the resolution of MLLs, which is defined by the thickness of their thinnest layers, it is necessary to prepare as small structures as possible. With regard to the structural stability of the layers a lower limit of the layer thickness can be determined. While using, the X-ray optic may be exposed to elevated temperatures so that a precise knowledge about the thermal stability of these multilayer systems is also required. Several measurement techniques like X-ray reflectometry (XRR including IMD simulations), X-ray diffraction (XRD) and transmission electron microscopy (TEM) were applied to study the

structure after preparation and *in situ* the phase transformations of the components during heating. The observed results are discussed with respect to the processes occurring during annealing of the multilayers (structural changes, crystallization of the amorphous oxides, changes in the oxygen content of the layers,...).
[1] T. Liese, V. Radisch, and H.U. Krebs, Rev. Sci. Instrum. 81 (2010) 073710.

DS 37.19 Thu 15:00 Poster E

Influence of the deposition geometry on the microstructure of sputter-deposited V-Al-C-N coatings — Susan Darma[1], •Bärbel Krause[1], Stephen Doyle[1], Stefan Mangold[1], Sven Ulrich[2], Michael Stüber[2], and Tilo Baumbach[1] — [1]ISS, Karlsruher Institut für Technologie — [2]IAM-AWP, Karlsruher Institut für Technologie

Multi-element hard coating materials such as V-Al-C-N are of great interest for many technological applications. Their mechanical properties depend on the composition and microstructure of the coating. In order to determine the optimum composition and deposition conditions of these complex materials, many samples are required. One powerful tool for reducing the number of experiments is based on the so-called combinatorial approach for thin film deposition: many different thin film samples can be realized simultaneously, exploiting the deposition gradient resulting from codeposition of several materials. We will present an X-ray diffraction study of the influence of the deposition geometry on the microstructure of V-Al-C-N coatings. The films were deposited by reactive RF magnetron sputtering from a segmented target composed of AlN and VC. Synchrotron radiation measurements where performed at the beamline PDIFF at ANKA. Significant texture changes were observed which can be attributed to the deposition geometry, as verified by calculations of the flux distribution. We conclude that codeposition can accelerate significantly the screening of new materials, under the condition that the desired property is not significantly influenced by the microstructural changes due to the deposition geometry.

DS 37.20 Thu 15:00 Poster E

Study of laser deposited W/Si multilayers for high-resolution transmission X-ray optics — •Christian Eberl, Florian Döring, Tobias Liese, and Hans-Ulrich Krebs — Institut für Materialphysik, Georg-August-University, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

High quality non-periodic W/Si multilayers were pulsed laser deposited (PLD) at 248 nm for the use as high-resolution transmission X-ray optics (multilayer Laue lenses) and studied by thickness monitoring, SEM, TEM, and X-ray reflectometry (XRR). Due to the large difference in melting point, the ablation threshold, deposition rate as well as droplet formation of the both components W and Si strongly differ. Furthermore, during deposition of W/Si multilayers thickness deficits up to 2 nm due to resputtering and WSi_2 interlayers occur. Thus, in order to ensure a defined deposition of high-quality multilayers, two distinct element specific sets of optimized preparation conditions had to be worked out. In this contribution, this process of optimization is described in detail and the underlying mechanisms are discussed, also in comparison with SRIM simulations.

DS 37.21 Thu 15:00 Poster E

Spray deposition of polymer thin films investigated by in situ muGISAXS — •Adeline Buffet, Jan Perlich, Matthias Schwartzkopf, Gerd Herzog, Mottakin M. Abul Kashem, and Stephan V. Roth — DESY, Hamburg, Germany

Over the past few years organic-based hybrid devices have attracted increasing interest in both academy and industry because of their potential for low-cost production and flexible device applications [1]. Recently, the novel technique of airbrush deposition was used in the fabrication of organic-based multilayer devices such solar cells [2]. This technique allows for performing rapid deposition of organic-based thin film showing high homogeneity over large areas [3]. We used the versatile technique of microfocus beam Grazing Incidence Small Angle X-ray Scattering (muGISAXS, [4]) to investigate in situ the formation of a polymer thin film on a flat silicon wafer during spray deposition. Given the high photon flux available at the MiNaXS beamline of the PETRA III storage ring at DESY (Hamburg, Germany) in situ investigation of the polymer thin film build-up and of the nanostructure growth kinetics could be achieved with an exceptional time resolution of 50 ms. [1] Kaune et al., Eur. Phys. J. E 26, 73-79 (2008) [2] Green et al., Appl. Phys. Lett. 92, 03330 (2008) [3] Buffet et al., Adv. Eng. Mat. Journal, 12, 1235 (2010) [4] Roth et al., Appl. Phys. Lett., 82, 1935 (2003)

DS 37.22 Thu 15:00 Poster E

Characterization of the ferecrystals $[(SnSe)_{1+x}]_m[MSe_2]_n$ (M= Ta, V) — •Corinna Grosse[1], Saskia F. Fischer[1], Ryan Atkins[2], Wolfgang Neumann[2], and David C. Johnson[2] — [1]Novel Materials, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Department of Chemistry, University of Oregon, Eugene OR 97401-3753, USA

Ferecrystals are layered intergrowth compounds consisting of different types of nanolayers with in-plane crystallinity and cross-plane turbostratic disorder. Layered structures of WSe_2 prepared by the modulated elemental reactants (MER) method have exhibited the lowest thermal conductivity ever observed in a fully dense solid [1]. However, the structural and electronic properties of many ferecrystals are still unknown. In this study, the ferecrystals $[(SnSe)_{1+x}]_m[MSe_2]_n$ (M= Ta, V) were synthesized by the MER method. Structural investigations of $[(SnSe)_{1+x}]_m[TaSe_2]_n$ were made by (scanning) transmission electron microscopy. The structure of the SnSe and $TaSe_2$ layers was resolved and compared to that of the binary compounds. Respective TEM investigations of $[(SnSe)_{1+x}]_m[VSe_2]_n$ will be made. The in-plane electrical resistivity will be measured as a function of temperature and layer sequence (m and n) using the van der Pauw method. Since the complex nanostructure and small deviations in composition can critically influence the electrical properties, the structural investigations will be correlated to the results of the electrical measurements.

[1] C. Chiritescu, D. G. Cahill, N. Nguyen, D. C. Johnson et al., Science 315, 351 (2007).

DS 37.23 Thu 15:00 Poster E

Shallow donors in rf plasma deposited ZnO:H thin films — •Jan M. Philipps, Jan Stehr, Achim Kronenberger, Angelika Polity, Detlev M. Hofmann, and Bruno K. Meyer — I. Physikalisches Institut, JLU Giessen, Germany

The rf-sputter deposition of ZnO using H_2 as a reactive gas allows modifying the carrier concentration of the films over more than six orders of magnitude. Electron concentrations from $5x10^{14}$ cm^{-3} up to $3x10^{20}$ cm^{-3} can be obtained by varying the H_2/O_2-ratio in the sputter gas. This makes the material attractive for applications such as TCO (transparent conducting oxides) or heatable windows. In order to investigate the properties of the incorporated donors we performed electron paramagnetic resonance experiments (EPR). In all samples the shallow donor resonance at g $\sim$ 1.96 could be detected with similar signal intensity. This was somewhat unexpected since high carrier concentrations above the Mott limit ($\sim 5x10^{18}$ cm^{-3}) should alter the resonance properties due to motional effects or electric shielding (skin effect). We found that high carrier concentrations have clear effect on the saturation behaviour of the EPR signals causing short relaxation times. The results will be discussed considering the polycrystalline structure of the films.

DS 37.24 Thu 15:00 Poster E

Surface plasmon resonances of Ag and Ag-Au nanoparticles embedded in thin glass surface layers — Manfred Dubiel[1], Jörg Haug[1], Martin Stiebing[1], Maximilian Heinz[1], and •Armin Hoell[2] — [1]Martin Luther University of Halle-Wittenberg, Institute of Physics, Von-Danckelmann-Platz 3, D-06120 Halle — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Institute of Applied Materials, Albert-Einstein-Strasse 15, D-12489 Berlin

Nano-sized metal particles embedded in glass are of great interest because of their potential application as non-linear material for photonic devices. By sequential high-dose ion implantation of Ag+ and Au+ ions as well as by ion exchange processes of Au-containing glasses metal nanoparticles have been formed in a surface-near region of the soda-lime silicate glass. The measurements of the surface plasmon resonances indicate the generation of homogeneous pure Ag and Au particles, of bimetallic Ag-Au particles or of core-shell structures. With it, the surface plasmon resonance could be adjusted between the resonance of pure Ag and Au nanoparticles by the variation of the composition of particles. In addition, surface plasmon resonances well above 600 nm were found which could be assigned to hollow nanoparticles.

The evaluation of the experimental data of the optical absorption spectra in combination with experiments of transmission electron microscopy and small angle X-ray scattering experiments allowed to explain the processes of nucleation and growth of such particles and to identify their compositions and structures. The optical changes have been examined for different penetration depths of particles.

DS 37.25 Thu 15:00 Poster E

Production and structural characterization of nanolayers of *LiNbO*$_3$ by wetchemical synthesis — •Doreen Eger, Emanuel Gutmann, Hartmut Stöcker, Erik Mehner, and Dirk-Carl Meyer — TU Bergakademie Freiberg, Inst. für Exp. Physik

There are many known applications of pyroelectrics. Some new ideas, e.g. disinfecting and biocatalytic surfaces, require thin pyroelectric layers on a substrate. A substance with high pyroelectric coefficient is lithium niobate. There, basic investigations of a new method for manufacturing thin layers of lithium niobate are presented.

The thin layers are produced by dip coating of fused silica in a solvens of lithium niobate. Samples with different drawing speed and reaction temperature are manufactured. The resulting layers are characterized by reflected light microscopy (RLM), atomic force microscopy (AFM) and X-ray diffraction (XRD).

It is proven by XRD that the layers consist of lithium niobate. AFM and RLM show that samples with low drawing speed become so thick that clefts are formed.

Therefore, the manufacturing of nanolayers of lithium niobate with dip coating is possible and reasonable. For an optimization of process parameters for deposition of a defined layer thickness more improvement of the method is necessary, e.g. adding a wetting agent or a conditioning step of the substrate.

DS 37.26 Thu 15:00 Poster E

Production and structural characterization of nanolayers of Ruddlesden-Popper phases SrO(SrTiO$_3$)$_n$ with n=1, 2 und 3 — •Diana Karsch, Emanuel Gutmann, Hartmut Stöcker, Erik Mehner, and Dirk-Carl Meyer — TU Bergakademie Freiberg, Inst. für Exp. Physik

The strontium titanate Ruddlesden-Popper phases (STO-RP) represent ordered compounds of strontium oxide and strontium titanate with prominent piezoelectric, dielectric and photocatalytic properties. Two different methods for manufacturing nanolayers consisting these compounds are analyzed.

The first method follows the citrate route while the second aimes at additional networking using a modified Pechini route. The prepared sols were characterized by their molecular structure with magnetic resonance spectroscopy and regarding their wetting behavior with viscosity measurements. The films, produced using both methods with different process parameters, were characterized by reflected light microscopy, atomic force microscopy, X-ray reflectometry, X-ray diffraction and spectroskopic ellipsometry.

It turns out that the modified Pechini route results in no additional networking. The annealed films possess a thickness of 75...180 nm and contain solely STO-RP phase $n = 1$ only by adapting the tempering parameters, all STO-RP phases $n = 1, 2$ and $n = 3$ occur together.

DS 37.27 Thu 15:00 Poster E

Strontium Titanate Thin Film Deposition – Structural and Electronical Characterization — •Florian Hanzig[1], Juliane Hanzig[1], Michael Franke[2], Hartmut Stöcker[1], Erik Mehner[1], Barbara Abendroth[1], and Dirk C. Meyer[1] — [1]TU Bergakademie Freiberg, Institut für Experimentelle Physik — [2]TU Bergakademie Freiberg, Institut für Elektronik- und Sensormaterialien

Strontium titanate is on the one hand a widely-used model oxide for solids which crystallize in perovskite type of structure. On the other hand, with its large band-gap energy and its mixed ionic and electronic conductivity, SrTiO$_3$ is a promising isolating material in metal-insulator-metal (MIM) structures for resistive switching memory cells. Here, we used physical vapour deposition methods (e. g. electron-beam and sputtering) to produce strontium titanate layers. Sample thicknesses were probed with X-ray reflectometry (XRR) and spectroscopic ellipsometry (SE). Additionally, layer densities and dielectric functions were quantified with XRR and SE, respectively. Using infrared spectroscopy free electron concentrations were obtained. Phase and element composition analysis was carried out with grazing incidence X-ray diffraction and X-ray photoelectron spectroscopy. Subsequent temperature treatment of samples lead to crystallization of the initially amorphous strontium titanate.

DS 37.28 Thu 15:00 Poster E

Preparation and characterization of Ge2Sb2Te5 phase change films on elastic substrates by pulsed laser deposition — •Hongbing Lu, Erik Thelander, Julia Benke, and Bernd Rauschenbach — Leibniz Institute of Surface Modification, 04318 Leipzig

Ge2Sb2Te5 (GST) thin films have attracted a great deal of interest as an active layer for data storage media due to its high switching rate and extremely good reversibility. Here we demonstrate the preparation of high-quality GST films on elastic polyimide substrates by pulsed laser deposition (PLD). The composition and chemical state of the films were investigated by energy dispersive x-ray spectroscopy (EDX) and x-ray photoelectron spectroscopy (XPS), respectively. The effect of annealing temperature on the crystalline nature of the films was also studied. As-deposited films were found to be amorphous. Crystalline phases with face-centered cubic and hexagonal structures appeared at 180 and 300 degrees, respectively. Importantly, no phase separation could be seen in the annealed films. Furthermore, reflectivity measurements were performed to characterize the as-deposited and annealed films, showing a high reflectivity contrast (up to 23%) between full crystalline and amorphous films. Our results indicate that PLD deposited GST film on polyimide substrate is a promising candidate for use in future flexible memory devices.

DS 37.29 Thu 15:00 Poster E

The ferroelectric transition in the phase-change material GeTe — •Franziska Schlich, Peter Zalden, and Matthias Wuttig — 1. Physikalisches Institut IA, RWTH Aachen University, 52074 Aachen, Germany

Phase-change materials can be cycled between the amorphous and the crystalline phase. This transition is accompanied by a significant change of the electrical resistance. The materials on the pseudo binary line between GeTe and Sb$_2$Te$_3$ are particularly suitable for memory devices. The meta-stable crystalline phase of Ge$_2$Sb$_2$Te$_5$ has a cubic symmetry and is characterised by atomic displacements and configurational disorder which leads to a localization of charge carriers and semiconducting properties. Also GeTe in its low temperature α-phase is claimed to have pronounced local distortions. Nevertheless in the literature two scenarios have been presented which can explain the transition to the cubic α-phase. One is based on a displacive transformation (Chattopadhyay et al.; J. Phys. C 20, p.1431, 1987) while the second one (Fons et al.; Phys. Rev. B 82, p.1431, 2010) utilizes an order-disorder phase transition.

Therefore we have investigated the phase transition of GeTe whose transition temperature is reported to depend critically on the stoichiometry. We have sputter deposited thin films of approx. 300 nm thickness and obtained Ge$_{53}$Te$_{47}$. X-ray diffraction (XRD) patterns which include information about the thermal and static disorder of the crystal lattice, have been recorded during heating. From these data we obtain important insight on the nature of the phase transition.

DS 37.30 Thu 15:00 Poster E

Spectroscopic Investigation of LaAlO$_3$ - SrTiO$_3$ Heterointerfaces — •Uwe Treske[1], Andreas Koitzsch[1], Martin Knupfer[1], Kathrin Dörr[2], and Bernd Büchner[1] — [1]IFW-Dresden — [2]MLU Halle-Wittenberg

In recent years epitaxial growth of transition metal oxides became possible and exotic phenomena were found at their interfaces. A prominent example is the formation of a high-mobility two-dimensional electron gas at the interface of LaAlO$_3$ grown on TiO$_2$-terminated SrTiO$_3$ substrates. Such heterointerfaces fabricated by pulsed laser deposition under various growth conditions were investigated with soft x-ray photoemission spectroscopy. We focused on stoichiometric aspects as well as in-gap states and differences in the core levels. Deviations from an abrupt interface without defects were found.

DS 37.31 Thu 15:00 Poster E

Ultra-thin TiO$_x$ films on Pt(111): effect of the preparation parameters on the electronic and local structure. — •Mathias Glaser and Thomas Chassé — Universität Tübingen, Institut für Physikalische und Theoretische Chemie, Auf der Morgenstelle 18, 72076 Tübingen

Ultra-thin TiO$_x$ films on Pt(111) are promising model systems for the investigation of catalysis and are well suited for the investigation of oxide-oxide interphases. Carefully controlled preparation conditions are necessary during reactive evaporation of Ti in an O$_2$ environment to obtain high quality films.

We investigated the electronic structure and the oxidation states of the different chemical elements of such ultra-thin films by x-ray photoelectron spectroscopy (XPS). The comparison of Ti2p core level spectra of different TiO_x films shows the influence of different preparation parameters like evaporation and substrate temperature.

In order to investigate the local structure we used electron diffraction methods. Some of the films show the same patterns described in literature [1] before but were prepared by using other preparation parameters.

[1] F. Sedona et al., J. Phys. Chem. 2005, 109, 24411-24426.

DS 37.32 Thu 15:00 Poster E

Texture analysis of MgO layers in MgO-CoFeB thin film systems by HRTEM — •Patrick Peretzki[1], Vladyslav Zbarsky[2], Marvin Walter[2], Henning Schuhmann[1], Filip Podjaski[1], Markus Münzenberg[2], and Michael Seibt[1] — [1]IV. Physikalisches Institut, Georg-August-Universität Göttingen — [2]I. Physikalisches Institut, Georg-August-Universität Göttingen

Magnetic tunnel junctions (MTJs) consisting of two ferromagnetic amorphous CoFeB electrodes separated by a crystalline MgO tunnel barrier are good and well-studied candidates for industrial use of the tunnel magnetoresistance (TMR) effect for a variety of applications. Practical use requires a clearly defined nanostructure of the MgO barrier which is only a few monolayers thick and tends to crystallize in a textured grain structure. However, the exact influence of the degree of texturing on the MTJ behaviour, for example the TMR value or the mechanism of dielectric breakdown, is not clear. To clarify this, first steps were taken in developing a quantitative assessment of the MgO degree of texturing in several layer stacks with varying deposition temperature, layer order and thicknesses. Two approaches have been implemented and evaluated to quantitatively analyse the MgO layer texture from High Resolution Transmission Electron Microscopy (HRTEM) images obtained from the layer stacks. They use Fourier transform and Hough transform of the images, respectively. Results indicate a cumulative roughness effect in the stacks with layers having high degrees of texturing. We thank the DFG for funding through SFB 602.

DS 37.33 Thu 15:00 Poster E

Spatially Resolved MOKE Spectroscopy — •Peter Richter, Michael Fronk, Alexander Kopylov, Dietrich R.T. Zahn, and Georgeta Salvan — Semiconductor Physics, Chemnitz University of Technology, 09107 Chemnitz

The measurement of the magneto-optic Kerr-effect (MOKE) yields information on the magnetic properties of para- and ferromagnetic thin films and can be used to characterize them with regard to spin polarization. This helps to assess their potential for spintronic devices or for modern magnetic data storage. Since samples of such materials often show structures on the micro- and nanoscopic scale, the use of a divergent light source with a large spot size (*e.g.* a Xe-lamp) for spectroscopic MOKE measurements provides averaged information. This work presents the experimental realization of a MOKE setup which uses a supercontinuum white light source ($\lambda = 450$ to 1000 nm) to achieve a μm-scale resolution for spatially resolved spectroscopic MOKE measurements. This setup furthermore allows measurements in the polar and in the longitudinal MOKE geometry, with the latter allowing materials with in-plane magnetic anisotropy to be investigated. The layout of the new setup and important hardware parts are described in detail. Finally, exemplary spatially resolved spectroscopic MOKE measurements of cobalt and nickel micro-electrodes for spintronic devices are presented.

DS 37.34 Thu 15:00 Poster E

Investigation of local texture and crystallite size in thin FePtCu films via EBSD — •Nathanael Jöhrmann, Herbert Schletter, Christoph Brombacher, Manfred Albrecht, and Michael Hietschold — Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz

FePt shows a very high uniaxial magnetocrystalline anisotropy in its chemical ordered $L1_0$ phase. Therefore thin FePt films are a promising candidate to raise the storage density of magnetic storage devices. For such applications it is necessary to grow films with (001) texture. The addition of copper can improve the texture formation during annealing [1].

In this work a FePtCu alloy with 9 at.% Cu was investigated via electron backscatter diffraction. The film was prepared by magnetron sputtering of 0.6 nm Cu and 4.4 nm FePt at room temperature on a thermally oxidized Si(100) substrate, followed by rapid thermal annealing to 600 °C for 30 s. Because of the small observed crystallite sizes in a range of 10 - 100 nm it proved difficult to obtain good electron backscatter diffraction patterns. To improve spatial resolution, the acceleration voltage of the electrons in the scanning electron microscope was optimized. In another approach, the substrate was thinned from the back to a thickness of approximately 100 nm, to reduce the interaction volume of the primary electrons.

[1] M. L. Yan et al., J. Appl. Phys. 99, 08G903 (2006)

DS 37.35 Thu 15:00 Poster E

STM studies of epitaxial grown iron films on MgO(001) — •Christian Otte, Martin Suendorf, and Joachim Wollschläger — Barbarastr. 7, 49076 Osnabrück

Due to their electric and magnetic properties, ultra thin iron films are a considerable candidate for spintronic applications. Therefore, ultra thin epitaxial grown iron films were prepared on MgO(001) under UHV conditions and investigated using Scanning Tunneling Microscopy. Au contatcs were applied to the substrate via Molecular Beam Epitaxy (MBE) prior to film depostition in order to provide electrical contact to the film. The films were deposited by MBE using different depostition rates and substrate temperatures.

A strong depency between the growth of the films and the substrate temperature was observed which results in different kinds of growth mode, island shape and island size. A transition from *Volmer-Weber-growth* to *Frank-van der Merve growth* was observed with increasing substrate temperature.

DS 37.36 Thu 15:00 Poster E

Oxidation of iron films on MgO(001) — •Tobias Schemme, Martin Suendorf, Frederic Timmer, and Joachim Wollschläger — Barbarastr. 7, 49076 Osnabrück

The oxidation of ultrathin iron films on MgO(001) substrates was investigated by photoelectron spectroscopy and electron diffraction. First a layer of iron was deposited on the substrate using molecular beam epitaxy (MBE) at room temperature. The iron films were annealed several times in a thin oxygen atmosphere ($p(O_2) = 10^{-6}$ mbar). To determine the dependence of the annealing temperature on the oxidation process, the iron films were heated up to different temperatures (RT until 573 K). The stoichiometric composition and the structure of the iron oxide films were investigated by X-ray Photoelectron Spectroscopy (XPS) and Low Energy Electron Diffraction (LEED), respectively. Analyzing the Fe 2p and the Fe 3p signal, the iron oxide films show stronger oxidation at high temperatures. While the iron films were not completely oxidized to Fe_2O_3 after a few oxygen treatsments at low temperatures, the iron films annealed at higher temperatures showed full oxidation to stoichiometric Fe_2O_3.

DS 37.37 Thu 15:00 Poster E

Novel high-temperature films consisting of mass selected carbon clusters — •Artur Böttcher, Seyithan Ulas, Patrick Weis, and Manfred Kappes — KIT, Institut für Physikalische Chemie, Karlsruhe

Cluster beam deposition has been established as a method for preparation of monodisperse films consisting of tailored building blocks. We fabricated thick films via aggregation of small fullerene cages, C_n ($48 < n < 70$). Such carbon cages are created by electron-impact inducend ionization/fragmentation of IPR cages: C_{70}+ e→ C_{68}+C_2 → C_{66}+C_2 →... Film growth is governed by the formation of -C_n-C_n- oligomers interlinked by covalent bonds constituted by nIPR-nIPR bridges. All C_n films created are semiconducting with electronic and vibronic properties depending on the size of the C_n building blocks (IP, HOMO-LUMO-gap, valence band, etc.). The thermal stability of the C_n films can be related to the mean number of non-IPR sites in C_n cage. Some Raman bands confirm the role of the covalently stabilized oligomers as the species responsible for unique mechanical and thermal properties. The C_n solids exhibit mechanical properties comparable to graphite. Annealing the C_n solids up to 1100 K results in stable chains of fused C_n cages (HT-C_n solids).

DS 37.38 Thu 15:00 Poster E

The impact of phase segregation on the electrical properties of $GeTe_{1-x}$ $SnTe_x$ alloys — •Felix Lange, Hanno Volker, Peter Zalden, and Matthias Wuttig — 1. Physikalisches Institut IA, RWTH Aachen University

Phase-change alloys are a unique class of materials that can be reversibly switched between their amorphous and crystalline phase. This transition is accompanied by a significant change in physical properties such as reflectivity and electrical conductivity. Especially the current induced phase transition within nanoseconds [1] makes PCM valuable for non volatile RAM application.

The common PCMs are tellurium based chalcogenides with an average number of three p-electrons per atom in their outer electronic shell. Since the p-band is half-filled it is expected that these alloys develop a band-gap due to Peierls distortions resulting in a thermally activated charge transport. However, experimentally PCM are found to be degenerate semiconductors with carrier concentration in the range of 10^{20} 1/cm^3. Edwards *et al.* [2] recently showed that it is favorable in GeTe to formvacancies on the cation site that shift the Fermi-level well inside the valence band.

This work focuses on the electrical properties of GeTe$_{1-x}$SnTe$_x$ alloys. Low temperature electrical conductivity data are interpreted in terms of phase segregation in crystalline GeTe$_{1-x}$SnTe$_x$ and amorphous Ge.

[1] G. Bruns *et al.*, Appl. Phys. Lett. **95**, 043108 (2009)
[1] Edwards *et al.*, Phys. Rev. B **73**, 045210 (2006)

DS 37.39 Thu 15:00 Poster E

Preparation and Characterisation of LIPON thin films — •Susann Nowak, Frank Berkemeier, and Guido Schmitz — Westfälische Wilhelms-Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str. 10, 48149 Münster

We present the preparation of LIPON (lithium phosphorous oxynitride, $\mathrm{Li_3N_x(PO_4)_{1-x}}$) thin films by reactive ion-beam sputtering, and the characterization of the films by temperature-dependent electrochemical impedance spectroscopy (EIS), X-ray diffraction (XRD) and transmission electron microscopy (TEM). Despite LIPON is widely discussed as a suitable electrolyte for all solid-state thin film batteries, there are only a few publications reporting on films that exhibit a thickness below 1 μm. Therefore, in this work we investigate the properties of LIPON films with a thickness between 50 and 500 nm. Ion beam sputter deposition results in amorphous LIPON layers, as observed by XRD and TEM. Temperature dependent measurements of dc-conductivity by EIS give a conductivity of $5 * 10^{-7}$ S/cm at 30°C and an activation enthalpy of (58 ± 2) kJ/mol, and hence allow to operate the LIPON films in all-solid state batteries at room temperature, with a reasonable charge/discharge performance. Additionally, thin film batteries have been prepared by depositing a LIPON layer between two metallic electrodes (e.g. Pt and Ag). It is shown that during the first cycle of cyclic voltammetry measurements, electrochemically active interface regions are formed, serving as anode and cathode, respectively, and thus forming a complete electrochemical thin-film cell, which is further investigated by means of EIS and TEM.

DS 37.40 Thu 15:00 Poster E

Towards circularly polarized (sub-) femtosecond XUV pulses for ultrafast pump-probe experiments — •Jürgen Schmidt[1], Alexander Guggenmos[2], Michael Hofstetter[2], Soo Hoon Chew[1], Mihael Kranjec[1], and Ulf Kleineberg[1] — [1]LMU München, Physik-Department, Garching — [2]MPQ für Quantenoptik, Garching

Circularly polarized (CP) XUV radiation has been demonstrated to be a useful probe for the experimental investigation of electronic effects in magnetic materials such as magnetic circular dichroism, spin-polarized photoemission, magneto-optical Kerr-effect and others. On the laboratory scale, High Harmonic (HH) gas jet sources which inherently provide coherent and ultrashort linearly polarized XUV pulses in the sub-fs domain, suitable to study ultrafast dynamics, have emerged. In our setup we aim at incorporating in-house fabricated broadband transmission multilayer phase shifters into a laser driven 10kHz repetition rate HH Source in the 50-70eV photon energy range. To our knowledge only little investigation on such polarizers intended for use in HH radiation has been made so far. We examine our phase shifters regarding tunability of energy range, phase retardation, transmission efficiency and spectral bandwidth. For this purpose we use a home-made XUV flat-field spectrometer and a multilayer mirror based polarization analyzer. Combining the expected CP pulses with our TOF-PEEM and ARPES spectrometer will pave the way towards time resolved measurements of exchange-coupled electron dynamics.

DS 37.41 Thu 15:00 Poster E

Multilayer zone plates for x-ray focusing fabricated by pulsed laser deposition — •Florian Döring, Christian Eberl, Tobias Liese, and Hans-Ulrich Krebs — Institut für Materialphysik, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

X-ray microscopy in the soft and hard regime is a highly useful technique for biological and materials sciences, polymer research, colloidal science and even earth science. One alternative approach for two-dimensional x-ray focusing is to prepare non-periodic multilayer structures. They can be designed in zone plate geometry by depositing high quality non-periodic multilayers on wires according to the Fresnel zone plate law. For this, ZrO$_2$/Ti and W/Si multilayers with high optical contrast in the soft and hard x-ray region, respectively, were pulsed laser deposited (PLD) at 248 nm. In this contribution, the growth of multilayers on flat and curved surfaces (studied by electron microscopy after focused ion beam preparation) is compared, and the fabrication steps of different zone plate structures are presented.

DS 37.42 Thu 15:00 Poster E

Atomically precise deposition control of multilayer mirrors-towards attosecond water window experiments — •Alexander Guggenmos[1,2], Michael Hofstetter[1,2], Ferenc Krausz[1,2], and Ulf Kleineberg[1,2] — [1]Ludwig-Maximilians-Universität München, Garching, Deutschland — [2]Max-Planck-Institut für Quantenoptik, Garching, Deutschland

Extending current attosecond technology to the water window range (300-500 eV) may not only enable the generation of ever shorter pulses; it will further allow for the investigation of the underlying electron dynamics of fundamental biological processes such as photosynthesis.

Only aperiodic multilayer optics can exhibit the required degree of freedom for the synchronization and tailored shaping of attosecond pulses in that energy range.

With typical layer thicknesses of less than 1 nm, atomically precise knowledge of the intrinsic built-up of the individual layers and atomically precise control over the deposition process is required. As will be shown, ion beam sputter deposition in combination with sophisticated measurement techniques succeeds the required precision and enables a statistical accuracy far beyond 1 Angstrom.

We will present results from these elaborate calibrations, which enabled the fabrication of even three and four material aperiodic attosecond water window multilayer mirrors. These mirrors pave the way towards taylor-made attosecond pulses in the water window spectral range.

DS 37.43 Thu 15:00 Poster E

Pulsed DC Magnetron Sputtered TiO$_2$ Layers Optimized for Photocatalytic Efficiency — •Bodo Henkel, Thomas Strunskus, Vladimir Zaporojtchenko, Stefan Rehders, and Franz Faupel — Institute for Materials Science, Kiel, Germany

Pulsed DC Magnetron Sputtering was used to produce highly photocatalytically active TiO$_2$ layers on quartz glass. For measuring photocatalytic efficiency, degradation of methylene blue in combination with in situ UV-vis measurement was used. UV LEDs with 365 nm wavelength were taken to irradiate the TiO$_2$ layer. The influence of various sputter parameters was examined as well as post annealing time and temperature. To indicate correlation to effective surface area, roughness and crystallinity, AFM and XRD measurements were done.

DS 37.44 Thu 15:00 Poster E

Functional thin films prepared by high power impulse magnetron sputtering — •Vitezslav Stranak[1], Harm Wulff[1], Robert Bogdanowicz[1], Henrike Rebl[2], Carmen Zietz[3], Zdenek Hubicka[4], Kathleen Arndt[5], Barbara Nebe[2], Rainer Bader[3], Andreas Podbielski[5], and Rainer Hippler[1] — [1]University of Greifswald, Institute of Physics, Felix-Hausdorff Str. 6, 17489 Greifswald, Germany — [2]University of Rostock, Biomedical Res. Center, Schillingallee 69, 18057 Rostock, Germany — [3]University of Rostock, Dept. of Orthopaedics, Doberaner Str. 142, 18057 Rostock, Germany — [4]Academy of Sciences of the Czech Republic, Inst. of Physics, Na Slovance 2, 180 00 Prague, Czech Republic — [5]University of Rostock, Dept. of Med. Microbiol., Virology and Hygiene, Schillingallee 70, 18057 Rostock, Germany

Antibacterial effect of thin titanium/copper (Ti-Cu) films in combination with growth of human osteoblastic cells on the surface is reported. Thin films were prepared by dual-High Power Impulse Magnetron Sputtering (dual-HiPIMS). The quality and properties of deposited films are influenced by internal plasma parameters (mainly by the energy of particles incoming to the growing film). The Ion Velocity Distribution Function (IVDF) was measured by a retarding field analyzer (RFA). It was found that films are copper rich with a density close to pure bulk Cu material (investigated by GIXD and XR techniques). This effect, together with larger domain size, results from the high energy of sputtered particles during HiPIMS pulses.

DS 37.45 Thu 15:00 Poster E

CO2-Methanation by Catalytic Conversion — •Klaus Müller, David Hoffmannbeck, Georg Kirner, Matthias Staedter, and Dieter Schmeisser — Angewandte PhysikII/Sensorik, BTU Cottbus, Konrad Wachsmann Allee 1, 03046 Cottbus

The utilization of CO2 as raw material is an important component of a program for CO2 reduction. A possibility is the production of methane. At a moderate temperature of around 350°C, hydrogenation of CO2 to methane is possible by the Sabatier reaction CO2 + 4H2 ->CH4 +2H2O. Prerequisite for an efficient kinetics of the Sabatier reaction is the application and optimization of catalysts. In this contribution, we present investigations of Ru and Ni catalysts on different substrates. For Ru/Al2O3 catalysts, we found stable operation without degradation within 500 hours with a conversion rate of 80% at 350°C. For NiO/SiO2 catalysts, a conversion rate of 90% was found for temperatures of 350-405°C. We also show the investigation of cross sensitivities against SOx and NOx, which are typical contaminations of CO2, generated by the industrial oxyfuel process. In our work the morphology (REM, AFM, specific surface), chemical composition (FTIR, XPS) and phase composition (XRD) of the catalysts are characterized. In addition, we report on thermodesorption (TDS) measurements at atmospheric pressure to determine the amount of adsorbed CO2 under real conditions. The project is funded by the German Ministry of Research and Education (BMBF-GeoEn).

DS 37.46 Thu 15:00 Poster E

Thermal conductivity measurements of $(\mathrm{GeTe})_{1-x}(\mathrm{SnTe})_x$ phase-change alloys — •Kai Hugenroth, Karl Simon Siegert, Felix Lange, Roland Sittner, and Matthias Wuttig — 1. Physikalisches Institut IA, RWTH Aachen, 52064 Aachen

Phase-change materials (PCM) are a versatile class of materials with a broad range of applications, for instance as memory cells. For decades, PCM's were the standard material for optical data storage applications, such as CD-RW's and DVD-RW's. They are also promising for the development of electronic memories, such as Random Access Memory (PC-RAM), capitalizing on the rapid crystalline-amorphous phase-transition which occurs within nanoseconds.

This work focuses on the thermal conductivity κ of phase change materials, along the pseudo binary line from GeTe to SnTe [1]. κ is a central attribute for memory applications. Low thermal conductivities enable the design of very small memory-cells in the order of a few nanometers, thus allowing further miniaturization of mobile electronic devices. This is a highly important aspect, concerning feature sizes of alternative approaches, such as classic D-RAM or Flash-memory.

The measurements of κ are conducted at low temperatures from 40 K to 300 K, using the 3ω-method. A new measurement scheme for low temperatures is developed. The impact of different heater materials is taken into account, since deposition, adhesion and temperature stability as well as 3ω-compatibility are important aspects for successful analysis.

[1] D. Lencer et al. Nature Materials 7, 972-7 (2008).

DS 37.47 Thu 15:00 Poster E

Non-invasive measurement and control of the temperature of Pt nanofilms on Si supports — •Jan Philipp Meyburg[1], Ievgen Nedrygailov[1], Eduard Karpov[2], Eckart Hasselbrink[1], and Detlef Diesing[1] — [1]Fakultät für Chemie, Universität Duisburg-Essen, D-45117 Essen, Germany — [2]Department of Civil & Materials Engineering, University of Illinois, Chicago, IL 60607, USA

A direct, non-invasive thermometry method based on the temperature dependence of the in-plane electrical resistance of Pt nanofilms deposited on commercial n-Si (111) substrates was developed in order to study the water formation reaction. At the calibration stage, the entire sample was slowly heated by external means. Experiments were carried out for hydrogen−oxygen mixtures in different molar ratios and pressures in the range of 2−30 mbar. To ignite the hydrogen−oxygen mixtures the Pt nanofilm was directly heated up to 500 °C by passing an electric current through it. Both, surface-catalyzed heterogeneous and homogeneous gas-phase reactions were identified. During the reaction process the resistance of the Pt nanofilm was monitored. The temperature of the Pt nanofilm was calculated using the Callendar−Van Dusen equation which describes the relationship between the temperature and the resistance of Pt thermometers. The accuracy of the present method for dynamical temperature measurement is found to be significantly better than that of a standard approach using a Pt RTD sensor. The validity of this method for Pt nanofilms on silicon is discussed.

DS 38: Poster III: Resistive switching (jointly with DF, KR, HL); Thermoelectric materials (Focused session); Micro- and nanopatterning (jointly with O); Ion irradiation effects

Time: Thursday 17:30–19:00 Location: Poster E

DS 38.1 Thu 17:30 Poster E

Electrical and thermal properties of phase change line cell devices — •Martin Wimmer, Lukas Küpper, and Martin Salinga — 1. Institut of Physics, RWTH Aachen University, Germany

The characteristic electronic properties of phase change materials are the reason for their recent success in electronic data storage devices. While the current versions of phase change memory are used as a replacement of Flash memory, the potential to write information within a nanosecond offers the opportunity to replace even DRAM with this non-volatile technology.

Within this work, electrical and thermal properties of lateral phase change line cells produced by electron beam lithography are studied. This low cost cell design provides excellent scalability down to tens of nanometers. Due to the easy variability of the line cell geometry the threshold and memory switching behaviour, in particular the threshold field and the scalability of energy consumption, can be systematically investigated.

DS 38.2 Thu 17:30 Poster E

Numerical simulations of threshold switching effect in phase change memory devices — •Sascha Cramer, Martin Wimmer, and Martin Salinga — 1. Institut of Physics, RWTH Aachen University, Germany

Phase change materials are one of the most promising candidates for future universal memory technologies. In this class of materials information can be stored by using the huge contrast in electrical resistivity between the amorphous and crystalline phase. While the permanent switching is commonly understood as a structural change between those two phases, there exists another transient switching phenomenon. The latter is observed as a strong non-linearity in the current-voltage characteristic of the amorphous state: At a critical voltage a sudden drop of resistivity is observed, the so-called threshold switching. The physical understanding of this effect is still controversially discussed today. In this work numerical simulations are performed based on two different models (Ielmini*s Poole-Frenkel-model and an alternative generation-recombination-model) and compared with experimental data.

DS 38.3 Thu 17:30 Poster E

Resistance drift in amorphous phase change thin films — •Christian Dellen, Martin Wimmer, Rüdiger M. Schmidt, Martin Salinga, and Matthias Wuttig — 1. Institut of Physics, RWTH Aachen University, Germany

While phase change materials have been successfully applied in rewriteable optical data storage, they are also used for novel non-volatile electronic memory devices. The material has the ability to be switched within nanoseconds between two phases, which show large contrast in electrical resistivity. One approach to improve the information density of such a phase change memory device is to store several logic bits in one physical cell by distinguishing between different states of partial crystallization. For this so-called multilevel storage device it is important that the resistance of this device is stable over many orders of magnitude in time. While for the crystalline phase this condition is sufficiently fulfilled, the amorphous phase shows a strong time dependence of the resistance, the so-called resistance drift. In literature this effect is often ascribed to relaxation of mechanical stress or to a change of electronic defects. In this work experimental data of the resistance drift are analyzed for a variety of different phase change materials and compared to models reported in literature.

DS 38.4 Thu 17:30 Poster E

Continuum modeling of phase formation in phase change materials — •fatemeh tabatabaei[1], markus apel[2], and efim brener[1] — [1]Peter Grünberg Institut (PGI-2), Forschungszentrum Jülich, 52428 Jülich — [2]Access e.V., RWTH Aachen, 52072 Aachen

Recently, the use of phase change materials (PCM) in non-volatile rewritable memory devices has expanded substantially. For memory applications a stable crystalline and a metastable amorphous state can be utilized for the data recording.To obtain a quantitative understanding of the kinetics of writing and erasing data, gaining insights into the energy transport and phase boundary movement during the phase transformation is aimed. One of the governing parameters for the transformation kinetics is the mobility of the liquid-solid interface. However, only limited knowledge and models for it is available. We carried out phase field modeling as a continuum simulation technique in order to study rapid crystallization processes in AgInSbTe. We performed spatio-temporal simulations of the crystallization of a molten area in a PCM layer stack initiated by a laser pulse. We refined the simulation concerning experimental conditions for the measurement of the crystallization kinetics. Simulations are performed for different substrate temperatures, i. e. for temperatures close to the melting point of AgInSbTe down to the glass temperature when the amorphous state is involved. The effect of the interface mobility on the solidification kinetics is investigated. A non-linear dependence of the interface kinetic coefficient on temperature is necessary to explain the temperature dependent crystallization velocity observed in experiments.

DS 38.5 Thu 17:30 Poster E

Thermal Conductivity as sensor for defects in homoepitaxial SrTiO3 — •Thilo Kramer[1], Jonas Lindner[1], Stefanie Wiedigen[1], Manuel Feuchter[2], Marc Kamlah[2], Inga Knorr[1], Cynthia Volkert[1], and Christian Jooss[1] — [1]University of Göttingen, Institute for Materials Physics — [2]Forschungszentrum Karlsruhe, Instiute for Materials Research II

SrTiO3 is a promising material for various future applications in the fields of thermoelectric, oxide electronics or resistive switching, where the control of point defect structure is of high importance. Such defects control the strain and doping level, and, may be involved in resistive switching. Because a direct measurement of defect type and concentrations is difficult, we evaluate whether thermal conductivity can indirectly give access to the desired information via point defect induced phonon scattering. Thin homoepitaxial SrTiO3 films are fabricated with Ion Beam Sputtering. The balance between ion beam induced defect generation and dynamic healing and thus the resulting net defect concentration can be influenced by varying the deposition temperature. The temperature dependence of the thermal conductivity of the thin films is reliably measured by the 3w method in combination with finite element simulations of the thermal conditions. We present systematic study of thermal conductivity as a function of varying preparation conditions. X-ray diffraction, TEM and mechanical measurements allow for detailed insights into the degree of epitaxy and the stress strain state of the films. The combination of all used methods gives evidence that charge neutral Schottky defects are the dominating defect type.

DS 38.6 Thu 17:30 Poster E

Pulse length dependence of resistive switching in $Pr_{0.7}Ca_{0.3}MnO_3$ noble metal sandwich structures — •Björn-Uwe Meyer, Malte Scherff, Johannes Maier, Jörg Hoffmann, and Christian Jooss — Institute of Materials Physics, University of Göttingen, Germany

Time-resolved electric transport studies are an important approach for the analysis of the underlying mechanisms of resistive switching. Pulsed voltage experiments of sputtered $Pr_{0.7}Ca_{0.3}MnO_3$ films sandwiched by noble metal electrodes are performed with pulse length variation between 20ns and 1s in a temperature range between 300K and 165K. Due to the interaction of the opposing metal-oxide-interfaces in an asymmetric interface geometry, switching polarity inversion is observed. The inversion and the dependence of the switching amplitude on the pulse length can be used to demonstrate an equivalence of voltage amplitude and pulse duration. Especially, the switching amplitude strongly changes at lower temperature. These results will be compared with other findings such as a variation of electrode materials, device geometry and PCMO deposition parameters. Microstructure and chemical composition before and after switching is characterized for selected samples by transmission electron microscopy.

DS 38.7 Thu 17:30 Poster E

Multifunctional oxides and the influence of defects on the ferroic properties — •S. Gemming[1], T. Weissbach[2], M. Zschornak[1,2], H. Stöcker[2], D. C. Meyer[2], T. Leisegang[2,3], I. Ronneberger[1], and K. Potzger[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany. — [2]Institute of Physics, TU Bergakademie Freiberg, Freiberg, Germany. — [3]SAXRAY GmbH i.G., Dresden-Rossendorf, Germany.

Transition metal oxides exhibit many physical phenomena, among them ferroic properties such as ferroelasticity, ferroelectricity and ferromagnetism, or their combination in multiferroics. The stoichiometry of transition metal oxides depends on the oxygen partial pressure and changes conductivity and ferroic properties. Ternary/quaternary oxides are discussed, which correlate local defect-induced structure changes with changes of the elastic, polarization and magnetic properties. The microscopic interactions are determined by density functional theory as basis for more large-scale simulations with effective Hamiltonians. Oxygen vacancies in $SrTiO_3$ accumulate in an external electric field and reduce the hardness. For Sr/O excess $SrO(SrTiO_3)_n$ phases with additional SrO planes occur, which change the X-Ray reflectivity. Ion-irradiation triggers additional point defects which can form stable aggregates. In YMn_2O_5 several antiferromagnetic phases coexist with ferroelectricity; $YFeMnO_5$ exhibits only one commensurable ferrimagnetic phase. Based on spin-polarized DFT calculations a Heisenberg model yields the coupling constants of the two compounds and relates them to crystal-field interactions.

DS 38.8 Thu 17:30 Poster E

UHV-compatible setup for alcohol-assisted chemical vapor deposition of metals — •Fedor Strigunov, Volkmar Zielasek, and Marcus Bäumer — Universität Bremen, Institut für Angewandte und Physikalische Chemie, Leobener Str. NW2, 28359 Bremen, Deutschland

Due to the importance of thin metal films in the functionality of magnetic, superconductive, optical and microelectronic devices, there is high interest in chemical vapor deposition (CVD) techniques that fit industry requirements of reliability, sustainability and ease of use. So far, however, metal CVD had often been linked to toxic precursors or low quality of the resulting film.

A recently developed hydrogen-free approach to metal-CVD uses pulsed spray evaporation delivery of simple and commercially available non-toxic metal-organic precursors in alcohols [1]. We will present the design of a CVD reactor for pulsed spray deposition of metal organic precursors and alcohols that is integrated into an UHV system for thin film analysis. Sample transfer between the chambers for thin film preparation and for analysis via XPS, STM, LEED or IR spectroscopy can proceed without breaking vacuum. The results of preliminary experiments on the deposition of Co films on various substrates will be shown. The efficiency of the Co growth process and the quality of the resulting film depend on several parameters such as concentration of the precursors, deposition pressure, carrier gas flow rate, substrate temperature, deposition duration, spray pulse frequency and pulse width.

[1] P. A. Premkumar et al., Chem. Vap. Deposition, 13 (2007) 219.

DS 38.9 Thu 17:30 Poster E

Nonvolatile resistive switching in Au/BiFeO3/Pt — •Yao Shuai[1,2], Chuangui Wu[2], Wanli Zhang[2], Shengqiang Zhou[1], Danilo Bürger[1], Stefan Slesazeck[3], Thomas Mikolajick[3], Manfred Helm[1], and Heidemarie Schmidt[1] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, P. O. Box 510119, Dresden 01314, Germany — [2]State Key Laboratory of Electronic Thin Films and Integrated Devices, — [3]Namlab gGmbH, Nöthnitzer Strasse 64, 01187 Dresden, Germany

Nonvolatile bipolar resistive switching has been observed in an Au/BiFeO3/Pt structure, where a Schottky contact and a quasi-Ohmic contact were formed at the Au/BiFeO3 and BiFeO3/Pt interface, respectively. By changing the polarity of the external voltage, the Au/BiFeO3/Pt is switched between two stable resistance states without an electroforming process. The resistive switching is strongly dependent on the deposition pressure of the BiFeO3 thin films, and the resistive switching property of the Au/BiFeO3/Pt stack has been significantly improved by carefully tuning the oxygen pressure during the growth, and a large switching ratio of ˜4500 has been achieved. The deposition pressure modifies the concentration of oxygen vacancies and the rectifying behavior of the Au/BiFeO3 junction, and consequently influences the resistive switching behavior of the whole stack.

DS 38.10 Thu 17:30 Poster E

Massive parallelisation in Phonon transport calculations — •Robert Henrich, Michael Czerner, Michael Bachmann, and Christian Heiliger — I. Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany

In the last years a huge progress was archived in fabrication of nanostructured materials. Typical nano structures are super lattices, quantum dots, and nano tubes. For many applications in such structures the control of the heat flow is an essential issue. The heat flow is carried by electrons and phonons whereas in semi-conductors the phonon contribution dominates. The calculation of the phonon heat flow in nano materials is quite challenging: Although the underlying physics are the same as for bulk systems, the number of simulated atoms are much higher since in nano materials the assumptions of periodic boundary conditions in all directions does not hold. A common tool to calculate phonon transport is the so called atomistic Green's function method [1]. We present a method to calculate phonon transport in systems that contain millions of atoms within a reasonable time. For this task the most time consuming calculations in the atomistic greens function method has to be parallelized with MPI to handle the extreme huge matrices. Furthermore we are using GPU's as a co-processor to gain an enormous speed up for the matrixoperations.

[1], W.Fisher, T.Mingo, N.Numerical Heat Transfer, Part B: 2007, 51, 333

DS 38.11 Thu 17:30 Poster E

Semi ab initio phonon tunneling calculations in Au/Slab/Au by using non equilibrium Green's function formalism — •Saeideh Edalati Boostan, Michael Bachmann, Michael Czerner, and Christian Heiliger — I. Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany

Heat can be conducted across a nanometer-sized vacuum gap something that was deemed impossible until 2010 [1]. In this work we performed ab initio calculations using the abinit package to obtain the interatomic force constants of gold separated by a vacuum slab. These force constants are used in the non equilibrium Green's function formalism to calculate the transmission function and the temperature dependence of the thermal conductivity in the linear ballistic response regime [2, 3]. We analyze the phonon transport across the vacuum slab as a function of the thickness of the vacuum slab.

[1] Igor Altfeder, Andrey A. Voevodin, and Ajit K. Roy, Phys. Rev. Lett. 105, 166101 (2010)

[2] S. Datta, Electronic Transport in Mesoscopic Systems, Cambridge Univeristy Press (1995)

[3] P. E. Hopkins, P. M. Noris, M. S. Tsegaye, and A. W. Ghosh, J. Appl. Phys. 106, 063503 (2009)

DS 38.12 Thu 17:30 Poster E

Measurements at a Thermoelectric Nanowire Characterisation Platform (TNCP) — •D. Kojda[1], R. Mitdank[1], Z. Wang[2], M. Kröner[2], P. Woias[2], and S.F. Fischer[1] — [1]Neue Materialien, Humboldt-Universität zu Berlin, D-10099 Berlin — [2]IMTEK, University of Freiburg, D-79110 Freiburg

Nanowires are expected to improve the thermoelectric efficiency [1]. To date, the thermoelectric characterisation of a single nanowire involving the measurements of the Seebeck coefficient, the electrical and the thermal conductivity remains challenging.

For this purpose IMTEK designed the **T**hermoelectric **N**anowire **C**haracterisation **P**latform (**TNCP**), which was established by the means of silicon micromachining [2]. It contains two symmetric Si cantilevers where the nanowire takes place in between. Thin Pt microheaters on each cantilever create a temperature gradient.

Aiming to determine the platforms' characteristics, we measured the specific I-V-curves of the heater and the wire contact points in the temperature range between 5 K and 295 K. We detected the temperature-dependant resistance and the generated temperature difference as a function of power. Starting with a residual resistance of $54\,\Omega$, the heaters resistance increases linearly above 30 K up to $351\,\Omega$ at room temperature. Our next investigations will cover the applicability of dielectrophoresis in order to bridge the two cantilevers with a single wire.

[1] K. Nielsch *et al.*, Advanced Energy Materials, October 2011

[2] Z. Wang *et al.*, Transducers Conference, June 2011

DS 38.13 Thu 17:30 Poster E

Phase-Change materials as thermoelectrics — •Roland Sittner, Karl Simon Siegert, Felix Lange, and Matthias Wuttig — 1.Physikalisches Institut IA, RWTH Aachen, 52064 Aachen

Phase-change materials (PCMs) offer a unique combination of physical properties. They possess a high contrast in optical reflectivity and electrical resistivity and in addition a nanosecond switching capability between the amorphous and the crystalline state [1]. These properties make PCMs predestinated for the technological application in the field of data storage. Here they are already used as an active layer in rewritable optical data storage media (e.g. DVD±RW) and are promising candidates for the next generation of non-volatile electrical data storage applications (PRAM). Another potential field of application for PCMs are thermoelectrics (TEs). PCMs are close to common TE materials in their atomic composition and offer favourable low thermal conductivities in combination with high electrical conductivity values.

This work focuses on the potential of PCMs for thermoelectric applications by evaluating their figure of merit ZT. Several PC thin films were created by sputter deposition. The related physical properties κ, σ and S are measured with the 3ω method, the van der Pauw method and a self-made setup for determining the Seebeck coefficient. Special focus is set on the measurement of the thermal conductivity.

[1] Bruns et al., Appl. Phys. Lett. 95, 043108 (2009)

DS 38.14 Thu 17:30 Poster E

Thermal conductance of ballistic point contacts — •Alina Tittel, Thorben Bartsch, Christian Heyn, and Wolfgang Hansen — Institut für Angewandte Physik, Jungiusstr. 11, D-20355 Hamburg, Germany

We study the thermal conductance of ballistic point contacts that are realized as few nanometer long pillars. The pillars were fabricated using molecular beam epitaxy, with a combination of in situ local droplet etching and ex situ selective chemical wet-etching of a sacrificial layer [1]. They have typical length between 2 nm and 8 nm and diameters of about 100 nm. Because of the short pillar length, which is significantly smaller than the phonon mean free path up to room temperature, the thermal conductance is dominated by ballistic thermal transport. [2] The fabrication technique allows for control of composition, geometry and density of the pillars. Here we present investigations of the influence of such modifications on the thermal conductance. The measurements were performed with the 3w method.

[1] Ch. Heyn et al., Appl. Phys. Lett. 98, 033105 (2011). [2] Th. Bartsch et al. submitted , published on arXive: http://arxiv.org/abs/1111.1164

DS 38.15 Thu 17:30 Poster E

Magnesium- and fluorine co-doping of vanadium dioxide films — •Marc K. Dietrich, Andreas Laufer, Angelika Polity, and Bruno K. Meyer — I. Physics Institute, Justus-Liebig-University Gießen, Heinrich-Buff-Ring 16, 35392 Gießen, Germany

Thermochromic Mg- and F-doped VO_2 thin films, which enable new possibilities as an intelligent window coating, were deposited by rf sputtering. The appliance of VO_2 for energy efficient fenestration is so far limited by some properties of the bulk material. The alternation of luminous transmittance of bulk VO_2, which is caused by a reversible metal-semiconductor phase transition, will appear at temperatures about 68°C. By doping with Mg or F this transition temperature can be decreased to practical values. Furthermore, the Mg-doping level is associated with a blue shift of the band gap energy and is connected with an increase of luminous transmittance.

DS 38.16 Thu 17:30 Poster E

Doped Amorphous Si/Ge Nanostructured Thin Films via Glancing Angle Deposition — •Jens Bauer, Christoph Grüner, and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung, Permoserstrasse 15, D-04318 Leipzig, Germany

The preparation of efficient thermoelectric nanomaterials is a big challenge in modern material science. Key research fields are the defined adjustment of structure geometry, size and orientation on one hand and the structural material optimization on the other hand. For this purpose we present PVD investigations on self-organized a-Si and a-Ge nanostructures by a recent nanofabrication technique, the glancing angle deposition (GLAD). Nanostructure shape and distribution can be controlled via the geometrical deposition parameters, i.e. the polar and azimuthal particle incidence angle. Multicomponent nanomaterials as up-right nanocolumns with incorporated axial Si/Ge multiheterojunctions are realized by sequential deposition and a fast azimuthal rotation speed. For structural material customization the amorphous materials were passivated by atomic hydrogen. The hydrogen incorporation was verified via effusion tests, X-ray reflection, SIMS and FTIR measurements. Furthermore, in situ B and Sb doping was investigated. SIMS analyses showed high doping levels up to the solid solubility limits. Hydrogen effusion experiments revealed no difference between continuous films and GLAD nanostructures. However, B doping was found to strongly enhance the hydrogen release. Since hydrogen effusion started at temperatures >320℃ in a-Si without doping, with B doping hydrogen released already above room temperature.

DS 38.17 Thu 17:30 Poster E

Thermoelectric transport coefficients of bismuth compound nanomaterials — •Daniel Huzel[1,2], Heiko Reith[1,2], Matthias C Schmitt[1,2], Friedemann Völklein[1], and Michael Huth[2] — [1]IMtech, Hochschule RheinMain, Am Brückweg 26, D-65428 Rüsselsheim — [2]Physikalisches Institut, Goethe-Universität, Max-von-Laue-Str. 1, D-60438 Frankfurt am Main

Thermoelectric transport properties show a strong dependency on composition, crystallinity and geometric structure of a sample. With a decrease in size and dimensionality the conductivity decreases, therefore nanostructures are a promising field for materials / structures aiming at a high thermoelectric figure of merit (ZT).

Our work focuses on the determination of the thermoelectric transport coefficients of bismuth and bismuth compound nanowires. We present the Z-Chip, a platform for the combined measurement of Seebeck-coefficient, thermal and electrical conductivity on a single thermoelectric nanowire which allows the characterization of ZT of the wire. Results of bismuth telluride nanowires are shown but the measurement platform can be used for different nanostructures as well.

Additionally, a setup for the steady-state measurement of cross-plane thermal conductivity for embedded nanowires is demonstrated. Results obtained by this method are presented as well.

With regard to future applications, stability and reliability results on bismuth antimonide films are also shown.

DS 38.18 Thu 17:30 Poster E

In-plane thermal conductivity measurements of ZnO-, ZnS-, and YSZ thin-films on glass substrates — •David Hartung, Florian Gather, Achim Kronenberger, Florian Kuhl, Bruno K. Meyer, and Peter J. Klar — I. Physikalisches Institut, Justus-Liebig-University, Heinrich-Buff-Ring 16, 35392 Giessen

In this work we present in-plane thermal conductivity measurements of ZnO-, ZnS-, and YSZ thin-films. Borosilicate glass with a thickness of 50 microns and low thermal conductivity for improving the signal to noise ratio was used as substrate material. The above different films are deposited by rf-sputtering and have a thickness of about 1 micron. Our approach is a steady-state measurement. A wide metal wire on the film is used as a heater and two parallel lying narrow wires at distances of 100 microns and 200 microns from the heater wire, respectively, serve as the temperature sensors. The wire structure design is transfered on to the thin films by photolithography and metal evaporation. Measurements of the in-plane thermal conductivities of the above mentioned materials are presented and compared with corresponding results in the literature.

DS 38.19 Thu 17:30 Poster E

Investigation of the thermal conductivity of $\mathbf{ZnO_{1-x}S_x}$ thin films — •Florian Gather, Achim Kronenberger, Peter J. Klar, and Bruno K. Meyer — I. Physikalisches Institut, Justus-Liebig-University, Heinrich-Buff-Ring 16, 35392 Giessen

We investigated the thermal conductivity κ of rf-sputtered $ZnO_{1-x}S_x$ thin films. For a reliable measurement of the thermal conductivity of thin films, the 3ω-method is supposed to yield the best results. Measurements, performed using a self-constructed 3ω measurement system, show a reduced κ of the $ZnO_{1-x}S_x$ samples compared to bulk crystals. Using Raman spectroscopy we found indications for local phonon modes of oxygen in zinc-sulfide and sulphur in zinc-oxide, respectively. Presumably these local phonon modes cause the reduction of κ observed in the experiments.

DS 38.20 Thu 17:30 Poster E

Fabrication of a CuO/ZnO thin film thermoelectric generator — •Tobias Lind, Gert Homm, Peter J. Klar, Bruno K. Meyer, Achim Kronenberger, Torsten Henning, Daniel Reppin, and Stefan Lautenschlaeger — I. Physikalisches Institut, Justus Liebig University, Heinrich-Buff-Ring 16, 35392 Giessen

Cuprous oxide and zinc oxide are promising candidates for thermoelectric applications as an alternative to the well known Te-based thermoelectric materials, since they are stable up to high temperatures, environmentally friendly and available in abundance. A further advantage is their processability down to the micrometer range. Thin films of about 400 nm thickness were either CVD grown on MgO substrates or sputtered on glass substrates. These films were microfabricated by photolithography and wet chemical etching to create the p-type legs of a thermoelectric generator (TEG). In a second lithography and sputter depostion step the n-type legs of the TEG, created from 400 nm of ZnO, were placed in between the CuO legs to create the desired p-n-leg structure of the thermoelectric generator. The legs were connected by metallic microcontacts made from Ti/Au on ZnO or Au on CuO, respectively. First measurements of the thermoelectric voltage and the output power of the generator are presented.

DS 38.21 Thu 17:30 Poster E

Optimizing thermoelectric Properties: Microstructure Analysis of $\mathbf{Ag_{1-x}Pb_{18}Sb_{1+y}Te_{20}}$ — •Susanne Perlt[1], Thomas Höche[2], Jayaram Dadda[3], and Eckhard Müller[3] — [1]Leibniz Institute of Surface Modification, Leipzig — [2]Fraunhofer Institute for Mechanics of Materials, Halle — [3]German Aerospace Center, Institute of Materials Research, Köln

The feasible recovery of waste-heat energy as it is generated by industrial and vehicle engines has led to increasing research interest in thermoelectrics (TE). In order to get TE materials with high performance, i.e. with a large figure of merit ZT, one needs to tune electronic and phononic properties. A promising candidate is the quaternary compound $Ag_{1-x}Pb_{18}Sb_{1+y}Te_{20}$ (Lead-Antimony-Silver-Tellurium, LAST) for applications in the mid-temperature range. While the self-organized nanostructures assumed to act as phonon scatterers decrease the lattice thermal conductivity κ_L, the volume fraction of Sb and Ag and their ratio in the matrix have a significant influence on the electronic properties of the material. This study reports microstructure investigations at the micrometer and nanometer scale regarding SEM and TEM analysis, as well as measurements concerning TE properties. An attempt is made to derive a structure-property relationship.

DS 38.22 Thu 17:30 Poster E

Investigations on the $\mathbf{Ti_{0.5}Zr_{0.25}Hf_{0.25}NiSn_{1-x}Sb_x}$ system. — •Michael Schwall and Benjamin Balke — Institute of Inorganic Chemistry and Analytical Chemistry, Johannes Gutenberg - University, Mainz

Heusler compounds with $C1_b$ structure were reported from several groups in Asia and the USA as suitable for thermoelectric applications. Thereby, is the best published Figure of Merit $ZT = 1.5$ for a n-type material was found in the $Ti_{0.5}Zr_{0.25}Hf_{0.25}NiSn_{1-x}Sb_x$ system and presented by Toschiba and Toyota already in 2005. Since then, nobody was able o reproduce these results. Now, we were able to - almost - reach their high ZT values. In this study, we investigated the reasons for this outstanding thermoelectric properties in the $Ti_{0.5}Zr_{0.25}Hf_{0.25}NiSn_{1-x}Sb_x$ system. The effect of the microstructure on the transport properties will be described in details. The authors gratefully acknowledge the financial support by the "thermoHeusler" Project (Project No. 0327876D) of the German Federal Ministry of Economics and Technology (BMWi).

DS 38.23 Thu 17:30 Poster E

Nano structuring of $\mathbf{XCoSb}$ based Heusler compounds with $\mathbf{C1_b}$ structure as thermoelectric materials. — •Elisabeth Rausch, Michael Schwall, and Benjamin Balke — Institute of Inorganic Chemistry and Analytical Chemistry, Johannes Gutenberg - University, Mainz

This work reports on the experimental investigations of XCoSb (X= Ti, Zr or Hf) based Heusler compounds discussed as potential p-type thermoelectic materials. A lot of n-type materials are known and exhibt high ZT values (ZT_{max}=1.5), but there are only a few p-type materials which can achieve ZT values above 0.5. We tried to improve the thermoelectric properties by nano structring the materials. The samples were mechanical alloyed by means of a high energy ball mill. The thermoelectric properties could be enhanced due to the nano structuring of the material. We will present structural and physical properties of the synthized coumpounds including a complete high temperature thermoelectric characterisation. The authors gratefully acknowledge the financial support by the "thermoHeusler" Project (Project No. 0327876D) of the German Federal Ministry of Economics and Technology (BMWi).

DS 38.24 Thu 17:30 Poster E

Evolution of Si surface topography during ion beam erosion at high incidence angles — •Marc Teichmann, Jan Lorbeer, Frank Frost und Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstr. 15, D-04318 Leipzig

The self-organized pattern formation on Si(001) by low-energy ion beam sputtering at high incidence angels ($\alpha \geq 65$ deg) with and without sample rotation is studied.

At ion incidence angles between 65 deg and 85 deg, ripple patterns oriented perpendicular to ion beam direction evolve at low fluences. However, after a certain erosion time, isolated protuberances oriented parallel to the beam direction and with higher amplitude were formed. At a certain fluence the ripple structures vanish with increasing angle of incidence. The amplitude of these protuberances, or columnar structures increases continuously in the fluence range analyzed, i. e. up to $1.3 \times 10^{19}\,\mathrm{cm}^2$. These facets are suppressed if the samples are rotated where dot-like structures evolve. The height and size of the dots decreases with increasing rotational speed.

These observations suggest that the angle-dependent sputter yield Y is responsible for the formation of these columnar structures, that is also supported by TRIM.SP [1] calculations. At high angles the slope of the sputter yield curve is much larger than for small angles, i. e. small variations in the surface gradient produce large changes of Y and hence in the local erosion rate.

Support by DFG through FOR 845 is gratefully acknowledged.

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

DS 38.25 Thu 17:30 Poster E

Pattern formation on ion beam eroded quartz glass surfaces — •Jan Lorbeer, Marc Teichmann, Frank Frost, and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstr. 15, D-04318 Leipzig

The surface evolution quartz glass by low-energy ion beam erosion with and without simultaneous sample rotation is investigated. In detail the influence of the ion incidence angle ($\theta = 0-85$ deg), ion energy ($E_{ion} = 800 - 2000$ eV), ion species, fluence ($\Phi \approx 2 \times 10^{18} - 1.5 \times 10^{19}$ cm^{-2}) and speed of rotation ($N = 1/60 - 30$ rpm) were evaluated.

For the non-rotating samples ripple pattern starts to form at ion incidence angles between 40 and 50 deg. For increasing erosion times the ripple structures reveal a distinct faceting and coarsening. The faceting can be explained by gradient dependent sputtering as an important topography evolution mechanism on fused silica [1]. The observed surface coarsening is explained by the contribution of reflected ions resulting in an incessantly vanishing of smaller facets [2].

These experiments where repeated with substrate rotation. It is shown, that the size of the emerging surface features decreases with increasing speed of rotation. The correlation between the speed of rotation and the emerging pattern allows an insight to the associated time scale of the underlying mechanism and the growth kinetics.

Support by Deutsche Forschungsgemeinschaft through Forschergruppe 845 is gratefully acknowledged.

[1] J. Völlner et. al., J. Appl. Phys. **109**, 043501 (2011)

[2] W. Hauffe, Phys Status Solidi A **35**, K93 (1976)

DS 38.26 Thu 17:30 Poster E

Optical investigation of Au coated nanostructured surfaces — •Tammo Böntgen[1], Jan Lorbeer[2], Marc Teichmann[2], Frank Frost[2], Rüdiger Schmidt-Grund[1], Michael Lorenz[1], and Marius Grundmann[1] — [1]Universtät Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, Germany — [2]Leibniz-Institut für Oberflächenmodifizierung e.V., Permoserstr. 15, Leipzig, Germany

Nanoscale ripple pattern on SiO_2 and Al_2O_3 surfaces were formed with low-energy ion beam erosion ($E_{ion} < 2\,\mathrm{keV}$) at oblique ion incidence angles. Depending on process parameters (ion species, erosion time, ion energy,) ripple pattern with different wavelengths and amplitudes are formed. Using spectroscopic ellipsometry an anisotropy in the structures optical response was found. This anisotropy is only visible if the wavelength of the light is on the same scale as the periodicity of the pattern. By coating the surface with a thin gold film, the present plasmon resonances transfer the structural anisotropy to a dielectric anisotropy. This manifests in a shift of the resonance frequency depending on the in-plane orientation of the sample. For Au plasmonic structures deposited on patterned surfaces we found a distinct resonance frequency for k parallel and perpendicular to the ripple pattern. The wavelength of the pattern also affects the strength of the anisotropy. For structures with a wavelength of $\approx$100 nm only a very weak anisotropy is observed whereas the anisotropy is much stronger for structures with a shorter wavelength.

DS 38.27 Thu 17:30 Poster E

Saturation of Plastic Deformation by Swift Heavy Ion Irradiation: Ion Hammering vs. Surface Effects — •Redi Ferhati[1], Knut Dautel[1], Monika Fritzsche[2], and Wolfgang Bolse[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart — [2]Helmholtz-Zentrum Dresden-Rossendorf

Swift heavy ion (SHI) induced plastic deformation is a subject of current research and scientific discussion. This *Ion Hammering* phenomenon was first observed 30 years ago in amorphous materials like metallic glasses [1]. About 10 years ago, Feyh et al. [2] have shown that stress generation and *Ion Hammering* result in self-organization of thin NiO-films on Si-wafers into a sub-micron lamellae-like structure under grazing angle irradiation. The growth of the lamellae was found to saturate as soon as they have reached a thickness of a few hundreds of nm. Here we will show our latest results on the restructuring of pre-patterned thin oxide films by SHI under various irradiation conditions. The experiments were performed by employing (in-situ) scanning electron microscopy [3], and were complemented by (in-situ) energy dispersive x-ray analysis and atomic force microscopy. As we will show, the saturation behavior can be understood as a competition of *Ion Hammering* and surface energy effects, while the unexpected fact, that the initially crystalline films undergo *Ion Hammering* can possibly be attributed to oxygen loss and thus amorphization during irradiation. [1] S.Klaumünzer et al., Phys. Rev. Lett. 51 (1983), [2] W. Bolse et al., Appl. Phys. A77 (2003), [3] S. Amirthapandian et al., Rev. Sci. Instr. 81 (2010)

DS 38.28 Thu 17:30 Poster E

Manipulating the aspect ratio of Si surface nanopattern with low energy ion sputtering and reactive ion etching — Hans Hofsäss, •Kun Zhang, Ulrich Vetter, Omar Bobes, and Christoph Brüsewitz — II. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

A periodic self-forming surface nanostructure can be produced with low energy ion sputtering. The wavelength of such nanopattern can be controlled very well, by varying the energy and the incident angle of ion-beam. A low energy N_2^+ ion beam produces not only nanoripples on Si surface, but also forms a thin silicon nitride layer on the ridges of the ripples. This thin silicon nitride layer has a thickness from some nm to 20 nm (depending on the ion energy and the incident angle) and acts as an inert nanomask for reactive ion etching process, resulting in formation of deep grooves [1]. The depth of the grooves depends on the etching time. By combining the low energy N_2^+ ion beam sputtering and reactive ion etching, the formation of surface nanopattern with controllable average values of wavelength, ridge width and groove depth on Si surface can be realized. This surface nanostructured silicon with controllable features could be widely used in nanotechnology, including so-called black silicon for solar cells. Here, we will report on the formation of nanoripple patterns by low energy N_2^+ ion beam ($\leq$ 10keV), and the modification of these nanopatterns by reactive ion etching. In addition, the optical properties of the nanostructured silicon surfaces will be discussed. [1] V. K. Smirnov et al., Nanotechnology 14 (2003)709.

DS 38.29 Thu 17:30 Poster E

Ripple pattern formation on single crystalline magnesium oxide. — •Omar Bobes, Hans Hofsäss, and Kun Zhang — II. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Magnesium oxide MgO is a highly ionic bound crystal with cubic rock salt structure. Because of its high ionicity MgO is almost impossible to amorphize by ion irradiation. MgO could therefore act as a model system to investigate pattern formation by ion beam erosion on a crystalline substrate. Furthermore, the sputter yield is quite low and therefore MgO could be also a model system to investigate the role of sputtering itself for pattern formation. We have irradiated single crystalline MgO samples at 60° incidence angle with 1 keV Ar^+- and O_2^+-ions at room temperature. The sputter yield under these conditions is 3.5 for oxygen and 4.2 for magnesium. The maximum projected ion range is only about 3 nm. The as grown samples were flat with rms roughness < 0.7 nm. Only μm wide weak wavy structures could be seen in AFM. After irradiation with fluence of 1*10^{18} Ar/cm^2 a complex ripple structure with rms roughness of 5.3 nm and maximum ripple amplitudes of 10-20 nm are observed. The pattern consists of ripples with up to 400 nm in length oriented perpendicular to the projected ion beam direction. The width of the ripples varies between about 30 nm and 100 nm. For O_2^+-irradiation, dot-pattern appears at the ion fluence of 1*10^{18} Ar/cm^2. With increasing the ion fluence, these dots tend to orient along the direction perpendicular to ion-beam. The pattern formation is discussed based on existing models.

DS 38.30 Thu 17:30 Poster E

Influence of Phase Separation for Surfactant Driven Pattern Formation during Ion Beam Erosion — Hans Hofsäss, •Kun Zhang, Ulrich Vetter, Omar Bobes, Andre Pape, Hans-Gregor Gehrke, and Marc Brötzmann — II. Phys. Institut, Uni Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

We will present results on metal surfactant driven self-organized pattern formation on surfaces by ion beam erosion, with a focus on the role of phase separation for the initial steps of pattern formation. Si substrates were irradiated with 5 keV Xe ions at normal incidence and ion fluences up to 5*10^{17} Xe/cm^2 under continuous deposition of surfactant atoms. In the absence of such surfactants uniform flat surfaces are obtained, while in the presence of Fe and Mo surfactants pronounced patterns like dots, combinations of dots and ripples with wavelengths around 100 nm are generated [1]. The surfactant coverage and deposition direction determine the pattern type and the pattern orientation, respectively. A critical steady-state coverage for onset of dot formation and onset of ripple formation is in the range of 10^{15} and 5*10^{15} /cm^2. The steady-state surface region consists of a thin amorphous metal silicide layer with high metal concentration in the ripple and dot regions. Pattern formation is explained by ion induced diffusion and phase separation of the initially flat amorphous silicide layer and subsequent ion beam erosion with composition dependent sputter yield. To investigate the role of initial phase separation we additionally compare the pattern formation for different other metal surfactants. [1] H. Hofsäss et al., New J. Phys. 13 (2011) 013033

DS 38.31 Thu 17:30 Poster E

Transport anisotropy of $LaAlO_3$/$SrTiO_3$ interfaces on chemically patterned $SrTiO_3$ — •Michael Foerster[1], Romain Bachelet[1], Vladimir Laukhin[1,2], Josep Fontcuberta[1], Gervasi Herranz[1], and Florencio Sanchez[1] — [1]Institut de Ciència de Materials de Barcelona ICMAB-CSIC, Campus de la UAB, 08193 Bellaterra, Catalonia, Spain — [2]Institució Catalana de Recerca i Estudis Avançats (ICREA), 08010 Barcelona, Catalonia, Spain

A few years ago high mobility electronic transport was found at the interface between the wide bandgap insulators $SrTiO_3$ and $LaAlO_3$ [1]. This conductive layer is confined to a few unit cells around the interface and it appears when $LaAlO_3$ layers with thickness above 3-4 unit cells are grown on $SrTiO_3$. It is known that TiO_2/LaO interfaces are conductive, while SrO/AlO_2 interfaces are insulating.

Here we exploited this way to control the interface properties to produce large scale functional nanostructures. TiO_2/AlO - SrO /LaO_2 modulated interfaces have been prepared using thermally treated $SrTiO_3$ surfaces with self-organized patterned chemical termination. The interface transport properties are found to be controlled according to these interface patterns. While the influence of the interface topology, e.g. terrace steps, is negligible, a strong transport anisotropy is observed when large-scale well oriented chemical patterns are realized. Our results show that bottom-up engineering of the interface chemical composition is a suitable strategy to influence the transport properties on large scales.

References [1] A. Ohtomo and H.Y. Hwang, Nature 427, 423 (2004).

DS 38.32 Thu 17:30 Poster E

Deposition of ZnO on Micro-structured Electrodes for the Characterization as a Field Effect Transistor — •Martina Stumpp, Christopher Keil, and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen

Zinc oxide (ZnO) films were electrodeposited in pulses of controlled current on micro-structured silver and gold electrodes on insulating SiO_2 on Si wafers using aqueous solutions of 0.1 M $Zn(NO_3)_2$. The growth of ZnO crystals on top of the metal fingers and between the fingers on the SiO_2 was analyzed. In some cases the film deposited between the fingers was conductive enough to even induce deposition on neighboring fingers which were not connected to the potentiostat. Depending on the applied current density, a different concentration profile of the precursors in solution was established leading to ZnO films with different surface morphologies. The deposited ZnO within the gaps of the microstructures formed a thin semiconducting film which subsequent to the deposition served as active layer of a field-effect transistor (FET). Electrical measurements were performed in different environments, in order to characterize the efficiency of the ZnO layer as a transistor channel.

DS 38.33 Thu 17:30 Poster E

Diffusion-controlled Electrochemical Growth of Porous ZnO on μ-structures — •Christian Lupo and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen

Porous ZnO films were prepared by electrochemical deposition on interdigitated microstructures of gold-, silver- or platinum band electrodes. The electrodeposition was realized at a constant electrode potential of a rotating electrode from an aqueous $ZnCl_2$ solution in the presence of the xanthene dye $EosinY$. The deposition conditions were kept constant, except the deposition time and the rotation speed. The interdigital electrode size, gap width and the number of electrode bands were varied. The growth of ZnO was characterized by the observed deposition current and by scanning electron microscopy. The comparison with a model of spherical diffusion reveals limitations of mass transport towards the edges of the bands during extended growth. Application of this model to the process of electrochemical deposition provides useful contributions to the further development towards a controlled growth of semiconducting oxide films on microelectrodes. Additional options and limitations of the model in this respect will be discussed.

DS 38.34 Thu 17:30 Poster E

Plasma functionalization of self-organized Polystyrene Nanospheres — •Lienhard Wegewitz[1], Alexandra Prowald[2], Sebastian Dahle[1], Oliver Höfft[2], Frank Endres[2], and Wolfgang Maus-Friedrichs[1] — [1]Institut für Energieforschung und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany — [2]Institut für Mechanische Verfahrenstechnik, TU Clausthal, Arnold-Sommerfeld-Str. 6, 38678 Clausthal-Zellerfeld, Germany

Polystyrene nanospheres are currently under investigation as litography masks and templates for the production of hollow inorganic spheres which have promising applications in catalysis and energy storage. In this regard the chemical functionalization and stabilization of the polystyrene framework is crucial.

Thin films of ordered polystyrene nanospheres with diameters of about 600 nm have been exposed to dielectric barrier discharges in different atmospheres and were subsequently chemically treatet in DMDCS and OMCTS. For the investigation of each treatment X-Ray Photoelectron Spectroscopy (XPS) and Atomic Force Microscopy (AFM) are applied. The plasma treatment of the spheres in oxygen yields a significant increase of carbon-oxygen bonds at the surface whereas a silane-plasma covers the spheres with a closed silicon nitride layer. After the wet chemical treatment silicon dioxide is detectable at the surface. Furthermore first experiments of electrochemical deposition with modified nanospheres as substrate will be shown.

DS 38.35 Thu 17:30 Poster E

Nanopatterning by molecular polygons — •Stefan-Sven Jester, Eva Sigmund, and Sigurd Höger — Rheinische Friedrich-Wilhelms-Universität Bonn, Kekulé-Institut für Organische Chemie und Biochemie, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany

Self-assembled monolayers of shape-persistent macrocycles at the solid/liquid interface (here: 1,2,4-trichlorobenzene/HOPG) are investigated by scanning tunneling microscopy. The macrocycles are accessible from cyclooligomerization of the respective half-rings and subsequent separation of the respective crude product. The chemical structure includes dithiophene corner units connected via linear phenylene-ethynylene-butadiynylene rod units. The resulting cyclooligomers (of oligomerization degree n = 3-6) can be viewed as equilateral two-dimensional polygons with three to six sides and diameters in the range of 2-5 nm. The distinct shapes allow the formation of predictable surface patterns with lateral periodicities of up to 19 nm. The results include the 2D crystallization of molecular pentagons as well as the formation of binary mixtures of triangles and hexagons and thus provide an insight into how the symmetry of molecules is translated into periodic structures. [1] S.-S. Jester, E. Sigmund, S. Höger, *J. Am. Chem. Soc.* **2011**, *133*, 11062.

DS 38.36 Thu 17:30 Poster E

Phase Change of Tetrahedral Amorphous-Carbon by Low Energy Electrons in a Scanning Tunnelling Microscope — •Frederik Klein and Thomas Mühl — Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden

Low energy electron-based energy deposition in tetrahedral amorphous-carbon thin films by a scanning tunnelling microscope leads to a local phase change of the carbon. Both the mass density and the electrical resistivity are reduced indicating a graphitization. We expose nano-sized surface areas to field emitted low energy electrons under high vacuum conditions and investigate the temperature and electron energy dependence of the carbon phase change process. Supplementary topography measurements are performed by atomic force microscopy.

DS 38.37 Thu 17:30 Poster E

Deep X-Ray Lithography at DELTA — •Thorsten Brenner, Daniela Lietz, Michael Paulus, Christian Sternemann, and Metin Tolan — Technische Universität Dortmund/DELTA, 44221 Dortmund, Germany

DELTA (Dortmund, Germany) is a synchrotron light source with a electron energy of 1.5 GeV and a maximum current of 130 mA. DELTA beamline BL-1 is dedicated to deep x-ray lithography (DXRL). DXRL is a method to produce various microstructures with a height up to several millimeters. Microstructures are applied in optics, micro mechanics, fluidic, or medical devices. It is possible to reach a high aspect ratio of about 100 and a lateral resolution up to $2\,\mu$m for microstructures using DXRL [1]. A well-established process for production of microstructures using lithography is the LIGA process. It includes the process steps (xray) lithography, electroplating, and molding. The aim is to produce microparts with high quality. For that reason silicon wafers with SU-8 photoresist are exposed and chemically developed. Here, process parameters (x-ray spectrum, mask types, dose, post exposure bake) are tuned for optimization of exposure process. SEM images are made to determine aspect ratio, roughness of surfaces and walls and adhesion between substrate and resist. Furthermore, a new endstation for BL-1 at DELTA is under construction. Here, improvements for the exposure process are of central interest.

[1] V. Saile, U. Wallrabe, O. Tabata, J.G. Korvink, O. Brand, G.K. Fedder, C. Hierold (Eds.):, LIGA and its applications, Wiley-VCH (2009).

DS 38.38 Thu 17:30 Poster E

Simulation-free determination of structural grating parameters with GISAXS — •Jan Wernecke, Michael Krumrey, and Frank Scholze — Physikalisch-Technische Bundesanstalt (PTB), Abbestr. 2-12, D-10587 Berlin

New technologies such as next-generation semiconductor and lithography techniques rely on complex surface structures with characteristic dimensions in the nanometre range. The functionality of such structures depends greatly on their feature size, thus, dimensional nanometrology is essential for precise control of nanostructured devices. Grazing Incidence Small Angle X-ray Scattering (GISAXS) is a tool for non-destructive length measurement in the nanometre range. Structure parameter retrieval from GISAXS scattering data generally requires simulation of the morphology due to the loss of phase information during image acquisition. Here we present an approach to obtain dimensional parameters of highly ordered surface structures directly from the scattering data without the need of simulation. Line gratings have been investigated with GISAXS and important parameters such as line and groove width, etching depth and period length can be obtained from scattering images by Fourier transformation. The analysis method was applied to different test grating structures as well as to simulated scattering patterns for validation. The experiments were performed at the Four-Crystal Monochromator (FCM) beamline in the PTB laboratory at the electron storage ring BESSY II using the SAXS setup of the Helmholtz-Zentrum Berlin (HZB).

DS 38.39 Thu 17:30 Poster E

Hierarchical Fabrication of Gecko-Mimicking Nano- and Microstructures by Hot Embossing and Hot Pulling — •Guénola Etienne, Michael Röhrig, Farid Oulhadj, Marc Schneider, Matthias Worgull, and Hendrik Hölscher — Karlsruher Institut für Technologie, Institut für Mikrostrukturtechnik, Postfach 3640, 76021 Karlsruhe, Deutschland

Hierarchical dry adhesives have been fabricated by hot embossing and hot pulling. Three levels of hierarchy mimic the gecko*s tiny tilted hairs which ramify into smaller structures covering its toes. Gecko-like adhesives offer a large amount of interesting applications, like pick-and-place systems or adhesive bandages inside the human body. However, such products have to be cost-effectively fabricated on large areas. This can be achieved by three-fold hierarchical dry adhesives, fabricated by hot embossing and hot pulling. These techniques enable the large-area fabrication of delicate polymer fibrils with high aspect ratios and diameters in the nanometer range. The fabricated structures are very compliant and achieve a high real contact area even to rough substrates. This causes high adhesion originating from van-der-Waals forces.

DS 38.40 Thu 17:30 Poster E

Laser thinning of titanium foils — •Regina Moser, Adrian Zacherle, Gerhard Heise, and Heinz Huber — Munich University of Applied Sciences, Lothstrasse 34, 80335 Munich, Germany

Electron beam guns with powers of approximately 100 kW are used for drying printing colors. The exit window for the electron beam consists of a 10 um thin titan foil. By thinning this window, electron transmission can be increased reducing the required acceleration voltage and power consumption for the electron gun. In fact, the minimal achievable thickness in an industrial rolling process is about 10 um. To keep the thin foils vacuum proof and to retain their mechanical stability, we are reducing the foils thickness locally using ultra short pulse laser ablation. For this purpose, different overlap values, fluencies and structuring strategies as well as sample mounting methods are examined to reduce foil thickness maintaining optimal surface quality and suppressing the observed foil benching.

DS 38.41 Thu 17:30 Poster E

Towards nanofocusing of attosecond XUV pulses — •Christian Späth[1], Alexander Guggenmos[2], Soo Hoon Chew[1], Kellie Pearce[1], Michael Hofstetter[2], Jürgen Schmidt[1], and Ulf Kleineberg[1] — [1]Ludwig-Maximilians-Universität München, Fakultät Physik, 85748 Garching — [2]Max-Planck-Institut für Quantenoptik, 85748 Garching

Attosecond pulses are finding more and more applications in measuring electron dynamics in atoms and molecules as well as electronic phenomena at surfaces and nanostructures. Nanofocusing of such pulses, for intensity enhancing at the sample position or for microscopic investigations, has not been successfully performed yet. We report on first towards diffractive polychromatic nanofocusing optics for XUV pulses at 90 eV photon energy.

Circular and elliptical zone plate structures have been written by advanced e-beam lithography in different resists (PMMA and HSQ) on ultrathin Si3N4 membrane windows.

Combining diffractive with refractive lenses on the same element results in increased usable bandwidth as required for focusing of sub femtosecond pulses. We will discuss the capabilities and limitations of these new optics and report first steps towards their experimental fabrication.

DS 38.42 Thu 17:30 Poster E

Damage formation in SiC ion implanted at 625 K — Elke Wendler[1], •Philipp Schöppe[1], Thomas Bierschenk[1], Steffen Milz[1], Werner Wesch[1], Nick G. van der Berg[2], Erich Friedland[2], and Johan B. Malherbe[2] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Physics Department, University of Pretoria, 0002 Pretoria, South Africa

Damage formation in 4H-SiC during ion implantation at 625 K is studied applying Rutherford backscattering spectrometry (RBS) in channeling configuration. For comparison two selected samples are analysed by cross section transmission electron microscopy (TEM). The results for dual implantation of the self-ions Si and C with the ratio 1:1 are compared with those obtained for Ag ion implantation. It is found that the evolution of damage as a function of the number of displacements per lattice atom proceeds in two steps and is almost independent of the ion species implanted. The second significant increase of the damage concentration starts obviously when the relative volume increase introduced by the implanted ions exceeds a critical value of about $6 \cdot 10^{-3}$. The damage produced at high ion fluences consists of point defect clusters and, probably, extended defects.

DS 38.43 Thu 17:30 Poster E

Ion beam induced density changes and plastic phenomena — Tobias Steinbach, •Emanuel Schmidt, Aaron Reupert, Mathias Schmidt, and Werner Wesch — Institute of Solid State Physics, Friedrich Schiller University Jena

Conventional ion irradiation is a well-established standard doping method in semiconductor processing for effective modification of electrical, mechanical, optical and chemical properties. However, in the low energy range the ions are stopped mainly by elastic scattering with the lattice atoms, which results in the displacement of target atoms and consequently in lattice damage. This ion beam induced damaging and amorphization process is accompanied by three different radiation-induced deformation phenomena: densification, radiation enhanced viscous flow and anisotropic deformation. The change of stress associated with these effects can be investigated during irradiation by observing the bending of freestanding thin crystalline samples by means of an in situ scanning laser reflection technique, which was recently established at the FSU Jena. We present ion beam induced stress evolution as a function of fluence for the irradiation of semiconductors (Ge and Si) as well as for insulators ($LiNbO_3$). In case of Ge and Si, the formation and relaxation of stress will be discussed as a function of fluence, nuclear energy deposition, projected ion range and irradiation temperature. In addition, the significant stress increase during beam interruption will be explained. In $LiNbO_3$, the observed stress evolution depends on the crystallographic orientation and will be discussed based on the preferential rearrangement of displaced lattice atoms.

DS 38.44 Thu 17:30 Poster E

Ion beam nano-patterned surfaces as biomaterials — •Falk Wyrwa, Steffanie Kosan, Jessica Hönig, Raphael Niepelt, Jana Sommerfeld, and Carsten Ronning — Institute of solid state physics, Friedrich Schiller University of Jena, Helmholtzweg 3, 07743 Jena

We prepared wave-like ripple structures in the nanometer scale on silicon and titanium dioxide substrates using low energy sputtering with nobel gas ions. The ions were accelerated up to 20 keV hitting the target with a specific angle about 70° to the surface normal. Different ripple wavelengths and amplitudes could be achieved by varying the acceleration energy and the erosion time, which will lead to new surface characteristics without changing the chemical stoichiometry. Especially a different adsorbent behavior for protein molecules was established, which also depends on the substrate material itself. Motivated by the many possibilities to apply silicon and titanium dioxide in the biomedical field, we investigated their interaction with the biological environment, which will be presented in this contribution.

DS 38.45 Thu 17:30 Poster E

Scanning ion irradiation of polyimide films — •Stefan Lücken, Yuri Koval, and Paul Müller — Department of Physics and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg

Recently we found, that the surface of nearly any polymer can be converted into conductive material by low energy ion irradiation. The graphitized layer consists of nanometer sized graphene and graphite flakes [1]. In order to enhance the conductivity and to increase the size of the flakes we applied a novel method of scanning irradiation [2]. We investigated the influence of various irradiation parameters on the conductivity of the graphitized layer. We show, that the conductance vs. temperature can be described in terms of weak Anderson localization. At approximately 70 K, a crossover occurs from 2-dimensional to 3-dimensional behavior. This can be explained by a decrease of the Thouless length with increasing temperature. The crossover temperature can be used to estimate the thickness of the graphitized layer.

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

[2] S. Lücken Scanning irradiation of polyimide by low-energy Ar ions Diplomarbeit, Erlangen (2011)

DS 38.46 Thu 17:30 Poster E

Modification of diamond-like carbon by ion irradiation — •Hanna Bukowska[1], Benedict Kleine Bussmann[1], Dirk Walecki[1], Florian Meinerzhagen[1], Marc Brötzmann[2], Hans-Gregor Gehrke[2], Hans Hofsäss[2], and Marika Schleberger[1] — [1]Universität Duisburg-Essen, Fakultät für Physik, Lotherstraße 1, 47057 Duisburg, Germany — [2]Universität Göttingen, Fakultät für Physik, Bunsenstraße 13, 37073 Göttingen, Germany

Diamond-like carbon (DLC) films were irradiated with swift heavy ion beams of varying energy and angles of incidence. The irradiation created electrically conducting tracks in the DLC-films by transforming sp^3 into sp^2 bonds. The DLC-films were analyzed by conductive atomic force microscopy. The images were used to identify ion impact sites, and I-V-Spectroscopy was applied to determine the conductivity of the tracks. High energy ions (2,2 GeV, Au^{25+}) created tracks with ohmic conductivity in the case of perpendicular bombardment, whereas grazing irradiation results in tracks that show mainly tunneling behavior. Low energy ions (100 MeV, Xe^{23+}) created tracks which exhibit tunneling behaviour after perpendicular incidence irradiation, but irradiation under 1° did not result in conductive tracks.

DS 38.47 Thu 17:30 Poster E

Monte Carlo Simulations of Silicon Sputtering by Argon Ions and an Approach for Comparison with Molecular Dynamic Results — René Feder, Frank Frost, Stefan G. Mayr, Horst Neumann, and •Carsten Bundesmann — Leibniz-Institut für Oberflächenmodifizierung e.V., Permoserstr. 15, 04318 Leipzig, Germany

Ion beam sputter processes deliver some intrinsic features influencing the growing film properties. Utilisation of these features needs to know how primary ion properties and geometrical process conditions influence the energy and spatial distribution of the sputtered and scattered particles. Beside complex experiments simulations are helpful to explain the correlation between primary parameters and thin film properties.

The paper presents first results of two simulation codes with completely different approaches: Monte Carlo (MC) calculations with help of the well known TRIM.SP code [1] and Molecular Dynamics calculations with an in-house developed code. First results of both simulation principles are compared for Argon ion bombardment on a Silicon target. Furthermore, a special experimental setup is outlined for validation of modelling. The setup allows the variation of ion beam parameters (ion species, ion energy, ion incidence angle on the target) and the measurement of the properties of sputtered and scattered particles.

Financial support by DFG within project BU2625/1-1 is gratefully acknowledged.

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

DS 38.48 Thu 17:30 Poster E

Tuning the conductivity of vanadium dioxide films by swift heavy ion irradiation — •Paul Ehrhardt[1], Hans Hofsäss[1], Hans-Gregor Gehrke[1], Johann Krauser[2], Christina Trautmann[3], and Shriram Ramanathan[4] — [1]II. Physikalisches Institut, Fakultät für Physik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Hochschule Harz, University of Applied Sciences, Friedrichstraße 57-59, 38855 Wernigerode, Germany — [3]Gesellschaft für Schwerionenforschung, Planckstrasse 1, 64291 Darmstadt, Germany — [4]Harvard School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, USA

We demonstrate the generation of a persistent conductivity increase in vanadium dioxide thin films by irradiation with swift heavy ions at room temperature. VO2 undergoes a temperature driven metal-insulator-transition (MIT) at 67 °C. After the ion irradiation the conductivity of the films we observe a strong increase in conductivity below the transition temperature proportional to the ion fluence. This change in conductivity is persistent and remains after several cycles of heating. Low temperature measurements down to 15 K show no further MIT below room temperature. Although the conductivity increase after irradiation at such low fluences is due to single ion track effects, atomic force microscopy (AFM) measurements do not show surface hillocks, which are characteristic for ion tracks in other materials. AFM measurements with conducting tip give no evidence for conducting ion tracks but indicate the existence of conducting regions around poorly conducting ion tracks, possible due to stress generation.

DS 38.49 Thu 17:30 Poster E

Ion beam assisted deposition of nano-structured C:Ni films — G. Abrasonis[1], M. Krause[1,2], A. Mücklich[1], R. Heller[1], K.-H. Heinig[1], •S. Gemming[1], and W. Möller[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany. — [2]Institute of Physics,TU Dresden, Dresden, Germany.

Nanostructures influence material properties dramatically due to size, shape and interface effects. Thus the control of the structure at the nanoscale is a key issue in nanomaterials science. The interaction of hyperthermal ions with solids is confined to the nanometer scale. Thus, it can be used to control the morphology evolution during multiphase film deposition. Ion-induced displacements occur in a thin surface layer of the growing film where they increase the atomic mobility for the phase separation. Here the growth-structure relationship of C:Ni (˜15 at.%) nanocomposite films grown by oblique incidence (˜45°) ion beam assisted deposition is reported. The influences of the flux of an assisting Ar+ ion beam (0-140 eV) as well as of an elevated substrate temperature have been studied. The formation of elongated nickel nanoparticles is strongly promoted by the ion beam assistance. Moreover, the metal nanocolumns no longer align with the advancing surface, but with the incoming ions. A window of conditions is established within which the ion assistance leads to the formation of regular composition modulations with a well defined periodicity and tilt. As the dominating driving force for the pattern formation is of physical origin, this approach might be applicable to other immiscible systems.

DS 39: Resistive switching I (jointly with DF, KR, HL)

Time: Friday 9:30–10:45 Location: H 0111

DS 39.1 Fri 9:30 H 0111

Ab-initio studies of metal-insulator transitions in defective perovskites — •Gustav Bihlmayer and Kourosh Rahmanizadeh — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Resistive switching in perovskite materials can be triggered by a variety of external stimuli, like electric fields or oxygen partial pressure. While the role of oxygen defects for the electronic transport is in many cases established, the nature of the metal-insulator transition has still to be explored. Density functional theory calculations including strong correlation effects on a model level can help to gain an understanding here.

We investigate the transition between an insulating state of a correlated, localized level and a partially filled conductive band as function of electron concentration. The band filling can be controlled in a chemical way or via electric fields. A ferroelectric polarization can screen or enhance the effects at the boundaries of a ferroelectric material. We study the localization of defect states in model systems of structurally simple perovskites like $SrTiO_3$ or $PbTiO_3$ to gain a coherent picture of the conductive states that are manipulated in the resistive switching process.

Financial support of the EU grant NMP3-LA-2010-246102 (IFOX) is gratefully acknowledged.

DS 39.2 Fri 9:45 H 0111

Elucidation of the resistive switching in $SrTiO_3$ MIM-structures by μXANES — •Christian Lenser[1,2], Alexei Kuzmin[3], Alexandr Kalinko[3], Juris Purans[3], Rainer Waser[1,2,4], and Regina Dittmann[1,2] — [1]Peter Grünberg Institut 7, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Jülich-Aachen Research Alliance, Section Fundamentals of Future Information Technology (JARA-FIT), Germany — [3]Institute of Solid State Physics, University of Latvia, Kengaraga Street 8, LV- 1063 Riga, Latvia — [4]Institut für Werkstoffe der Elektrotechnik, RWTH Aachen, 52056 Aachen, Germany

The resistive switching effect in Fe-doped $SrTiO_3$ thin films is investigated on 100 μm^2 metal-insulator-metal (MIM) structures by chemical mapping in the μm regime. X-ray absorption fine structure (XAFS) - measured at beamline ID03, ESRF - with a x-ray beam focused to several μm provides information about the absorption fine structure modulations at the Fe K-edge. The increase of pre-edge intensity characteristic of oxygen vacancies in the first coordination shell of the transition metal dopant shows the films to be highly oxygen deficient after growth. In addition to an increase of the $\text{Fe-V}_O^{\bullet\bullet}$ concentration over the whole electrode area after electroforming, μm-sized mapping of a MIM-structure reveals the location of the conducting filament by a strong local change in the absorption edge, which is localized to a size of the order of 1 μm. The change of the absorption characteristics is interpreted with full multiple-scattering XANES simulations, suggesting oxygen vacancy clustering around Fe as the likely explanation.

DS 39.3 Fri 10:00 H 0111

A ferroelectric switchable tunnel junction: $KNbO_3/SrTiO_3$ — •Kourosh Rahmanizadeh, Gustav Bihlmayer, Daniel Wortmann, and Stefan Blügel — Peter Grünberg Institut (PGI-1) & Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The properties of thin oxide films and multilayers are strongly influenced by defects and, therefore, can be controllably tuned by the defect concentration at the interface. For example, due to the charge discontinuity at the $SrTiO_3$/KO-$KNbO_3$-NbO_2/$SrTiO_3$ interface only one direction of polarization in $KNbO_3$ film is stable. A switchable polarization in $KNbO_3$ can be realized by creating (oxygen) defects at the interfaces.

We carried out density functional theory (DFT) calculations based on the full potential linearized augmented planewave (FLAPW) method as implemented in the `FLEUR` code [1] for studying the polar interface $SrTiO_3/KNbO_3$ and a $SrRuO_3/SrTiO_3/KNbO_3$ tunnel junction. The electronic transport properties of the switchable multiferroic $SrRuO_3$/$SrTiO_3$/KO-$KNbO_3$-NbO_3/$SrTiO_3$/$SrRuO_3$ heterostructure have been investigated using an embedded Green-function approach [2]. A strong dependence of the (magneto electric) transport properties on the polarization is observed. The work was conducted under the auspices of the IFOX consortia under grant agreement NMP3-LA-2010-246102.

[1] http://www.flapw.de

[2] D. Wortmann, H. Ishida, and S. Blügel, PRB **66**, 075113 (2002)

DS 39.4 Fri 10:15 H 0111

Resistive switching in different forming states of Ti/ $Pr_{0.48}Ca_{0.52}MnO_3$ junctions — •Chanwoo Park[1], Anja Herpers[1], Rainer Bruchhaus[1], Johan Verbeeck[2], Ricardo Egoavil[2], Francesco Borgatti[3], Giancarlo Panaccione[4], Francesco Offi[5], and Regina Dittmann[1] — [1]PGI-7, FZ Jülich — [2]EMAT, University of Antwerp, Belgium — [3]ISMN-CNR, Bologna, Italy — [4]Laboratorio Nazionale TASC-INFM-CNR, Trieste, Italy — [5]CNISM and Dipartimento di Fisica, Università Roma Tre, Rome, Italy

We investigated the resistive switching (RS) characteristics of Ti/$Pr_{0.48}Ca_{0.52}MnO_3$ (PCMO) junctions. RS characteristics were observed after a first forming (1stF) procedure, which changes the initial resistance state to a high resistance state (HRS) which shows a clear area dependence. By performing Hard X-ray Photoelectron Spectroscopy for different resistive states, we found a change of the Ti2p peak intensity after the 1stF which is associated with the formation of TiO_2 at the interface. Moreover, the shape and position of the Mn2p peak hints on the reduction of Mn. The formation of TiO_x at the Ti/PCMO interface after the 1stF was confirmed by cross-sectional Transmission Electron Microscope investigations. The results indicate that the 1stF step is related to a redox process at the Ti/PCMO interface. Moreover, we were able to perform a second forming step which changes the HRS to the low resistance. The area dependence disappeared after the second forming. This implies that conducting filaments might form at the Ti/PCMO interface.

DS 39.5 Fri 10:30 H 0111

Remanent resistance changes in metal- PrCaMnO-metal sandwich structures — •Malte Scherff, Bjoern Meyer, Julius Scholz, Joerg Hoffmann, and Christian Jooss — Institute of Materials Physics, University of Goettingen, Germany

The non-volatile electric pulse induced resistance change (EPIR) seems to be a rather common feature of oxides sandwiched by electrodes. However, microscopic mechanisms are discussed controversially. We present electrical transport measurements of sputtered $Pr_{0.7}Ca_{0.3}MnO_3$ films sandwiched by metallic electrodes with variation of electrode materials, device geometry and PCMO deposition parameters. Cross-plane transport measurements have been performed as function of temperature and magnetic field. Specifically, the transition from dynamic resistance changes due to non-linear transport to remanent switching is analyzed. By analyzing changes of magnetoresistance at low temperatures in different resistance states we aim for separation between interface and film contributions to switching. Comparing switching behavior in symmetric and asymmetric electrode configuration allows for identification of the active, single interface in the switching process and the origin of an observed switching polarity inversion[1]. The influence of excitation field and power on the switching characteristics of different noble metal electrodes is discussed. Samples from macroscopic devices and in situ stimulated sandwich structures were studied in a transmission electron microscope in order to investigate the induced structural, chemical and electronic changes. [1] M. Scherff et al, J.Appl.Phys. 110, 043718 (2011)

DS 40: Resistive switching II (jointly with DF, KR, HL)

Time: Friday 11:00–12:30 Location: H 0111

DS 40.1 Fri 11:00 H 0111

Resistive switching mechanism of Ti/HfO$_2$/TiN RRAM cells studied by nondestructive hard x-ray photoelectron spectroscopy — •Małgorzata Sowińska[1], Thomas Bertaud[1], Damian Walczyk[1], Christian Walczyk[1], Sebastian Thiess[2], Wolfgang Drube[2], and Thomas Schroeder[1] — [1]IHP, Im Technologiepark 25, 15236 Frankfurt/Oder, Germany — [2]DESY, Notkestrasse 85, 22607 Hamburg, Germany

A variety of different metal-insulator-metal (MIM) multilayered structures reveal reversible changes in resistance upon applying bias voltages across the layers. The physical mechanism of this resistive switching effect in such MIM cells is mostly unknown up to nowadays, although different models depending on the switching behaviour (unipolar or bipolar) and the conducting path type (filamentary or interface) have been proposed. In order to identify whether the resistance variation in the Ti/HfO$_2$/TiN system is related to local changes in the chemistry or to charge distribution we performed ex-situ and in-situ hard x-ray photoelectron spectroscopy (HAXPES) studies. This technique is well suited for investigating the buried interface of our resistive random access memory (RRAM) cell in a nondestructive way. In result, spectral differences observed between as-deposited and electrically switched devices lead us to the conclusion that the Ti/HfO$_2$ interface was modified, which can be associated with an interface-type model. Furthermore, we have also better revealed the impact of the current compliance on the HAXPES spectra of our device.

DS 40.2 Fri 11:15 H 0111

Pulse-induced resistive switching of CMOS embedded HfO$_2$-based 1T1R cells — •damian walczyk, christian walczyk, thomas bertaud, małgorzata sowińska, mindaugas lukosius, steffen kubotsch, thomas schroeder, and christian wenger — IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany.

Low-cost embedded nonvolatile memories (eNVMs) with high-density, high-speed, and low-power are of interest for many different system applications in Si-based CMOS technologies, including consumer electronics, high-end and mobile computing, various sensor and medical health care devices. The rising importance of embedded NVM technologies in recent years has pushed Resistance change Random Access Memory (RRAM) into the spotlight. However, despite numerous integration efforts, the driving mechanism for the resistive switching effect of HfO$_2$-based RRAM is still under debate [1]. Progress in the development has mainly been delayed due to the lack of control over the switching parameters. To achieve an application relevant endurance, the capability to control the resistance by an access device is addressed in this talk. Moreover, this work considers the pulse-induced resistive switching of memory cells with an area down to 1×1 μm^2. It is observed that the pulse width range for the set process is between 60 ns and 80 ns while the reset encompasses a pulse width range of 10-30 μs. Due to the intrinsic current compliance of the access transistor, low set currents of 10 μA and reset currents of 1 μA are obtained.

[1] C. Walczyk et al., IEEE Trans. Electron. Devices, vol. 58, no. 9, pp. 3124-3131 (2011).

DS 40.3 Fri 11:30 H 0111

Resistive switching on HfO$_2$-based metal-insulator-metal structures: effects of the top metal electrode and the oxygen partial pressure — •Thomas Bertaud[1], Damian Walczyk[1], Christian Walczyk[1], Steffen Kubotsch[1], Malgorzata Sowinska[1], Thomas Schroeder[1], Christophe Vallée[2], Vincent Jousseaume[3], and Christian Wenger[1] — [1]IHP, Im Technologiepark 25, 15236 Frankfurt Oder, Germany — [2]LTM Université Joseph Fourier, 17 Rue des Martyrs 38054 Grenoble, France — [3]CEA-LETI Minatec, 17 Rue des Martyrs 38054 Grenoble, France

Embedded nonvolatile memories (eNVM) are attractive for a growing number of applications. One promising candidate for next-generation eNVM is based on the electrically switchable resistance change between a high and a low resistive state of a metal-insulator-metal (MIM) structure, called resistance random access memory (RRAM). Due to the cost effectivity and BEOL compatibility with (Bi)CMOS technologies, this approach is highly attractive. In this talk, the resistive switching on HfO$_2$/bottom TiN based devices will be demonstrated. The work is focused on the impact of the top metal electrode on the switching behavior of the RRAM devices: Al, Hf and Ti (reactive non-blocking), and Cu, Pt and Au (non-reactive blocking) are used and lead to bipolar or unipolar switching, respectively [1]. The current and capacitance characteristics of the MIM diodes are studied by voltage sweeps and retention measurements under different gas ambient in order to highlight the effect of the oxygen partial pressure for a better understanding of the mechanism. [1] T. Bertaud et al., Thin Solid Films (2011).

DS 40.4 Fri 11:45 H 0111

A model for a non-volatile memory material: First principles study of Cu diffusion in α-cristobalite and α-quartz — •Martin Zelený[1], Jozsef Hegedüs[1], Adam. S. Foster[2], David. A. Drabold[3], Stephen. R. Elliott[4], and Risto. M. Nieminen[1] — [1]COMP/Dept. of Applied Physics, Aalto University School of Science, Espoo, Finland — [2]Dept. of Physics, Tampere University of Technology, Tampere, Finland — [3]Dept. of Physics and Astronomy, Ohio University, Athens, USA — [4]Dept. of Chemistry, University of Cambridge, Cambridge, UK

The switching mechanism of a new type of non-volatile memories can be based on electrochemical metallization occurring due to the migration of Ag or Cu ions in oxide glasses as for example SiO$_2$. In order to clarify this mechanism, we have performed simulations of Cu diffusion in the different modifications of SiO$_2$. All calculations in our study were carried out based on first-principles density-functional theory using the Vienna Ab initio Simulation Package (VASP).

We present a total-energy calculation of the barrier along a diffusion path of Cu between two equivalent interstitial positions in α-cristobalite and α-quartz. Our results for α-cristobalite show that the shape of the path strongly depends on the charge of the system, but the height of the migration barrier stays between 0.15-0.2 eV. On the other hand, the height of the barrier in α-quartz varies between 0.1 and 0.6 eV and depends on the directions of Cu motion. We also present results of molecular dynamics simulations of the drift of a Cu atom driven by an external electric field.

DS 40.5 Fri 12:00 H 0111

Transient Processes in Response to Electronic Excitation of Phase Change Materials — •Martin Salinga and Martin Wimmer — 1. Institut of Physics, RWTH Aachen University, Germany

In recent years a strong interest in phase change materials has been aroused by their potential for being utilized as the core element of a promising novel electronic memory technology. For such an application it is crucial to understand the characteristic switching mechanisms. Especially the electronic properties of the amorphous phase are of paramount importance. Thus, the strong non-linearity in the current-voltage-dependence of the amorphous phase, often referred to as threshold-switching, has drawn much attention.

In this work the transient current response of vertical Ge2Sb2Te5 devices to controlled voltage excitations is experimentally studied down to a time-scale of a few nanoseconds and analyzed with a particular focus on the delay-time before threshold switching and its dependence on the applied voltage. The results are compared to both experimental and theoretical studies in the literature and their implications for this field of research are discussed.

DS 40.6 Fri 12:15 H 0111

Nonvolatile resistive switching in Au/BiFeO3 rectifying

junction — •Yao Shuai[1,2], Chuangui Wu[2], Wanli Zhang[2], Shengqiang Zhou[1], Danilo Bürger[1], Stefan Slesazeck[3], Thomas Mikolajick[3], Manfred Helm[1], and Heidemarie Schmidt[1] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, P. O. Box 510119, Dresden 01314, Germany — [2]State Key Laboratory of Electronic Thin Films and Integrated Devices, Chengdu, China — [3]Namlab gGmbH, Nöthnitzer Strasse 64, 01187 Dresden, Germany

BiFeO3 thin films have been grown on Pt/Ti/SiO2/Si substrates with pulsed laser deposition. RF sputtered Au has been used for the top electrode. The transport properties of the BiFeO3 thin films have been previously demonstrated to be sensitive to the interface [1]. In the present work, an interface-related resistive switching behavior with large switching ratio up to 4500 has been observed in the Au/BiFeO3/Pt structure [2]. The different polarities of the external voltage induce an electron trapping or detrapping process, and consequently change the depletion layer width below the Au Schottky contact, which is revealed by capacitance-voltage measurements and by long-term low/high resistance state capacitance transient measurements at zero bias [3]. [1] Y. Shuai et al., Appl. Phys. Lett., 98, 232901 (2011). [2] Y. Shuai et al., Appl. Phys. Express. 4, 095802 (2011). [3] Y. Shuai et al., J. Appl. Phys. 109, 124117 (2011).

DS 41: Thermoelectric materials III: Heterostructures (Focused session – Organizers: Meyer, Heiliger)

Time: Friday 9:30–11:15 Location: H 2032

DS 41.1 Fri 9:30 H 2032

Phonon transport from *ab initio* in $ZnO_{1-x}S_x$ and $ZnS_{1-x}O_x$ — Michael Bachmann, •Michael Czerner, Saeideh Edalati-Boostan, and Christian Heiliger — I. Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany

We present results from *ab initio* calculations of $ZnO_{1-x}S_x$ and $ZnS_{1-x}O_x$. We focus our investigations on the Phonondensity of states and the inter atomic force constants in these systems. Furthermore the inter atomic force constants are used in an atomistic Green's function method [1] to obtain the phonon transmission function of the system. The transmission function can then be used to calculate the thermal lattice conductance within the linear response regime. Having the lattice conductance we can estimate the usability of such systems for thermoelectric applications.

DS 41.2 Fri 9:45 H 2032

Experimental determination of the thermoelectric figure-of-merit and optimal annealing condition of electrodeposited films. — •Hans-Fridtjof Pernau, Martin Jägle, Alexandre Jacquot, Benjamin Bayer, Karina Tarantik, Olivia Herm, Harald Böttner, Jan König, and Kilian Bartholomé — Fraunhofer Institut für Physikalische Messtechnik IPM, Heidenhofstr. 8, 79110 Freiburg, Deutschland

Thermoelectric characterization tools developed at the Fraunhofer-IPM can not only be used for the characterization of thermoelectric properties, but also for optimization purposes. For example, thin film samples can be monitored on-line during annealing. These tools optimiza-tion technique is applicable for sputtered or electroplated films. An overview on the 3-omega method in combination with other measurement techniques allowing a determination of the figure of merit will be given.

This work presents the on-going efforts of the Fraunhofer-IPM to measure the thermoelectric figure of merit of electrodeposited or sputtered films and the fast determination of optimal an-nealing conditions.

DS 41.3 Fri 10:00 H 2032

Epitaxial growth and control of sodium content in Na_xCoO_2 thin films grown by pulsed laser deposition — •Sandra Hildebrandt, Philipp Komissinskiy, Marton Major, Wolfgang Donner, and Lambert Alff — Institut für Materialwissenschaft, Technische Universität Darmstadt, 64287 Darmstadt, Germany

A variety of interesting phenomena such as large thermoelectric power and (possibly) unconventional superconductivity of the water-intercalated compound are observed in sodium cobaltate Na_xCoO_2 depending on sodium content[1,2]. We have grown *c*-axis oriented Na_xCoO_2 thin films on $SrTiO_3(100)$ using pulsed laser deposition. The sodium stoichiometry of the films is controlled within $0.38 < x < 0.84$ by varying the post-deposition annealing conditions in oxygen. Thus, low sodium content ($x < 0.5$) can be achieved without the commonly used chemical deintercalation of Na using a Br_2- (or I_2-) based solution. X-ray diffraction analysis demonstrates that the Na_xCoO_2 films grow in two twin domains rotated by 15 and 45 degrees relative to [100] $SrTiO_3$. After annealing for 15-20 minutes single-crystalline films are obtained with a full width at half maximum of the (002) reflection below 0.2 degrees.

1. I. Terasaki, Y. Sasago, and K. Uchinokura, Physical Review B **56**, 12685 (1997).
2. K. Takada, H. Sakurai, E. Takayama-Muromachi, F. Izumi, R. A. Dilanian, and T. Sasaki, Nature **422**, 53 (2003).

This study was supported by DFG through project AL560/6-1.

DS 41.4 Fri 10:15 H 2032

Thermal conductivity in $Pr_{1-x}Ca_xMnO_3$ and $SrTiO_3$ thin film systems — •Stefanie Wiedigen[1], Thilo Kramer[1], Manuel Feuchter[2], Kodanda R. Mangipudi[1], Jörg Hoffmann[1], Marc Kamlah[2], Cynthia A. Volkert[1], and Christian Jooss[1] — [1]Institute for Materials Physics, University of Göttingen, Germany — [2]Institute for Applied Materials, Karlsruhe Institute of Technology, Germany

Epitaxial multilayers and superlattices are one recent approach for the design of efficient thermoelectrics. To study the effect of phonon blocking and scattering on thermal conductivity of oxide multilayers, a combination of two perovskites with promising thermoelectric properties is selected: the orthorhombic $Pr_{1-x}Ca_xMnO_3$ and the cubic $SrTiO_3$. In order to investigate the effect of microstructure, interfaces and acoustic impedance mismatch on thermal conductivity κ high preparation quality is needed. Our thin films were prepared by ion-beam and magnetron sputtering. Structural analysis is done by XRD and TEM and will be presented in combination with thermal conductivity measurements using the 3ω method. Single layers of $Pr_{1-x}Ca_xMnO_3$ show low κ values and no significant increase of thermal conductivty with increasing doping. In homoepitaxial single layers of $SrTiO_3$ preparation conditions have a high impact on κ, most probably due to different concentrations of point defects. $Pr_{1-x}Ca_xMnO_3/SrTiO_3$ multilayers show a κ decreases systematically with increasing number of double layers. The results are discussed in the light of the theoretically calculated phonon dispersion and the experimentally observed microstructure.

DS 41.5 Fri 10:30 H 2032

Thermoelectric Transport in strained Si and Si/Ge heterostructures — Nicki F. Hinsche[1], Ingrid Mertig[1,2], and •Peter Zahn[1] — [1]Martin-Luther-Universität, Institut für Physik, Von-Seckendorff-Platz 1, D-06120 Halle — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle

Starting from bulk silicon, we study the change in thermoelectric properties due to symmetry breaking in strained Si which might be applied in nanostructured thermoelectrics.

In detail, the anisotropy of the electrical conductivity, the thermopower and the resulting power factor in the in-plane and cross-plane directions are studied in dependence on doping level, temperature, and strain in [001] and [111] direction. Our results show that tetragonal [1] and rhombohedral [2] distortions have a strong influence on the thermoelectric transport properties. The electronic structure is calculated self-consistently within the framework of density functional theory. The transport properties are studied in the diffusive limit applying the Boltzmann theory in relaxation time approximation [3].

Furthermore, we present results for strained Si/Ge heterostructures, showing an enhanced power factor in cross-plane direction under electron doping as suggested by Koga *et al.* [4].

[1] N. F. Hinsche, I. Mertig, and P. Zahn, *J. Phys.: Cond. Matt.* **23**, 295502 (2011). [2] N. F. Hinsche, I. Mertig, and P. Zahn, *to be published.* [3] I. Mertig, *Rep. Prog. Phys.* **62**, 237 (1999). [4] T. Koga, X. Sun, S. B. Cronin, and M. S. Dresselhaus, *Appl. Phys. Lett.* **75**,

2438 (1999).

DS 41.6 Fri 10:45 H 2032

Electric Characterization of Si/Ge Superlattices — •Markus Trutschel[1], Katrin Bertram[1], Bodo Fuhrmann[1], Alexander Tonkikh[2], Peter Werner[2], and Hartmut S. Leipner[1] — [1]Martin-Luther-Universität Halle-Wittenberg, Interdisziplinäres Zentrum für Materialwissenschaften, Heinrich-Damerow-Str. 4, D-06120 Halle, Germany. — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany.

Si/Ge superlattices are expected to have an increased figure of merit due to their two dimensional structure. The enhancement in the figure of merit can be attributed to a decreased thermal conductivity due to phonon scattering at the interfaces between the Si/Ge layers. For this reason applications are aspired in cross plane direction.

The measurement of electrical properties in cross plane direction of thin films with thicknesses in the nanometer range is strongly affected by measurement uncertainties. In this work, we studied the requirements of the electrical conductivity measurement cross plane using a modified transmission line model (TLM). For this purpose, a suitable mesa structure for TLM measurements was developed. In order to obtain more precise results, a finite element model was performed to simulate the current density distribution in the sample. Additionally we present experimental results in comparison to the calculated values. We thank the BMBF for financial support.

DS 41.7 Fri 11:00 H 2032

Thermoelectric Transport in Bi_2Te_3/Sb_2Te_3 heterostructures — •Nicki F. Hinsche[1], Bogdan Yu. Yavorsky[1], Ingrid Mertig[1,2] und Peter Zahn[1] — [1]Martin-Luther-Universität, Institut für Physik, Von-Seckendorff-Platz 1, D-06120 Halle — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle

Bi_2Te_3/Sb_2Te_3-heterostructures show a remarkable enhancement of the thermoelectric figure of merit compared to the bulk materials [1]. While gaining much attention in the last decade, the physical origin of this enhancement is still under debate. To contribute on this, we studied the electronic structure of Bi_2Te_3/Sb_2Te_3 heterostructures with a fully relativistic screened Korringa-Kohn-Rostoker Greens function method. The thermoelectric transport properties in-plane and cross-plane were calculated within the relaxation time approximation of the Boltzmann theory. The influence of composition, interfacial strain, and doping on the anisotropic thermoelectric properties were studied in detail [2,3].

[1] R. Venkatasubramanian, E. Siivola, T. Colpitts, and B. O'Quinn, *Nature* **413**, 597 (2001). [2] N. F. Hinsche, B. Yu. Yavorsky, I. Mertig, and P. Zahn, *Phys. Rev. B* **84**, 165214 (2011). [3] B. Yu. Yavorsky, N. F. Hinsche, I. Mertig, and P. Zahn, *Phys. Rev. B* **84**, 165208 (2011).

DS 42: Thermoelectric materials IV: Glass, sintered materials (Focused session – Organizers: Meyer, Heiliger)

Time: Friday 11:30–13:00 Location: H 2032

Topical Talk DS 42.1 Fri 11:30 H 2032

Employing laterally nanostructured ZnO-based thin-films as model systems for studying interface effects in themoelectrics — •Peter J. Klar — I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Germany

The morphology of the interface between two materials has a major impact on the transport properties across this interface. Interface properties at different length scales ranging from the atomic to the micrometer scale affect phonons and electrons differently. Controlling these effects allows one to tune and optimize the thermoelectric properties of materials. Laterally nanostructured thin-films offer the advantage that the interfaces between its constituents are easily accessible by local probes such as electron microscopy, micro-Raman and micro-photoluminescence spectroscopy as well as local transport measurements, which allows one to correlate the interface structure with global and local transport properties and thus to establish structure-property relationships. In particular, the controlled fabrication of interfaces of different morphology by self-aligned patterning combining lithographic steps, etching steps, and rf-sputtering will be introduced. Examples of the impact of the interface structure on the transport properties and the correlation between their global and local properties will be discussed for various series of laterally nanostructured ZnO thin-films. The results suggest that in many nanostructured thermoelectrics the impact of diffusion, band bending or percolation on thermoelectric properties is more significant than that of density of states changes and confinement anticipated at reduced dimensions.

DS 42.2 Fri 12:00 H 2032

Glass-ceramics as high-temperature thermoelectric materials — •Julian Lingner[1,2], Matthias Jost[1,2], Gerhard Jakob[1], and Martin Letz[2] — [1]Johannes Gutenberg-Universität Mainz — [2]Schott AG Mainz

The research on thermoelectric materials has progressed enormously over the last years and is still growing because of the global demand for eco-sensitive energy conversion. Innovative approaches like bulk-nanostructuring helped to increase the efficiency of the investigated materials. Especially the high temperature segment of thermoelectric materials seems to promise good yields concerning power generation because the efficiency is proportional to the temperature. Therefore it is important to find suitable materials in this regime. SiGe has been known to be a high-temperature thermoeletric but has the limited availability of Ge as a big disadvantage. This presentation focuses on a new material class for high temperatures in thermoelectrics - glass-ceramics. In a glass-ceramic, a certain crystal structure is embedded in a glass-matrix leading to many new properties of the material. Especially the possibility to induce small crystallites, the pore-free surface combined with the high-temperature durability of this material class support this approach. Measurements of different systems of glass-ceramic thermoelectric materials are presented.

DS 42.3 Fri 12:15 H 2032

$Ca_3Co_4O_9$ based ceramics and glass-ceramics as high temperature stable oxide thermoelectrics — •Matthias Jost[1,2], Julian Lingner[1,2], Martin Letz[2], and Gerhard Jakob[1] — [1]Johannes-Gutenberg Universität, Institut für Physik, Staudinger Weg 7, Mainz D-55128 — [2]Schott AG, Hattenbergstraße 10, Mainz D-55122

Oxidic thermoelectric materials are a good alternative to the now more common thermoelectric materials, such as PbTe, SiGe, BiSb or Bi_2Te_3, because of their thermal stability, chemical stability, low toxic level and good availability of the raw materials. In our presentation, we will give a brief review about the determined thermoelectric properties of our $Ca_3Co_4O_9$ ceramics and $Ca_3Co_4O_9$ glass-ceramics. $Ca_3Co_4O_9$ ceramics were first discussed by Ryoji Funahashi in 1999. The ceramics have been processed using conventional sintering. Therefor we mixed $CaCO_3$ and CoO powders. The mixture was ground, calcined, pulverized, and pressed into pellets. These pellets were cold isostatically pressed and after that sintered at different temperatures. The glass was melted in a platin-iridium crucible, casted into a steel mold, quenched and cooled down in an annealing lehr. After that, it was ceramized in an infrared-furnace. The ceramics/glass-ceramics were examined by X-ray diffraction and samples were prepared out of the pellets/glass-ceramic-blocks. Electrical conductivity, thermal resistivity and the Seebeck coefficient of these samples were measured for different temperatures and from these values ZT were calculated.

DS 42.4 Fri 12:30 H 2032

Nanocrystalline Diamond as Thermoelectric Material — •Nicolas Wöhrl[1], Markus Engenhorst[2], Gabi Schierning[2], and Volker Buck[1] — [1]University Duisburg-Essen and CeNIDE, Faculty of Physics, Duisburg, Germany — [2]University Duisburg-Essen and CeNIDE, Faculty of Engineering, Duisburg, Germany

The thermoelectric effect directly converts temperature differences into electric voltage and vice versa. The thermoelectric material has to have a high electrical conductivity because a high internal resistance will reduce the efficiency of the generator and a low thermal conductivity. Thus one promising way to design good thermoelectric materials is to manipulate phonons and electrons at the nanoscale making nanostructuring a possible way to achieve these materials. Introducing defects that scatter phonons but not electrons at the same degree can decrease the thermal conductivity without appreciably affecting the power factor. Another strategy is to scatter phonons at interfaces, leading to the use of nanostructured materials consisting of thin-film superlattices or mixed composite structures. Nanocrystalline diamond films were deposited by microwave-plasma CVD from an Ar/H2/CH4 plasma with admixtures of trialkylborane to obtain p-type semiconducting diamond and results shown here are indicating that nanostructured diamond films are a promising material for thermoelectric applications. Thermal conductivity lower than 10 W/mK and Seebeck coefficients above 50 μV/K were achieved.

DS 42.5 Fri 12:45 H 2032

Laser sintering of nanoparticles - morphologic and thermoelectric aspects — •Benedikt Stoib[1], Tim Langmann[1], Martin S. Brandt[1], Nils Petermann[2], Hartmut Wiggers[2], and Martin Stutzmann[1] — [1]Walter Schottky Institut, Technische Universität München, Am Coulombwall 4, 85748 Garching — [2]Institut für Verbrennung und Gasdynamik, Universität Duisburg-Essen, Lotharstraße 1, 47048 Duisburg

Bottom-up fabrication of nanoscale thermoelectrics in most cases requires annealing to improve the otherwise insufficient electrical performance. We apply a high-intensity short-pulse laser treatment to spin-coated films of crystalline nanoparticles, grown by plasma decomposition of silane and/or germane in a microwave reactor. The resulting films with sub-micrometer thickness are highly suited as a model system to systematically study the influence of Si/Ge ratio, doping, defects and grain size on the thermoelectrical potential of SiGe-based thin films. The morphology is discussed with special emphasis on porosity and its influence on macroscopic conductivity. The interdiffusion between nanoparticles of different composition during the partial melting is studied by Raman spectroscopy. The thermopower of the films indicates little variation of the Seebeck coefficient with respect to the morphological properties of the thin films.

DS 43: Thermoelectric materials V: Bulk materials (Focused session – Organizers: Meyer, Heiliger)

Time: Friday 13:30–16:00 Location: H 2032

Topical Talk DS 43.1 Fri 13:30 H 2032

Potential Seebeck Microprobe: Considerations on Accuracy and Spatial Resolution — •Pawel Ziolkowski, Gregor Oppitz, Gabriele Karpinski, and Eckhard Müller — German Aerospace Center - Institute of Materials Research, Linder Höhe, D-51147 Köln

Recent developments turned the Potential Seebeck Microprobe (PSM) into a powerful tool for functional materials characterisation. A wide spectrum of applications was demonstrated on a variety of thermoelectric material classes involving bulk and thin film samples. The principle involves a heated probe tip positioned at the surface of a sample coupled to a heat sink. The tip is heating up the sample in a micro-vicinity, forming a locally focused temperature gradient. The thermovoltage of the sample is measured by thermocouples, which are connected to the probe tip and sample respectively and form independent circuits containing the probe-sample contact. By these circuits, thermovoltages and the temperature drop over the gradient region are recorded, yielding the local Seebeck coefficient. Here, we give a summary on the determining factors for accuracy and spatial resolution during Seebeck coefficient measurements. Furthermore a theoretical approach will be presented, which provides the possibility to enhance the spatial resolution by means of a deconvolution algorithm based on the apparatus function, which can be derived from measurements on reference samples containing sharp material property transitions. Based on the idea of this theoretical approach a successor of the PSM was designed for transient operation. First results will be presented, which shall demonstrate the enhanced spatial resolution.

DS 43.2 Fri 14:00 H 2032

Annealed CoSb$_3$ thin films on various substrates — Martin Friedemann, •Marcus Daniel, Gunter Beddies, and Manfred Albrecht — Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany

Looking for new energy sources, thermoelectric becomes more and more important and especially CoSb$_3$ is a promising alloy for thermoelectric applications. Besides a high figure of merit, the thermal stability of the material has to be assured. Thermal treatment can yield to strain, cracks and formation of different crystal phases. During the annealing process of CoSb$_3$ thin films deposited on thermally oxidized Si substrates, cracks occur at the surface of the films. The reason for the cracks could be the difference of the thermal expansion coefficient of Si and CoSb$_3$. In this study, 40nm thick CoSb$_x$ films have been deposited via MBE at room temperature onto substrates with different expansion coefficient in the range of 0,5 - 12 $\cdot$ 10^{-6} K^{-1}. The samples were post-annealed in ultra-high vacuum for one hour at 500°C. The composition of the films were checked by RBS before and after annealing. The samples show small differences in composition and the Sb content of the annealed samples is slightly lower than that of the initial ones. The phase formation was analysed by XRD, where CoSb$_3$ could be found as major phase. The surface morphology and the roughness of the films was investigated by AFM. For a substrate thermal expansion coefficient between 9 and 11 $\cdot$ 10^{-6} K^{-1} crack formation could be prevented and a minima in roughness was found, resulting also in a minima of electric conductivity.

DS 43.3 Fri 14:15 H 2032

Electronic and Thermoelectric properties of RuIn$_{3-x}A_x$ (A=Sn, Zn) from first principles — •Deepa Kasinathan[1], Maik Wagner[1], Helge Rosner[1], and Klaus Koepernik[2] — [1]Max Planck Institute for Chemical Physics of Solids, Noethnitzer strasse 40, 01187 Dresden, Germany — [2]IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany

Recently, substitution derivatives of the intermetallic compound RuIn$_{3-x}A_x$ (A = Sn, Zn) have been shown to exhibit relatively high Seebeck coefficients. Substitution by Sn results in n-type behavior while p-type is the norm for substitution of In by Zn. We discuss in detail the electronic structure of the parent compound and the substitution derivatives obtained from density functional theory based calculations using the Full Potential Local Orbital code. The substitution effects have been studied using three different approximations: the simple virtual crystal approximation, the ordered supercell approach and the disordered coherent potential approximation. Both Sn and Zn prefer different site symmetry positions in the unit cell. While the parent compound RuIn$_3$ is a semiconductor, the substitution derivatives are not. For small doping concentrations, we observe a rather rigid-band-like behavior due to the parabolic nature of the bands forming the valence band maximum and the conduction band minimum. Transport properties calculated using the semi-classical Boltzmann transport equations based on the constant scattering approximation are consistent with the experiments. *Funding from the DFG via SPP1386 is acknowledged.*

DS 43.4 Fri 14:30 H 2032

Quantum Chemical Investigation of Filled Skutterudites as Thermoelectric Materials — Lukas Hammerschmidt and •Beate Paulus — Institut für Chemie und Biochemie, FU Berlin, Takustr. 3, 14195 Berlin

In the last few years Skutterudites attracted much interest as promising thermoelectric materials [1]. Thermoelectrics directly transform thermal energy into electric energy due to the so called “Seebeck-effect”. An enhanced thermoelectric figure of merit ZT is achieved by filling the icosahedral voids of the Skutterudite crystal structure by e.g. lanthanides, actinides, alkaline (earth) metals and other electropositive elements. In our study we apply plane-wave DFT methods implemented in the VASP program package [2] for the In, Ga and Tl doped CoSb$_3$ Skutterudites and study systematically the effects of the doping concentration on density of states (DOS), charges, energies and lattice constants.

[1] B. C. Sales, D. Mandrus, R. K. Williams *Science* 272 (1996) 1325.
[2] J. Hafner, *J. Comput. Chem.* 29 (2008) 2044; G. Kresse, J. Hafner, *J. Phys. Condens. Matter* 6 (1994) 8245.

DS 43.5 Fri 14:45 H 2032

Vibronic contribution to thermoelectric properties of Bi_2Te_3 and Bi_2Se_3 from first principles — •Martin Hölzer[1], Nicki F. Hinsche[2], Sergey Ostanin[1,2], and Arthur Ernst[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle/S. — [2]Martin-Luther-Universität, Institut für Physik, Von-Seckendorff-Platz 1, 06120 Halle/S.

We present *ab initio*-studies of the vibronic properties of Bi_2Te_3 and Bi_2Se_3 in the harmonic approximation. In this work, we used a multi-code-approach, consisting of pseudopotential calculations and a multiple scattering Green function method to investigate the phonon frequencies, electron-phonon-coupling, and the resulting thermoelectric properties for these materials. The influence of spin-orbit interaction, which is very important for the correct description of the electronic properties of these systens, will also be discussed.

DS 43.6 Fri 15:00 H 2032

Transport and thermal properties of single- and polycrystalline $NiZr_{0.5}Hf_{0.5}Sn$ — Siham Ouardi[1,4], Gerhard H. Fecher[1,4], Claudia Felser[1,4], •Christian G.F. Blum[2], Dirk Bombor[2], Christian Hess[2], Bernd Büchner[2], Eiji Ikenaga[3], and Sabine Wurmehl[2] — [1]Institut für Anorganische Chemie und Analytische Chemie, Johannes Gutenberg - Universität, Mainz, Germany — [2]Leibniz Institute for Solid State and Materials Research IFW, 01171 Dresden, Germany — [3]Japan Synchrotron Radiation Research Institute, SPring-8, Hyogo 679-5198, Japan — [4]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany

The thermoelectric properties of a Heusler compound with $NiZr_{0.5}Hf_{0.5}Sn$ composition were studied. A comparison of the properties of a single crystal and a polycrystal was carried out by measurements of the electrical conductivity, Seebeck coefficient, and thermal conductivity. The transport properties are directly compared to the valence band electronic structure measured by photoelectron spectroscopy. The single crystal shows a higher figure of merit (ZT=0.1) at room temperature which originates from the high electrical conductivity that is mediated by "in-gap" states observed by high energy photoemission spectroscopy.

DS 43.7 Fri 15:15 H 2032

TiNiSn and $Zr_{0.5}Hf_{0.5}NiSn$ superlattices for thermoelectrics — •Tino Jaeger[1], Michael Schwall[2], Xeniya Kozina[2], Benjamin Balke[2], Sascha Populoh[3], Anke Weidenkaff[3], Claudia Felser[2], and Gerhard Jakob[1] — [1]Institut für Physik, Universität Mainz, 55099 Mainz — [2]Institut für Analytische und Anorganische Chemie, Universität Mainz, 55099 Mainz — [3]EMPA, Ueberlandstrasse 129, 8600 Duebendorf, Switzerland

In order to increase the attractiveness of thermoelectric devices, their efficiency must be increased. Beside others, the properties of the thermoelectric material can be improved. That can be achieved by either increasing Seebeck coefficient or conductivity or by a depressed thermal conductivity along the thermal gradient. For thin films, superlattices or multilayers can be used to lower the cross plane thermal conductivity. As a bottom up approach, artificially layered films with a periodicity of about 5-6 nm are assumed to generate the most phonon scattering at the interfaces. If electrical properties remain unchanged or less effected, the thermoelectric efficiency is enhanced. Semiconducting Half-Heuslers are well studied thermoelectric bulk materials. Among others, TiNiSn and $Zr_{0.5}Hf_{0.5}NiSn$ are potential candidates. Essentially, their similar lattice constants enable epitaxial layers on top of each other. Furthermore, varied atomic masses of Ti, Zr and Hf generate the aspired alternating mass distribution. By rotating the substrate in between simultaneously burning cathodes, significant film thicknesses can be achieved by sputter deposition.

DS 43.8 Fri 15:30 H 2032

Investigations on the $Ti_xZr_yHf_zNiSn$ system. — •Michael Schwall and Benjamin Balke — Institute of Inorganic Chemistry and Analytical Chemistry, Johannes Gutenberg - University, Mainz

Half-Heusler compounds exhibit very promising thermoelectric properties for high temperature applications, combined with several additional advantages such as environmental friendliness, low production-costs and future availability of raw materials. The high thermoelectric potential can be mainly attributed to the high Seebeck coefficient and the low electrical resistivity values found recently in several half-Heusler alloys. The main obstacle is still their relatively high thermal conductivity. The best reported n-type materials are consisting of $Ti_xZr_yHf_zNiSn$ with different x ,y ,z (x+y+z=1). In this study, we investigated the reasons for this outstanding thermoelectric properties. The effect of the microstructure on the transport properties will be described in details. The authors gratefully acknowledge the financial support by the "thermoHeusler" Project (Project No. 0327876D) of the German Federal Ministry of Economics and Technology (BMWi).

DS 43.9 Fri 15:45 H 2032

Heusler compounds with $C1_b$ structure as promising p-type thermoelectric materials. — •Elisabeth Rausch, Michael Schwall, and Benjamin Balke — Institute of Inorganic Chemistry and Analytical Chemistry, Johannes Gutenberg - University, Mainz

This work reports on the experimental investigations of XCoSb (X= Ti, Zr or Hf) based Heusler compounds discussed as potential p-type thermoelectic materials. A lot of n-type materials are known and exhibt high ZT values (ZT_{max}=1.5), but there are only a few p-type materials which can achieve ZT values above 0.5. We tried to improve the thermoelectric properties by nano structring the materials. The samples were mechanical alloyed by means of a high energy ball mill. The thermoelectric properties could be enhanced due to the nano structuring of the material. We will present structural and physical properties of the synthized coumpounds including a complete high temperature thermoelectric characterisation. The authors gratefully acknowledge the financial support by the "thermoHeusler" Project (Project No. 0327876D) of the German Federal Ministry of Economics and Technology (BMWi).

DS 44: Poster IV: Thin film photovoltaics; Organic electronics and photovoltaics (jointly with CPP, HL, O); Organic thin films; Trends in atomic layer deposition (Focused session)

Time: Friday 9:30–12:00 Location: Poster E

DS 44.1 Fri 9:30 Poster E

Study of the optical properties of TiO2 Thin Films prepared by rapid thermal oxidation — Wafaa Al-Khayat[1,2] and •Gerhard Wilde[1] — [1]Institute of Materials Physics, WWU Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Collage of Science, Al-Mustansiriy University, Baghdad, Iraq

TiO2 thin films were deposited by the thermal oxidation method on glass substrates at room temperature. The X-ray diffraction patterns indicate an amorphous structure of the TiO2 thin films. The optical constants were characterized using the transmission spectra of the films obtained by uv-vis spectrophotometer. The optical band gaps were evaluated by the Tauce model. The optical properties of the thin films are discussed with respect of the film thickness and the oxidation condition.

DS 44.2 Fri 9:30 Poster E

Inhomogeneities in charge carrier transport properties of $Cu(In,Ga)Se_2$ solar-cells — •Melanie Nichterwitz[1], Christian Kaufmann[1], Raquel Caballero[2], Hans-Werner Schock[1], and Thomas Unold[1] — [1]Helmholtz-Zentrum Berlin, Germany — [2]Universidad Autónoma de Madrid, Spain

In this study, electron beam induced current (EBIC) in the cross section configuration is used to characterize charge carrier transport in $Cu(In,Ga)Se_2$ (CIGSe)/CdS/ZnO solar-cells. It is shown that charge carrier transport properties are (i) generation dependent and (ii) grain specific, i.e. spatially inhomogeneous. Within some grains of the CIGSe absorber layer, the collected short circuit current is reduced significantly for electron beam irradiation such that there is no generation at the heterojunction. Charge carrier transport is generation dependent in these grains for all used electron beam currents, i.e. generation densities (low injection). In other grains however, charge carrier transport is only generation dependent for the highest used electron beam current. In conjunction with numerical simulations, these results are used to derive a model for the electronic band diagram of the heterojunction region of the solar cell. It is based on the assumption of (i) a thin layer with a high density ($\approx 10^{17}$ cm^{-3}) of deep acceptor type defect states (p+ layer) and a lowered valence band maximum between the CIGSe and the CdS layer and (ii) donor type interface states at the p+ layer/CdS interface of some grains.

DS 44.3 Fri 9:30 Poster E

Post-deposition optimization of LPCVD grown ZnO:B as front TCO in thin film silicon solar cells — •Thomas Bienert, Oleg Sergeev, Karsten von Maydell, and Carsten Agert — NEXT ENERGY. EWE Forschungszentrum für Energietechnologie e.V., Oldenburg, Germany

Thin film solar cells with superstrate configuration have very specific requirements for optical and electrical properties of the front contact, like high transmittance and haze as well as a low sheet resistance. Transparent conductive oxides (TCO) have already been proven to be a good choice, but their optical and electrical properties can be improved even after the deposition by various means. The LPCVD grown ZnO:B TCO in this study has been treated with hydrochloric acid (HCl) and H_2-plasma prior to the deposition of μc-Si:H and a-Si:H pin-cells. The influence of such a treatment on optical and electrical properties of the TCO was investigated. The performance of the cells deposited on original and treated TCO was determined. It is shown that both treatments can be used to improve the overall TCO's properties. It has been found the etching enhances surface topography and haze while H_2-Plasma treatment decreases the sheet resistance significantly. The efficiency of both solar cell types (μc-Si:H as well as a a-Si:H pin) deposited on optimized LPCVD ZnO:B was increased by enhancement of the fill factor and of the photocurrent.

DS 44.4 Fri 9:30 Poster E

Photovoltaic energy conversion based on strongly correlated oxides — •Benedikt Ifland[1], Gesine Saucke[2], Jonas Norpoth[1], Jörg Hoffmann[1], and Christian Jooss[1] — [1]Institute of Materials Physics, University of Göttingen, Germany — [2]Institute for Condensed Matter Physics, University of Zürich, Switzerland

Materials with strong electron-electron or electron-phonon interaction offer promising opportunities in search for new fundamental mechanisms of light harvesting in solar cells via tuning their correlation interactions. We have studied two types of manganite-titanite pn-heterostructures, where p-doped manganites are deposited on single crystal substrate of n-type $SrTi_{1-x}Nb_xO_3$ (STNO) via ion beam sputter deposition: $Pr_{1-x}Ca_xMnO_3$ (PCMO) shows semiconducting behavior based on thermally assisted hopping of small polarons. In contrast, $La_{1-x}Sr_xMnO_3$ (LSMO) exhibits band like "metallic" conductivity and ferromagnetic order. It may form a Schottky like junction in electrical contact with STNO. Current-voltage-characteristics of the oxide junction in a temperature range between 25 and 300 K show strongly rectifying behavior. Although both p-type manganites have no optical band gap at 300K, the junctions reveal a photovoltaic effect. The open circuit voltage increases with decreasing temperature up to several hundred millivolts. Experimental results are discussed with respect to conventional semiconductor models, taken also into account the non-linear mobility of polarons in the presence of an electric field.

DS 44.5 Fri 9:30 Poster E

Physical vapor deposition of CdTe thin films at low temperature for solar cell applications — •Christoph Heisler, Michael Brückner, Felix Lind, Christian Kraft, Udo Reislöhner, Carsten Ronning, and Werner Wesch — Institute of Solid State Physics, University of Jena, Max-Wien-Platz 1, D-07743 Jena

Cadmium telluride is successfully utilized as an absorber material for thin film solar cells. Industrial production makes use of high substrate temperatures for the deposition of CdTe absorber layers. However, in order to exploit flexible substrates and to simplify the manufacturing process, lower deposition temperatures are beneficial. Based on the phase diagram of CdTe, predictions on the stoichiometry of CdTe thin films grown at low substrate temperatures are made in this work. These predictions were verified experimentally using additional sources of Cd and Te during the deposition of the CdTe thin films at different substrate temperatures. The deposited layers were analyzed with energy-dispersive X-ray spectroscopy. In case of CdTe layers which were deposited at substrate temperatures lower than 200 °C without usage of additional sources we found a non-stoichiometric growth of the CdTe layers. The application of the additional sources leads to a stoichiometric growth for substrate temperatures down to 100 °C which is a significant reduction of the substrate temperature during deposition.

DS 44.6 Fri 9:30 Poster E

Influence of the sintering process on the structure of Cu2ZnSnS4 nanocrystal thin films — •Kai Kornhuber[1], Jaison Kavalakkatt[1,2], Xianzhong Lin[1], Patryk Kusch[2], Ahmed Ennaoui[1], and Martha C. Lux-Steiner[1,2] — [1]Helmholtz Center Berlin for Materials and Energy, Berlin, Germany — [2]Freie Universität Berlin, Berlin, Germany

Cu_2ZnSnS_4 (CZTS) is a *p*-type emerging semiconductor solar absorber with optimal direct band gap energy of 1.5 eV and a large absorption coefficient above 10^4 cm^{-1}. It is structurally similar to Cu(In,Ga)Se_2 and contains only earth abundant, non-toxic elements. Recently promising energy conversion efficiencies of up to 10.1 % were demonstrated [D.Barkhouse, O.Gunawan, et. al, Prog. Photovolt: Res. Appl. (2011)]. So far, all preparation methods require an annealing step to improve the cristallinity. This process is not completely understood, suffering from the presence of secondary phases such as ZnS, Cu_xSnS_y and Cu_xS. In this work, a solution based approach to prepare CZTS-nanoparticle ink was used for CZTS thin film deposition on Mo-coated glass and FTO. The processing under different temperatures and atmospheres (Ar, H_2S) allowed to obtain compact film material. Combining X-ray diffraction and Raman spectroscopy as complimentary phase resolving techniques, identification of phases present in multiphase CZTS thin films was accomplished. The results of the Raman- and XRD-analysis of the phases formed and the advantages of using these techniques are presented. Furthermore UV-Vis-spectroscopy was applied to investigate changes of the optical properties.

DS 44.7 Fri 9:30 Poster E

Spectroscopic Characterization of Amorphous Silicon/Silicon Heterodiodes Prepared by DC Pulsed Magnetron Sputtering — •Philipp Schäfer[1], Frank Nobis[2], Ovidiu D. Gordan[1], Hartmut Kupfer[2], Frank Richter[2], and Dietrich R. T. Zahn[1] — [1]Semiconductor Physics, Chemnitz University of Technology — [2]Solid State Physics, Chemnitz University of Technology

Doped layers of hydrogenated amorphous silicon were prepared by dc magnetron sputtering onto oppositely doped crystalline silicon substrates. Defect levels of the thereby assembled heterostructure diodes were intensively studied using charge transient spectroscopy. During deposition the substrate temperature and hydrogen flow rate can be controlled individually. Energetic shifts of the defect levels occur with the variation of these key parameters. Furthermore, one can observe the influence of differently doped samples.

The influence of substrate temperature and hydrogen flow rate on the layer deposition is additionally studied by a variety of optical spectroscopy methods. Microstructure parameter as well as hydrogen content is derived from Si-H absorption in the infrared, while the Tauc-Lorentz band gap is derived from variable angle spectroscopic ellipsometry. Moreover, the parameters for which crystallization occurs were found by Raman spectroscopy. The combination of the variety of techniques provides a detailed insight in the optical, structural, and electrical properties of the samples studied.

DS 44.8 Fri 9:30 Poster E

Photoluminescence of $CuIn_XGa_{1-X}Se_2$ absorbers and solar cells — •Sven Schönherr[1], Jakob Haarstrich[1], Udo Reislöhner[1], Carsten Ronning[1], and Thorsten Rissom[2] — [1]Institut für Festkörperphysik, Friedrich Schiller Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Helmholtz Zentrum Berlin für Materialien und Energie, Solar Energy Research, Institute for Technology, Lise-Meitner-Campus, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Photoluminescence (PL) has been studied on high-efficiency CdS/CIGS solar cells. The sample layers were illuminated by a HeNe-Laser in a PL setup with a spot size of 1mm and in a micro-PL (μPL) setup, where the laser beam was focused by a microscope objective down to reach a spatial resolution of $\sim$1 μm at the focal spot on the sample. The samples were mounted in a LHe flow cryostat and studied as a function of temperatures from 3.5 to 300 K.

Photoluminescence spectra were measured from the front and the back site of the Cu(In,Ga)Se_2 absorber layers and different peak energies were detected corresponding to the typical band-gap grading of CIGS solar cells. Additionally, the micro-PL measurements have shown a lateral peak shift, which could be interpreted as varying grains or by different luminescence radiation of grains and grain boundaries.

DS 44.9 Fri 9:30 Poster E

Silicon Nanoparticle Sprayed Films and Their Characterization by Ellipsometry, Raman Spectroscopy, and Atomic Force Microscopy — •Falko Seidel[1], Iulia G. Korodi[1], Stephan Koth[2], Ronny Fritzsche[3], Ovidiu D. Gordan[1], Reinhard R. Baumann[2], Michael Mehring[3], and Dietrich R.T. Zahn[1] — [1]Semiconductor Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany — [2]Institute for Print and Media Technology, Chemnitz University of Technology, D-09107 Chemnitz, Germany — [3]Coordination Chemistry, Chemnitz University of Technology, D-09111 Chemnitz, Germany

The growth of single crystal Silicon (c-Si) for photovoltaic applications is an expensive, high temperature requiring process. Regarding thin film solar cells less expensive processes such as spray coating would be advantageous. In this work dispersions of silicon nanoparticles (Si NP) having nominal sizes of 6 nm and 40 nm dispersed in a solution are sprayed on 0.1 mm thick molybdenum foils. The spraying setup works in a glovebox under nitrogen atmosphere and an in-line spectroscopic ellipsometer (SE) enables to investigate optical properties during film deposition. In order to obtain microcrystalline Silicon (mc-Si), an high energetic light flash sinters the accumulated Si NP. Raman spectroscopy probes the sintering process while atomic force microscopy (AFM) probes the surface morphology and roughness. Eventually, results of these three methods are presented and discussed in the light of the potential of spray coating for producing low cost, large area photovoltaic devices.

DS 44.10 Fri 9:30 Poster E

Electrical Characterization of Doped a-Si:H/c-Si Heterojunctions, Produced by Magnetron Sputtering — •Frank Nobis, Hartmut Kupfer, Philipp Schäfer, Dietrich R. T. Zahn, and Frank Richter — Chemnitz University of Technology, Institute of Physics, 09107 Chemnitz, Germany

We investigate thin films of doped hydrogenated amorphous silicon (a-Si:H) with respect to their application in photovoltaics. Currently, chemical vapour deposition is widely used for the formation of such films providing comparably low defect density and relatively high efficiency of dopants. Our method of choice is pulsed dc magnetron sputtering because this method is well suitable to realize a high-efficiency inline technology for solar cells formation. Thereby a key question in our investigations is the amount of electrically active dopants which can be achieved in the magnetron sputtered films.

We deposited doped a-Si:H films onto oppositely doped silicon wafers. Crucial deposition parameters like substrate temperature and hydrogen partial pressure were varied. The resulting heterojunctions were characterized with respect to electrical film properties and doping efficiencies. Under certain conditions very good rectification ratios of the produced pn-junctions were achieved. This finding is correlated with the doping efficiency in the amorphous films.

DS 44.11 Fri 9:30 Poster E

Photoluminescence measurement of polycrystalline CdTe made of high purity source material — •Hannes Hempel, Christian Kraft, Christoph Heisler, Sebastina Geburt, Carsten Ronning, and Werner Wesch — Institute of solid state physics, Friedrich Schiller Universität Jena, Helmholtzweg 3, 07743 Jena

CdTe is a common material for thin film solar cells. However, the mainly used CdTe source material is known to contain a high number of intrinsic defects and impurities. In this work we investigate the defect structure of high purity CdTe by means of Photoluminescence, which is a common method to detect the energy levels of defects in the band gap of semiconductors. We used a 633nm HeNe-Laser at sample temperatures of 8 K. The examined samples were processed in a new vacuum system based on the PVD method. They yield significantly different spectra on as-grown samples compared to those measured on samples which are grown by the standard process, since the double peak at 1,55eV was hardly detectable and the A-center correlated transition vanished. Instead a peak at 1,50eV with pronounced phonon coupling was observed. The 1,50eV peak is known from other measurements but has not been characterized so far. The intention of this work is to characterize this new feature and the influence of post deposition treatments of the CdTe layers on the PL spectra.

DS 44.12 Fri 9:30 Poster E

Deposition control of thin-film silicon solar cells by optical emission spectroscopy — •Vitalij Schmidt[1], Wiebke Hachmann[1], Stefan Gruss[2], Helmut Stiebig[2], and Ulrich Heinzmann[1] — [1]Fak. f. Physik, Uni Bielefeld, Germany — [2]Malibu GmbH & Co. KG

The improvement of the layer quality is one key factor to the overall efficiency of thin-film silicon solar cells. Plasma-enhanced chemical vapor deposition (PECVD) is a widely applied production process for microcrystalline silicon layers (μc-Si). The μc-Si layer is used as a bottom cell material within a tandem stack.

Via in-situ spectroscopy we gain information on the deposition used as feedback for process control. The plasma emits light, characteristic for its composition. Research is done on the hydrogen dilution of silane as it affects the crystalline fraction of the grown layer. Observing the time development of the specific wavelengths for hydrogen and silane (H_α at 656 nm and SiH* at 414 nm) we determine the layer-thickness dependent crystallinity.

In order to achieve μc-Si layers with constant crystallinity we focus on monitoring and adjustment of the SiH*/H_α-ratio. This ratio can be used for a homogeneous μc-Si layer deposition.

DS 44.13 Fri 9:30 Poster E

Growth of large-size-two-dimensional pentacene crystalline for high performance organic transistors — Chuan Du, Wenchong Wang, •Liqiang Li, Harald Fuchs, and Lifeng Chi — Physikalisches Institut and Center for Nanotechnology (CeNTech) Universität Münster, 48149 Münster Germany

Organic field-effect transistors (OFETs) have been the focus of intense research in the last two decades. Several studies have been proposed to improve the field effect mobility, by optimizing the deposition of organic semiconductor films and modifying surface properties of the gate insulators. The interface between gate dielectric and organic film plays an important role in field-effect behavior because the first two to three molecular layers next to the dielectric interface dominate the charge transport. Self-assembled monolayer (SAM) has been widely used to modify the gate electric surface (SiO2).

Here we demonstrate that the use of SiO2 gate dielectric modified with a single molecular layer of PTCDI-C8 can yield a high-mobility organic semiconductor of pentacene. An average hole mobility about 1.71 cm2/VS is achieved, that is ten times higher than the mobility of devices fabricated on bare SiO2 under the same fabrication conditions (0.15 cm2/VS) and it is also higher than that of the devices with OTS treated SiO2. The differences in film morphology and grain size obtained from AFM-Images and the X-ray diffraction patterns could be used to explain the high mobility resulting from the modification of SiO2 with a single layer of PTCDI-C8.

DS 44.14 Fri 9:30 Poster E

Use of PEDOT:PSS as Gate Electrode on a PMMA Gate Dielectric in Transparent Organic Field Effect Transistors — •Steffen Heuser, Jan Hartel, Christopher Keil, and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen

Indium tin oxide (*ITO*) on glass was patterned to provide a transparent interdigitated source-drain electrode array. As an organic semiconductor, semitransparent 40 nm *pentacene* were prepared by physical vapor deposition (PVD) under fine vacuum conditions. As gate dielectric, a thin transparent polymer layer (500 nm) of *PMMA* (*poly*(*methylmethacrylate*)) was deposited by spin-coating on top of the *pentacene* layer. Finally, a layer of *PEDOT*:*PSS* was prepared by spin-coating and used as gate-electrode. The transistor structures were measured and as the characteristic properties the threshold voltage and the on/off ratio of the structures will be discussed.

DS 44.15 Fri 9:30 Poster E

Doping and Phase Separation in Mixtures of Differently Substituted Phthalocyanines Measured in-situ During Film Growth — •Lena Cornelius, Max Beu, Christopher Keil, and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen

Mixed films of the unsubstituted phthalocyaninato copper ($H_{16}PcCu$) and its perfluorinated derivative ($F_{16}PcCu$) with different molecular mixtures were prepared by co-evaporation and were analyzed in-situ by conduction measurements. High admixtures of $H_{16}PcCu$ in $F_{16}PcCu$ films disturbed the charge transport, presumably caused by phase separation and the presence of poorly conducting grains of $H_{16}PcCu$ in the conductive $F_{16}PcCu$ films. Very low admixtures increased the conductivity, indicating a successful doping of $F_{16}PcCu$ by $H_{16}PcCu$. For pure thin films of $F_{16}PcCu$ well-defined crystal structures ($\beta_{bilayer}$-structure and β-structure) were determined in the literature and correlated to optical absorption bands. Optical transmission spectroscopy performed for the present films revealed the presence of these structures as expected for the pure films of $F_{16}PcCu$ and also for low admixtures of $H_{16}PcCu$ but a disturbance of the $F_{16}PcCu$ solid state structure was seen for increased admixtures of $H_{16}PcCu$. The proportions of the $\beta_{bilayer}$-structure and the β-structure of $F_{16}PcCu$ were decreased indicating disturbance of the $F_{16}PcCu$ film growth by a large admixture of $H_{16}PcCu$.

DS 44.16 Fri 9:30 Poster E

Light-induced p-doping of P3HT and P3HT/Fulleren blends by oxygen studied by Photoelectron Spectroscopy — •Umut Aygül, Holger Hintz, Heiko Peisert, and Thomas Chassé — Universität Tübingen, Institut für Physikalische und Theoretische Chemie, Auf der Morgenstelle 18, 72076 Tübingen

Organic photovoltaic cells (OPVC) based on donor-acceptor blends present a quite new technique for environmental friendly energy conversion although their efficiency and lifetime is currently rather low compared to inorganic solar cells. Detailed unterstanding of the electronic properties and interface properties (e.g. electrodes or other organic materials) are required to increase efficiency and lifetime. We study the influence of oxygen and light (AM 1.5) on the energy level alignment of Poly(3-hexylthiophene) (P3HT) and P3HT/Fullerene blend films. The samples are alternately exposed to light and oxygen and then annealed. The electronic properties and interface properties are monitored subsequently by X-ray and ultraviolet photoelectron spectroscopy (XPS/UPS) in order to probe both changes in the electronic structure and the chemical composition of the film. The exposure to light and oxygen leads to reversible and irreversible effects. The reversible effect is an oxygen induced p-doping of the semiconductor whereas the irreversible part is the photooxidation of the polymer which does not alter the electronic structure.

DS 44.17 Fri 9:30 Poster E

Does NEXAFS provide valuable information on the electronic influence of functional groups? — •Christian Schmidt, Tobias Breuer, Michael Klues, and Gregor Witte — Molekulare Festkörperphysik, Philipps-Universität Marburg, Germany

Motivated by their possible application in organic electronic devices a variety of systematically modified acene derivatives is nowadays investigated. A question that frequently arises is whether the introduction of functional groups (e.g. electronegative fluorine atoms) affects the electronic system by intramolecular dipoles or by direct interaction with the aromatic system. From an experimental point of view this question is not easy accessible, especially for thin films. Our approach is to employ NEXAFS as a versatile tool that gives insight into both: geometric and electronic structure. We investigated differently substituted molecules and addressed functional groups directly by conducting angular dependent NEXAFS experiments at the corresponding absorption K-edge (e.g. F1s, O1s, N1s). In order to interpret these spectra, we contrast them with carbon K-edge spectra of the aromatic backbone and provide a detailed analysis of the origin and dichroism of related resonances. This systematic use of NEXAFS enables us to give further insight into the electronic properties of derivatized acenes.

DS 44.18 Fri 9:30 Poster E

The influence of typical degradative stresses on the constitutive parts of polymer/fullerene solar cells — •Vida Turkovic, Sebastian Engmann, Roland Rösch, Harald Hoppe, and Gerhard Gobsch — Technische Universität Ilmenau, Institut für Physik, Experimentalphysik 1, Weimarer Straße 32, 98693 Ilmenau

Improving the long time stability of organic photovoltaics is one of the key issues towards making them competitive with their inorganic counterparts. In order to separately investigate the degradation of the electrodes and the photoactive layer in thin film devices, we developed a simple approach based on ambient and inert atmosphere tests. The devices were characterized with standard spectroscopic measurements and electrical characterization, complemented by large-area imaging methods.

DS 44.19 Fri 9:30 Poster E

Influence of triplet excitons on the performance and lifetime of polymer-based organic light-emitting diodes — •Oili Pekkola[1], Fabian Etzold[2], Andrea Gassmann[1], Frédéric Laquai[2], Christian Melzer[1], and Heinz von Segger[1] — [1]Electronic Materials Department, Institute of Materials Science, Technische Universität Darmstadt, Petersenstr. 23, 64287 Darmstadt, Germany — [2]Max Planck Research Group for Organic Optoelectronics, Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Although large progress has been made in the development of polymer-based organic light-emitting diodes (PLEDs), their lifetime still remains a problematic issue. One of the topics in PLEDs studied to a lesser extent is the influence of the high density of non-emissive triplet excitons on the device lifetime.

In this work, PLEDs with a poly(p-phenylene vinylene) (PPV) derivative are utilized. The influence of triplet excitons on the fatigue of the PLEDs is investigated by increasing their amount in the PPV film. Therefore, PPV singlet excitons are converted to triplets by mixing different concentrations of the triplet sensitizer platinum (II) octaethylporphine ketone (PtOEPK) into the PPV matrix. The increase in the triplet population is characterized by photoluminescence and photoinduced absorption measurements. Both t50 and t90 lifetimes of the diodes are drastically shortened in the presence of PtOEPK, which indicates that the additional triplets might be harmful to the diode stability and lifetime.

DS 44.20 Fri 9:30 Poster E

Organic semiconductor devices in smart textiles: Challenges while approaching fibre shaped structures — •Tobias Könyves-Toth, Andrea Gassmann, and Heinz von Seggern — Electronic Materials Department, Institute of Materials Science, Technische Universität Darmstadt, Petersenstr. 23, 64287 Darmstadt, Germany

In the development of smart textiles already realized prototypes utilize embedded LEDs, displays or interactive communication devices based on inorganic semiconductor technology. Yet, these wearable smart textiles are not always comfortable since inorganic devices are stiff and rigid. On the other hand, organic electronic devices can be realized on flexible substrates employing very thin active layers of only about 100 nm thickness.

The aim of the present work is to process organic semiconductor based devices directly on fibre surfaces. This task is challenging as manufacturing related problems due to the cylindrical shape of the fibre substrates and their small diameter of about 0.2 mm have to be overcome. Here, we present our findings on the handling of fibre substrates in order to process working devices. In particular, the choice of proper fibre materials, ways to acquire smooth fibre surfaces and the structuring and encapsulation of fibre-shaped devices will be addressed. Additionally, methods to characterize the functionality of the devices will be presented.

DS 44.21 Fri 9:30 Poster E

IR spectroscopy on metal oxide p-doped thin films of organic semiconductors — •Sven Tengeler[1,4], Tobias Glaser[1,4], Sebastian Beck[1,4], Bernd Lunkenheimer[2,4], Daniela Donhauser[3,4], and Annemarie Pucci[1,4] — [1]Universität Heidelberg, Kirchhoff-Institut für Physik, INF 227, 69120 Heidelberg — [2]Universität Mainz, Institut für Physikalische Chemie, Jakob Welder Weg 11, 55099 Mainz — [3]Technische Universität Braunschweig, Institut für Hochfrequenztechnik, Schleinitzstr. 22, 38106 Braunschweig — [4]InnovationLab GmbH, Speyerer Str. 4, 69115 Heidelberg

To understand the underlying mechanisms of electrochemical doping of organic semiconductors, we investigated thin films of the organic ambipolar charge-transport materials N,N'-bis(1-naphtyl)-N,N'-diphenyl-1,1'-biphenyl-4,4'-diamine (α-NPD) and 4,4'-Bis(N-carbazolyl)-1,1'-biphenyl (CBP), each doped with the inorganic acceptor molybdenum oxide (MoO_3). The doping efficiency of MoO_3 was analyzed for various doping concentrations and substrate temperatures using in-situ infrared spectroscopy in a UHV setup. We introduce our experimental setup, explain the measured spectra and compare them with DFT-calculations for the neutral as well as the charged matrix molecules in order to estimate the charge-generation efficiency.

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

DS 44.22 Fri 9:30 Poster E

IR spectroscopic studies on charge transfer in thin films of donor-acceptor complexes — •Sebastian Beck[1,4], Diana Nanova[2,4], Andreas Fuchs[3,4], Christian Lennartz[3,4], Tobias Glaser[1,4], Michael Kröger[2,4], and Annemarie Pucci[1,4] — [1]Universität Heidelberg, Kirchhoff-Institut für Physik, INF 227, 69120

Heidelberg — [2]Technische Universität Braunschweig, Institut für Hochfrequenztechnik, Schleinitzstr. 22, 38106 Braunschweig — [3]BASF SE, 67056 Ludwigshafen — [4]InnovationLab GmbH, Speyerer Str. 4, 69115 Heidelberg

In the ongoing development of organic electronic devices, new materials with adjustable properties are needed in order to meet different specific requirements. Prototypical examples are the charge transfer complexes (CT complexes) with the acceptor 7,7,8,8-Tetracyanoquinodimethan (TCNQ). In this study, the degree of charge transfer in thin films of organic CT complexes of TCNQ which were deposited via thermal evaporation was determined with infrared spectroscopy. We demonstrate a linear relationship between the shift in the energy of the CN-stretching mode of TCNQ and the charge transfer in the CT complexes. The measured correlation very well agrees with DFT calculations. For Na-TCNQ we observe a splitting in the CN-stretching mode peak, which can be explained by the coupling of two modes and was confirmed by the calculations. In CT complexes with partial charge transfer the appearance of an electronic excitation is demonstrated.

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

DS 44.23 Fri 9:30 Poster E

Wavelength dependent pathways in the degradation of P3HT and PCPDTBT — •Ulf Dettinger[1], Holger Hintz[1], Catharina Sessler[1], Heiko Peisert[1], Hans Joachim Egelhaaf[2], and Thomas Chassé[1] — [1]Eberhard-Karls-University, Institute for Physical and Theoretical Chemistry, Auf der Morgenstelle 18, D-72076 Tübingen, Germany — [2]Konarka Technologies GmbH, Landgrabenstr. 94, D-90443 Nürnberg, Germany

Organic photovoltaic (OPV) present a promising and cost effective technology for the energy market of the future. Although the race for high efficiencies is still on the run, the stability of the single device materials becomes more and more important. Therefore photo degradation of P3HT and PCPDTBT thin films was investigated under both standard Air Mass 1.5 conditions and single wavelength illumination. The degradation of the materials was monitored using UV/VIS and FTIR transmission spectroscopy. Generally PCPDTBT exhibits an enhanced stability compared to the state of the art material P3HT. The effectiveness of the photo reaction does not follow the absorption spectrum in the case of P3HT suggesting a radical based mechanism which is not initiated by the polymer absorption[1].

[1] H. Hintz, H.J. Egelhaaf, L. Lüer, J. Hauch, H. Peisert, T. Chassé Chem. Mater., 2011, 23 (2), 145-154

DS 44.24 Fri 9:30 Poster E

Influence of different additives to an organic hole conductor for hybrid photovoltaics — •Ingolf Segger, Ulrike Kuck, Sascha Hackmann, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

In recent years, remarkably high power conversion efficiencies have been reported for dye sensitized solar cells (DSSCs). Therefore they are considered as a promising candidate for market-relevant thin-film solar cells. However, high performance DSSCs usually employ a liquid iodide-based electrolyte as an essential component for dye regeneration which introduces significant drawbacks for commercialisation like thermal instability and the requirement for highly reliable sealing techniques.

It has been shown that the organic hole conductor 2,2',7,7'-tetrakis(N,N-di-p-methoxyphenylamine)-9,9'-spirobifluorene (spiro-OMeTAD) has the potential to replace the liquid electrolyte in DSSCs. In order to achieve high power conversion efficiencies in such solid-state DSSCs, different additives to spiro-OMeTAD like Lithium bis(trifluoromethylsulfonyl)imide (Li-TFSI) and pyridine derivatives are required. Both optical properties and the electronic structure of materials used in photovoltaics play an important role for device performance. Therefore in this study spiro-OMeTAD thin-films with the addition of those different essential additives were investigated by means of photoluminescence spectroscopy, UV-VIS absorption spectroscopy and photoemission spectroscopy.

DS 44.25 Fri 9:30 Poster E

Transient spectroscopic studies of high performance PTB7-PCBM films for organic photovoltaics: the effect of processing additive and fullerene absorption — •Clare Dyer-Smith, Hannah Mangold, and Frédéric Laquai — Max-Planck Institut für Polymerforschung, Mainz, Germany

Photovoltaic blends of the thienothiophene-benzodithiophene polymer PTB7 with PC70BM have shown power conversion efficiencies exceeding 7%. Using transient absorption spectroscopy, we study the photoexcitation dynamics in PTB7:PC70BM and PTB7:PC60BM blend films across more than six orders of magnitude in time and across the entire spectral range from the visible to the near-infrared. We observe a fast spectral relaxation in the blend film, as well as a spectral relaxation in the pristine polymer emission detected using picosecond time-resolved fluorescence spectroscopy. We assign the latter to energetic disorder in the polymer, while the assignment of the former is the subject of ongoing investigation. Secondly, we characterize the dynamics of excited states in the heretofore unreported time range from 1 to 100 ns, crucial for the understanding of charge separation and recombination in organic solar cells. Our studies indicate that the use of the processing additive di-iodooctane produces longer lived charges in blend films, despite the presence of a more finely interpenetrating blend morphology and therefore a larger interfacial area. We also study the effect of varying the fullerene acceptor in the blend film to investigate the contribution of light absorption in the fullerene component to charge generation in the solar cell.

DS 44.26 Fri 9:30 Poster E

Metallic nano-particles embedded in small molecule organic solar cells (OSCs) : Optical and electrical effects. — •Till Hoheisel, Andreas Hille, André Merten, Moritz Riede, Lukas M. Eng, and Karl Leo — IAPP, TU Dresden

OSCs have the potential to provide electrical energy in a resource saving way by combining small material consumption with low temperature production processes in comparison to silicon solar cells. The thickness and absorption in OSCs is currently limited by the mobility of photo-generated excitons. We have systematically investigated the effect of plasmon active metallic nano-structures for enhancing the electromagnetic field close to the absorbing layers. We show that enhanced absorption inside typical organic solar cell material single layers is due to metallic nano-particles. The electrical effects of metallic nano-particles inside vacuum processed small molecule solar cells are investigated by varying the distance between the nano-particle layer and the absorber layer.

DS 44.27 Fri 9:30 Poster E

I-V Characteristics of Copper Phthalocyanine Based Laterally Stacked Devices Fabricated by Semiconductor Processing — •J. Ghosh[1], D. Reuter[1], M. Rennau[1], K. Hiller[1], G. Salvan[1], M. Fronk[1], D.R.T. Zahn[1], C. C. Bof Bufon[1,2], and O. Schmidt[1,2] — [1]Chemnitz University of Technology, Germany — [2]Institute for Integrative Nanosciences, IFW Dresden, Germany

This work presents a new approach of fabricating arrays of electrodes, separated by sub-micrometer gaps allowing the systematic investigation of electric properties of organic semiconductors. The laterally stacked devices are fabricated by using a trench isolation technique for separating different electrical potentials, as it is known for micromachining technologies like Single Crystal Reactive Ion Etching and Metallization (SCREAM). The essential part of this process is the patterning of sub-micrometer trenches onto the silicon substrate in a single lithographic step. Afterwards, the trenches are refilled by SiO_2 to allow the precise tuning of the electrode separation gap. The metal electrodes are formed via magnetron sputtering. This technological approach allows us to fabricate device structures with a transport channel length in the range of 100-250 nm by conventional photolithography. In this experiment, three different metals like Au, Co, and Ni were used as the electrode materials, while copper phthalocyanine, being deposited by thermal evaporation in high vacuum, was employed as the organic semiconductor under evaluation. The correlation, observed between the current across the junction and the gap between the electrodes, can be explained by the space charge limited current model.

DS 44.28 Fri 9:30 Poster E

Vibrational analysis of thin Zinc Tetraphenylporphyrin films on Si(111) — •Stephan Peter Kate[1], Karsten Hinrichs[1], Norbert Esser[1], Jörg Rappich[2], and Simona Pop[1] — [1]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Albert-Einstein Str. 9, Berlin, 12489, Germany — [2]Helmholtz-Zentrum for Materials and Energy GmbH, Kekulestraße 5, Berlin, 12489, Germany

The presented work includes micro-Raman spectroscopy for the analysis of the vibrational modes of the ZnTPP (Zinc Tetraphenylporphyrin) thin films. Resonant Raman spectra are taken with the 458 nm (2,71 eV) Ar-laser line which is located in the spectral range of the B-band.

The Raman frequencies are compared for samples with different film thicknesses and ZnTPP crystalline powder. A systematic shift with increasing film thickness is observed for some vibrational modes while others are not affected by the film thickness. The changes in the vibrational bands are discussed with respect to symmetry and in the vibration involved parts of the molecules.

DS 44.29 Fri 9:30 Poster E

Optical and structural properties of organic heterostructures: PTCDA and SnPc on Au(111) — •Kristin Wachter, Marco Gruenewald, Matthias Meissner, Falko Sojka, Roman Forker, and Torsten Fritz — University of Jena, Institute of Solid State Physics, Max-Wien-Platz 1, 07743 Jena, Germany

The optical and structural properties of organic heterostructures of ultrathin 3,4,9,10-perylenetetracarboxylic-dianhydride (PTCDA) and tin(II)-phthalocyanine (SnPc) films grown on the reconstructed Au(111) surface were investigated by Differential Reflectance Spectroscopy (DRS), Low Energy Electron Diffraction (LEED) and Scanning Tunneling Microscopy (STM) under ultra-high vacuum conditions. The film growth was carried out by organic molecular beam epitaxy (OMBE). In our optical spectra we find clear indications for a strong interaction between the substrate and the first monolayer SnPc and PTCDA, respectively. The overlying PTCDA, however, decouples from the first monolayer. Furthermore, from LEED measurements we conclude a commensurate structure of a SnPc monolayer film on Au(111) at room temperature.

DS 44.30 Fri 9:30 Poster E

Interface analysis of aluminum doped zinc oxide sputtered on copper phthalocyanine thin films — •Cathy Jodocy, Ingolf Segger, Patrick Ries, and Matthias Wuttig — Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

Organic electronics have attracted considerate attention due to their wide range of possible applications as well as their suitability for inexpensive and highly scalable processing techniques. Optoelectronic devices like organic solar cells and organic light-emitting diodes with a transparent top electrode are of interest since they allow a larger variety of organic-inorganic layer systems including semitransparent stacks.

We have deposited the transparent conductive oxide (TCO) material aluminum doped zinc oxide (ZnO:Al) as a top cathode above an organic layer. Copper phthalocyanine (CuPc) is an excellent material for the use as a donor in organic heterojunctions in organic solar cells. Furthermore its very rigid crystal structure is supposed to prevent degradation upon the impact of high kinetic energy particles generated during sputter deposition of the TCO. For the deposition of the ZnO:Al thin films we have used a dc magnetron sputtering process whereby layers with an excellent performance can be produced at low temperatures.

In this study a detailed investigation of the interface between sputtered ZnO:Al and the underlying CuPc layer is presented. The influence of sputter damage in the organic layer is characterized with photoelectron spectroscopy and x-ray diffraction measurements.

DS 44.31 Fri 9:30 Poster E

Study of excited states and a model for exciton-polaron interaction in P3HT — •Shine Philip[1], Klaus Müller[1], Matthias Richter[1], Marinus Kunst[2], and Dieter Schmeisser[1] — [1]Brandenburgische Technische Universität Cottbus, Angewandte Physik-Sensorik, 03046 Cottbus, Germany — [2]Helmholtz-Zentrum Berlin, Institut für Solare Brennstoffe (E-I6), Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Organic semiconductors efficiently harvest light in the region of the solar spectrum due to a high absorption/extinction coefficient.In our work we study the electronic structure and the charge carrier dynamics of polymeric organic semiconductor regioregular poly(3-hexylthiophen-2,5-diyl) (P3HT), an ideal p-type semiconductor and a widely used conjugated polymer, and blends with the fullerene derivative phenyl-C61-butyric acid methyl ester (PCBM), an electron acceptor material. The study was done with the help of time resolved microwave conductivity (TRMC) for contactless investigation of bulk carrier dynamics, optical spectroscopy, ultraviolet photoelectron spectroscopy(UPS) and high resolution X-ray absorption spectroscopy(XAS) which investigates excited states of rr-P3HT. From the data obtained we could infer the positions of the valence and conduction band, the existence of two excitons as well as the co-existence of one dimensional and two dimensional polarons. Based on our spectroscopic data we propose a model in which the scattering of virtual polarons and excitons are shown to create mobile polaronic charge carriers.

DS 44.32 Fri 9:30 Poster E

Influence of pre-structuring on self-organized pattern formation at organic-metal interfaces - experiment vs. modeling — •Florian Szillat and S.G. Mayr — Leibniz-Institut fuer Oberflaechenmodifizierung, Translationszentrum fuer regenerative Medizin und Fakultaet fuer Physik und Geowissenschaften der Universitaet Leipzig, 04318 Leipzig

Self-organized pattern formation observed during physical vapor deposition of organic materials on inorganic substrates leads to characteristic structure evolution up to film thicknesses of some tens of nanometers. By employing a combined experimental-computational approach we demonstrate the capability of a continuum model to describe structure evolution during poly(bisphenol A)carbonate deposition on rough copper surfaces [1]. The next step on the route to computer-assisted interface engineering is carried out by modeling poly(bisphenol A)carbonate deposition on pre-structured copper surfaces by means of stochastic rate equations. These predictions are compared with experiments on physical vapor deposition experiments with pre-patterned copper substrates, which are subsequently analyzed with atomic force microscopy. This allows conclusions on the underlying physical processes. This project is funded by the German BMBF, PTJ-BIO, Grant Number: 0313909.

[1] F. Szillat and S. G. Mayr, Phys. Rev. B 84, 115462 (2011)

DS 44.33 Fri 9:30 Poster E

Comparison of Structural Properties of Layers of Different Phthalocyanines on Reconstructed GaAs(001) **Surfaces** — •Linda Riele[1,2], Benjamin Buick[1], Ihor M. Kupchak[3], Bjorn-Ove Fimland[4], Patrick Vogt[2], and Wolfgang Richter[1] — [1]Università di Roma Tor Vergata, Rome, Italy — [2]TU Berlin, Berlin, Germany — [3]V. Lashkaryov Institute of semiconductor physics NAS, Kyiv, Ukraine — [4]Dept. of Electronics and Telecommunications, NTNU, Trondheim, Norway

The conductivity of organic layers depends crucially on the orientation and ordering of the molecules. Depending on the specific application in optoelectronic or electronic devices, a controlled growth of these layers on inorganic substrates is therefore desired. In this work we present a comparison of Raman scattering experiments of layers (up to 20 nm thick) of planar Cu phthalocyanines, and non-planar Pb phthalocyanines deposited on $c(4 \times 4)$ and (2×4) reconstructed surfaces of GaAs(001). The dependence of the molecular order on the surface reconstruction is analyzed by measuring the intensity of the Raman peaks as a function of sample rotation. We observe periodic intensity changes of the Pc vibrational modes with the rotation angle. These periodic changes have a fixed relation to the GaAs substrate phonons. This is an indication for well ordered Pc layers with a fixed geometrical relation to the substrate implying an epitaxial-like growth mode. DFT calculations allow a symmetry assignment of the vibrational modes (A_1, B_1, B_2, etc.) and allow consequently model calculations with the different Raman tensors.

DS 44.34 Fri 9:30 Poster E

Interrelation between Substrate Roughness and Thin-Film Structure of Functionalized Acenes on Graphite — •Tobias Breuer[1], Ingo Salzmann[2], Jan Götzen[1], Martin Oehzelt[2], Antonia Morherr[1], Norbert Koch[2], and Gregor Witte[1] — [1]AG Molekulare Festkörperphysik, Philipps-Universität Marburg, D-35032 Marburg — [2]Institut für Physik, Humboldt-Universität zu Berlin, D-12489 Berlin

We analyzed the growth of differently modified pentacenes (perfluoropentacene (PFP) and pentacenetetrone (P-TET)) on graphite and demonstrate that both, the resulting morphology and the crystalline structure of the films, critically depend on the microroughness of the substrate. On well-ordered highly oriented pyrolytic graphite (HOPG) surfaces prepared by exfoliation, both molecular materials form exceptionally smooth films, which consist of large-area molecularly flat islands yielding an overall low roughness. Interestingly, in these films molecules adopt a recumbent orientation, while on defective substrates, created by brief ion sputtering, the molecules adopt an upright orientation and form nonconnected islands exhibiting a significantly increased film roughness. Our study not only underlines the possibility to prepare very smooth films on a weakly interacting substrate but also emphasizes the importance of a proper substrate preparation and the significance of precise knowledge of substrate-surface properties to control the resulting structure of organic films.

[1] J. Götzen et al., Phys. Rev. B 81, 0854406 (2010).

[2] T. Breuer et al., Cryst. Growth Des. 11, 4996 (2011).

DS 44.35 Fri 9:30 Poster E

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

N,N'-Ditridecylperylene-3,4,9,10-tetracarboxylic diimide (PTCDIC-13) is a promising acceptor material for organic solar cells. To fully utilize the potential of this material, the growth of thin films of PTCDI-C13 has been studied. Particular attention has been devoted to understanding the electronic and chemical properties of the interface between the organic layer and the metal contact. The interaction between the PTCDI-C13 and the metal strongly influences the charge carrier transport mechanisms and thus the efficiency of the solar cell. In this study thin films of PTCDI-C13 with a thickness varying from single monolayers up to 20 nm, have been evaporated on Au, Ag, Cu and Al surfaces. The energy level alignment between the valence band of each metal and the frontier molecular orbitals of the subsequently deposited organic layer has been determined by Ultraviolet Photoelectron Spectroscopy (UPS). The chemical bonding is investigated by X-ray Photoelectron Spectroscopy (XPS). Finally, the nature of the interaction between the organic layer and the metal surface has been determined from the formation of interface states and the position of the energy levels.

DS 44.36 Fri 9:30 Poster E

A multitechnique investigation of substituted pentacene nanorods — •Sabine-Antonia Savu[1], Simon Schundelmaier[1], Sabine Abb[1], Christina Tönshoff[2], Holger F. Bettinger[2], Maria Benedetta Casu[1], and Thomas Chassé[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Tübingen, Deutschland — [2]Institut für Organische Chemie, Universität Tübingen, Tübingen, Deutschland

We report our investigation on nanorods of two newly synthesized substituted pentacenes by using X-ray photoemission spectroscopy (XPS), near edge X-ray absorption fine structure (NEXAFS) spectroscopy, and atomic force microscopy (AFM). The nanorods were deposited on Au(111). We have analyzed the photoemission spectra in detail by using a fitting procedure. XPS thickness dependent spectra show a different screening of the core-hole at the interface, while NEXAFS investigations suggest a molecular arrangement similar to what reported for pentacene thin films. In addition, the morphology of the nanorods has been investigated by using AFM, evaluating the nanorod characteristics also from a statistical point of view.

DS 44.37 Fri 9:30 Poster E

FePc/metals: Influence of the 3d-open shell on the interface properties — •Fotini Petraki[1], Heiko Peisert[1], Florian Latteyer[1], Umut Aygül[1], Johannes Uihlein[1], Antje Vollmer[2], and Thomas Chassé[1] — [1]Universität Tübingen, IPTC, Auf der Morgenstelle 18, 72076 Tübingen, Germany — [2]Helmholtz Zentrum Berlin für Materialien und Energie, Elektronenspeicherring BESSY II, Albert-Einstein-Str. 15, 12489 Berlin, Germany

The present work is focused on transition metal phthalocyanines (TMPcs) and in particular, on iron phthalocyanine (FePc), a two dimensional MPc where the central atom is a Fe2+ ion. The magnetic properties of such molecules depend strongly on the electronic configuration of the central metal atom, and in particular, the occupation of the 3d-related states. Recent studies, on TMPcs (TM: Co, Mn) by X-ray absorption (XAS) and resonant photoemission spectroscopy (ResPES) revealed a quite strong interaction between the TM and metallic substrates through charge transfer towards the 3d unoccupied electronic states.The investigation of FePc/ Au(100) and FePc/ Ag(111) interfaces by XAS and ResPES confirmed strong interactions also at these interfaces. The detailed electronic configuration however, depends on the substrate under consideration. Effects of chemical changes during the interface formation in terms of different oxidation state for the Fe-ion were detected also by XPS, confirming the partial filling of the 3d-open shell of Fe from electrons coming from the metallic substrate. From resonant PES measurements at the Fe-edge information on the local electronic structure of the occupied orbitals was also obtained.

DS 44.38 Fri 9:30 Poster E

Ultrathin oligothiophene films for organic electronics applications — •Nina Arzt[1], Benedikt Rösner[1], Andreas Späth[1], Norman Schmidt[1], Hannes Schulz[2], and Rainer Fink[1] — [1]Universität Erlangen-Nürnberg, Department Chemie u. Pharmazie, Physikalische Chemie II, Egerlandstr. 3, 91058 Erlangen, Germany — [2]Universität Erlangen-Nürnberg, Department Chemie u. Pharmazie, Theoretische Chemie, Egerlandstr. 3, 91058 Erlangen, Germany

Oligothiophenes are attracting major attention due to their potential application as semiconducting material for cheap, flexible and large-area electronic devices such as organic field effect transistors [1]. For their successful preparation homogenous and highly ordered thin films of the semiconductor material are required. We have successfully studied two different kinds of oligothiophenes with respect to their local arrangements. From low-energy electron diffraction (LEED) we deduce long-range ordered films of flat-lying molecules when deposited on Ag(100) single crystals. In contrast, the utilization of Si3N4 membranes, small domains are observed in scanning transmission X-ray microspectroscopy (STXM). Furthermore, NEXAFS studies using the PolLux-STXM installed at the Swiss Light Source offers more direct insight into the electronic structure of these microcrystalline films. We discuss the crystal growth properties considering the specific interface interactions. The work is funded by the BMBF, project 05 K10WEA.

[1] M. Halik, H. Klauk, U. Zschieschang, G. Schmid, S. Ponomarenko, S. Kirchmeyer, W. Weber, Adv. Mater., 2003, 15, 917-922.

DS 44.39 Fri 9:30 Poster E

Nucleation of Perylene films on SAM-covered Gold Surfaces — •André Pick and Gregor Witte — Molekulare Festkörperphysik, Philipps-Universität Marburg, Germany

Previous studies have demonstrated the ability to control the nucleation of organic semiconductor films on a micron scale by patterning of silicon dioxide substrates by means of micro contact printing of self-assembled monolayers. In that way arrays of organic micro-crystallites have been fabricated that are well suited for the fabrication of organic field-effect transistors (OFETS) [1]. It was found that the roughness of stamped domains of the used octadecyltrichlorsilane (OTS), the chemical termination and the mechanical contrast are critical parameters for selective crystal nucleation. To analyze microscopic mechanisms of this nucleation more qualitatively, we have studied the initial stage of growth of perylene (PER) films on gold surfaces that were pre-treated with aliphatic organothiol SAMs of various chain length and different chemical termination. Substrates were coated by the SAMs either homogeneously or selectively by using micro-contact printing. PER films were prepared by molecular beam deposition under vacuum conditions and the resulting film structures were characterized by means of atomic force microscopy. Moreover, to study the influence of substrate roughness these experiments have been carried out on single crystalline Au(111)/mica and poly-crystalline gold substrates. The observed variety of PER structures indicate that the actual film thickness of the thiol layer is an important parameter which will be discussed.

[1] A.L. Briseno et al., Nature Vol. 444, 913 (2006)

DS 44.40 Fri 9:30 Poster E

Structural properties of molecular mixtures of pentacene and diindenoperylene — •Antje Aufderheide[1], Katharina Broch[1], Jiří Novák[1], Alexander Hinderhofer[1], Roberto Nervo[2], Rupak Banerjee[1], Alexander Gerlach[1], and Frank Schreiber[1] — [1]Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen, Germany — [2]ESRF, 6 Rue Jules Horowitz, BP 220, 38043 Grenoble Cedex 9, France

We investigate mixtures of pentacene (PEN) and diindenoperylene (DIP) with different mixing ratios using x-ray reflectivity (XRR) and grazing incidence x-ray diffraction (GIXD). With a multilayer model we fit the reflectivity data including the first-order Bragg peak. Furthermore, we determine the coherent island size from the GIXD peak widths. Using the results of the in- and out-of-plane measurements we determine the ordering behavior which changes with the mixing ratio [1] and compare it with mixtures of similar molecules [2,3]. A first approach to a phenomenological description of the mixed film structure is made.

[1] A. Aufderheide et al., in preparation [2] A. Hinderhofer et al., J. Chem. Phys., **134**, 104702 (2011). [3] J. P. Reinhardt et al., in preparation

DS 44.41 Fri 9:30 Poster E

Impact of the 3d-electronic states of nickel and manganese phthalocyanines on electronic interface properties to metal substrates — •Johannes Uihlein[1], Umut Aygül[1], Fotini Petraki[1], Florian Latteyer[1], Patrick Hoffmann[2], Antje Vollmer[2], Heiko Peisert[1], and Thomas Chassé[1] — [1]Universität Tübingen, IPTC, Auf der Morgenstelle 18, 72076 Tübingen, Germany — [2]Helmholtz Zentrum Berlin für Materialien und Energie, Elektronenspeicherring BESSY II, Albert-Einstein-Str. 15, 12489 Berlin, Germany

In recent years there has been growing interest in the field of thin organic semiconducting films due to their successful application in optical and electronic devices. Transition-metal phthalocyanines (TMPc) are a promising class of organic semiconductors with remarkable electronic and magnetic properties and they are capable candidates for future applications. The electronic configuration of the central metal atom strongly affects the electronic properties of such molecules in thin films and of corresponding interfaces [1]. Interactions at the interface between transition-metal phthalocyanines (MnPc, NiPc) and single-crystalline metal substrates (Au(100), Ag(111)) are studied using X-ray absorption (XAS) and photoemission spectroscopy. In all cases, charge transfer processes from metallic substrates to the metal 3d levels of the phthalocyanine are found. However, the detailed electronic situation depends clearly on the system under consideration.
[1] F. Petraki et. al., J. Phys. Chem. C 115 (2011), 21334-21340.

DS 44.42 Fri 9:30 Poster E

Impact of Annealing of Structural, Optical and Electrical Properties of CoPc thin films — Husam El-Nasser[1], •Dominik Meyer[2], Philip Schulz[2], Christian Effertz[2], and Matthias Wuttig[2] — [1]Departement of Physics, Al al-Bayt University, Mafraq-Jordan — [2]I. Institute of Physics (IA), RWTH Aachen University, Germany

Organic materials are well known for their high potential as cost-efficient alternatives in the field of thin film based optoelectronic devices. Especially the wide range of possible materials offers promising opportunities to tailor crucial optical and electronic properties of the functional layers. Metal-phthalocyanines are commonly employed as p-type semiconducting layer in organic electronics. Yet the choice of the central metal atom has significant impact on the inter- and intramolecular characteristics. In this study we investigate structural, optical and electrical properties of cobalt-phthalocyanine (CoPc) as an alternative to the regularly used CuPc and ZnPc with a wide range of analytical setups. The XRD diffraction pattern present CoPc to be of high crystal order with a single sharp peak at $2\theta = 6.9\,^\circ$ corresponding to an interlayer spacing of $d = 12.72$ Å. Subsequent annealing revealed an increase of the mean grain size from 11 nm to 26 nm for the as deposited and annealed samples, respectively. The effect of annealing to optical constants as well as the charge carrier mobility is analyzed. Finally, we conclude on the impact of annealing affects to improve the suitability of this molecule for optoelectronic applications and to understand the driving forces in thin film formation and charge transport.

DS 44.43 Fri 9:30 Poster E

Influence of chemical transformation on molecular orientation and surface texture of aluminium and gallium phthalocyanines thin films — •Florian Latteyer[1], Tamara Basova[2], Vitaly Kiselev[3], Heiko Peisert[1], and Thomas Chassé[1] — [1]Universität Tübingen, IPTC, Auf der Morgenstelle 18, 72076 Tübingen, Germany. — [2]Nikolaev Institute of Inorganic Chemistry SB RAS, 630090 Novosibirsk, Russia. — [3]Institute of Chemical Kinetics and Combustion SB RAS, 630090 Novosibirsk, Russia.

The chemical transformation of aluminium and gallium phthalocyanines (AlClPc and GaClPc) in thin films to the mu-(oxo)dimers (PcAl)2O and (PcGa)2O has been investigated. IR, Raman, and XPS spectroscopies, as well as quantum chemical computations (DFT) were employed to study the structure of the films before and after annealing. It has been found that the annealing of AlClPc and GaClPc thin films in the presence of humidified nitrogen resulted in the formation of the corresponding mu-(oxo)dimers (PcAl)2O and (PcGa)2O. On the other hand, the annealing of the same films in the presence of oxygen led, beside to the formation of mu-(oxo)dimers, to a partial degradation and consequently to a parallel reaction. The structure changes of the thin films during annealing were studied using in situ Raman spectroscopy and AFM technique. Both, the initial AlClPc film and the obtained mu-(oxo)dimer (PcAl)2O film formed after annealing were disordered. At the same time, the molecules of the mu-(oxo)dimer (PcGa)2O formed out of GaClPc turned out to form a preferential standing orientation with respect to the substrate surface.

DS 44.44 Fri 9:30 Poster E

***In situ* X-ray diffraction on mixed pentacene - perfluoropentacene thin films** — •Christian Frank[1], Jiří Novák[1], Alexander Gerlach[1], Alexander Hinderhofer[1], Roberto Nervo[2], Katharina Broch[1], Giovanni Ligorio[1], and Frank Schreiber[1] — [1]Institut für Angwandte Physik, Universität Tübingen, Germany — [2]ESRF, Grenoble, France

Using X-ray diffraction [1] and optical spectrocopy [2] we have studied binary mixtures on SiO_x, consisting of pentacene (PEN) and perfluorinated-pentacene (PFP). For films with different mixing ratios we investigate the coexistence of the two mixed PEN:PFP phases together with the phases of the pure molecules. We show, that the σ-phase, with its long molecular axis oriented nearly perpendicular to the substrate is thermally stable, whereas the appearance of the λ-phase with its molecules lying flat, is induced by low temperatures. Based on previous results [1,3], the growth of these films is studied in real-time to measure the evolution of the coherent island size for both phases: We find that for PFP_1:PEN_2-mixtures the nucleation of the λ-phase is significantly retarded compared to PFP_2:PEN_1-mixtures. The study is complemented with a temperature series of pure PFP and post-growth measurements. [1] A. Hinderhofer, C. Frank, T. Hosokai, A. Resta, A. Gerlach, and F. Schreiber, *J. Chem. Phys.* **134** (2011), 104702. [2] K. Broch, U. Heinemeyer, A. Hinderhofer, F. Anger, R. Scholz, A. Gerlach, and F. Schreiber, *Phys. Rev. B* **83** (2011), 245307. [3] S. Kowarik, A. Gerlach, S. Sellner, F. Schreiber, L. Cavalcanti, and O. Konovalov, *Phys. Rev. Lett.* **96** (2006), 125504.

DS 44.45 Fri 9:30 Poster E

Interface Effects on Soret Band Excitations in Magnesium-Tetraphenylporphyrin Thin Films observed by Second-Harmonic Generation Spectroscopy — •Jan Metje, Klaus Stallberg, and Winfried Daum — Institute of Energy Research and Physical Technologies, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld

MgTPP films with thicknesses from 10 to 40 nm evaporated in UHV conditions on fused silica were studied using optical second-harmonic generation (SHG), UV-VIS absorption spectroscopy and AFM. The SHG spectra of the films exhibit two resonances in the spectral region of the Soret band of the molecule ($S_0 \rightarrow S_2$) at 2.95 eV and at about 2.7 eV. The 2.95 eV band agrees in energy with that of MgTPP molecules dissolved in benzene, indicating the presence of weakly interacting molecules. The 2.7 eV SHG band is strongly red-shifted with respect to the Soret band of the aggregated bulk molecules of the film, for which our UV-VIS spectra show an absorption band at 2.81 eV. SHG spectra from films deposited on oxidized Si(100) allow us to relate the SHG strength of the porphyrin bands to that of the silicon E_1 interband transitions. The comparatively weak porphyrin SHG signals indicate an interface effect. The low energy of 2.7 eV in comparison to the bulk transition energy points to strongly interacting molecules presumably located at the SiO_2/MgTPP interface.

Work supported by the NTH School for Contacts in Nanosystems

DS 44.46 Fri 9:30 Poster E

BioRef - the new, versatle reflectometer at HZB — •Marcus Trapp[1], Martin Kreuzer[2], Markus Strobl[3], Michael Grunze[1], Reiner Dahint[1], and Roland Steitz[2] — [1]Universität Heidelberg — [2]Helmholtz Zentrum Berlin — [3]European Spallation Source AB

The BioRef reflectometer was built in collaboration between the University of Heidelberg and the Helmholtz Zentrum Berlin (HZB). It offers the unique possibility to combine neutron reflectivity and in situ ATR-FTIR measurement on a sample at the same time. Despite these unique features an upgrade of the instrument is in progress in order to expand its capabilities even further.
The upgrade in progress will increase the available wavelength resolution up to 11% at a constant $\Delta\lambda/\lambda$ and will allow to resolve lateral structure with high resolution using the spin echo resolved gracing incidence technique (SERGIS).
The resent development of the instrument as well as further perspectives will be presented.

DS 44.47 Fri 9:30 Poster E

Investigation of the electronic properties of FePc by photoemission spectroscopy — •Quratulain Tariq, Susi Lindner, and Martin Knupfer — IFW Dresden, HelmholtzStr. 20, 01069 Dresden

Recently there has been much interest in the fundamental processes at the interfaces involving organic semiconductors and metals, since they represent a key factor in nearly all important aspects of device performance. Transition metal phthalocyanines have already obtained substantial attention of researchers due to many different potential applications in organic light emitting diodes, organic field effect transistors, organic photovoltaic cells and organic spintronic devices. Surface and interface analytical studies have generated critical insight into these fundamental processes at the interfaces. We investigate the electronic properties of iron phthalocyanine on noble metal single crystals using x-ray photoemission spectroscopy and valence band ultra-violet photoemission spectroscopy.

DS 44.48 Fri 9:30 Poster E

Spin-coating of Metal-organic Structures and (Magneto-) Optical Characterization — •Frank Lungwitz[1], Michael Fronk[1], Frederik Schleife[2], Dietrich R.T. Zahn[1], and Georgeta Salvan[1] — [1]Physics Department, Chemnitz University of Technology, Chemnitz, Germany — [2]Chemistry Department, Universität Leipzig, Leipzig, Germany

Optical and magneto-optical characterization of molecular complexes is an important tool for the development of molecular spintronic devices. The technique of spin-coating for preparing thin films (~ 50 nm to 100 nm) is often used for molecules which are not stable at higher temperatures required for preparation techniques like organic molecular beam deposition (OMBD). Here the spin-coating process is optimized for several organic molecules with multiple metal centres.

The silicon substrates are coated with a solution of the investigated material in a solvent, e.g. methanol. To prevent or at least minimize external influences the spin-coating process is performed in a glove-box under nitrogen atmosphere.

The first step of characterization is to determine the actual film thickness and the optical constants of the material using variable angle spectroscopic ellipsometry (VASE). In addition, layer properties like roughness, inhomogeneity, or optical anisotropy are derived from the VASE data. The polar magneto-optical Kerr effect measurements are used to determine magnetic properties and the Voigt constant of the material.

DS 44.49 Fri 9:30 Poster E

Influence of metal nanoparticles on the optical properties of molecular thin films — •Verena Kolb[1], Nadezda Tarakina[2], Jochen Manara[4], Andrès Guerrero Martìnez[3], and Jens Pflaum[1,4] — [1]Experimental Physics VI, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — [2]Experimental Physics III, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — [3]Departamento de Química Física, Universidade de Vigo, 36310 Vigo, Spain — [4]ZAE Bayern, D-97074 Würzburg

Utilization of plasmonic effects at metal nanoparticle surfaces provides an interesting approach to modify the optical properties of molecular thin films and thereby, to enhance their effective absorption. This enhancement is caused by an increase of the near-field component and the scattering of incident light and might be applied in e.g. organic photovoltaic (OPV) cells. In this contribution we present our latest results on synthesis and characterization of metallic nanoparticles. Silver nanocubes were prepared by wet-chemistry from CF_3COOAg-precursor. Complementary structural investigation by TEM, REM and X-ray confirmed the cubic morphology and single crystallinity. By UV-VIS spectrocopy the characteristic spectral features related to the plasmonic resonances of the nanoparticles were identified. Finally, the particles were embedded in an ITO/PEDOT:PSS/DIP layer structure, in analogy to standard OPV architectures, to analyze their influence on optical properties of the active molecular layer by Raman-spectroscopy.

DS 44.50 Fri 9:30 Poster E

Organophosphonate monolayer functionalization of planar and nano-porous aluminum oxide — •Anshuma Pathak[1], Björn Braunschweig[2], Achyut Bora[1], Hongdan Yan[3], Peter Lemmens[3], Winfried Daum[4], and Marc Tornow[1] — [1]IHT, TU Braunschweig, Germany — [2]LFG, University of Erlangen-Nuremberg, Germany — [3]IPKM, TU Braunschweig, Germany — [4]IEPT, TU Clausthal, Germany

Self-assembled monolayers (SAMs) of molecules on metal oxides are of increasing interest for organic electronics. We have deposited SAMs of aliphatic organophosphonates on different aluminum oxide substrates, including sapphire, polycrystalline Al/Al_2O_3 and nano-porous, amorphous aluminum oxide (AAO). Water contact angles in the range 95-120° and AFM measurements with RMS roughness down to $\sim$0.2 nm revealed homogeneous SAM formation. We used FTIR and Sum Frequency Generation (SFG) spectroscopy to investigate the molecular ordering of the layers. The positions of the asymmetric and symmetric CH_2 vibrational peaks determined by FTIR were below 2918 cm^{-1} and below 2850 cm^{-1}, respectively, indicating densely packed, crystalline layers. Remarkably, we observed only very small or even no intensity of CH2 peaks in the SFG spectra on sapphire and AAO. We conclude that the molecules in these SAMs are highly organized, practically in an all-trans conformation.

Work supported by the NTH School for Contacts in Nanosystems and by the Braunschweig International Graduate School of Metrology (IGSM).

DS 44.51 Fri 9:30 Poster E

Raman Spectroscopy on Potassium Doped Manganese Phthalocyanine Thin Films — •Michael Ludemann[1], Benjamin Mahns[2], Ovidiu D. Gordan[1], Martin Knupfer[2], and Dietrich R.T. Zahn[1] — [1]TU Chemnitz, 09126 Chemnitz, Germany — [2]IFW Dresden, 01069 Dresden, Germany

Alkali metals are well known as electron donors due to their strongly electropositive character. On the other hand, phthalocyanines are a known class of very stable organic molecules. Here, the influence of potassium intercalation on manganese phthalocyanine (MnPc), an archetype magnetic molecule, is investigated by *in situ* Raman spectroscopy. MnPc thin films ($\leq$ 10 nm) are prepared by organic molecular beam deposition (OMBD) in ultra-high vacuum (UHV) conditions and potassium is evaporated afterwards. Charge transfer from the potassium atoms to MnPc leading to negatively charged MnPc molecules is clearly observed by pronounced spectral changes in the Raman spectra. In combination with theoretical results the amount of charge per molecule was analysed.

DS 44.52 Fri 9:30 Poster E

Ellipsometry and UPS-IPS Measurements on MnPc Layers on Silicon — •Francisc Haidu, Daniel Lehmann, Michael Fronk, Georgeta Salvan, and Dietrich R. T. Zahn — Chemnitz University of Technology, Semiconductor Physics, D-09107 Chemnitz, Germany

Spectroscopic Ellipsometry (SE) is an elegant technique to monitor in situ changes in the optical response of thin films. Moreover, physical quantities, e.g. optical constants and optical band gap can be determined from the data evaluation. The transport band gap can be determined using the combination of Ultraviolet Photoelectron Spectroscopy (UPS) with Inverse Photoelectron Spectroscopy (IPS). Phthalocyanines, in general, are well known for their physical and chemical stability. Manganese Phthalocyanine (MnPc), in contrast, has high affinity towards oxygen. MnPc thin films were studied by in situ SE and UPS in combination with IPS. Monitoring by SE was performed during thermally evaporating onto Si substrates and during exposure of the MnPc films to air, clean oxygen, and nitrogen, respectively. We see changes in the optical response due to oxidation. The optical band gap as obtained from the SE data is compared to the transport gap derived from UPS-IPS measurements.

DS 44.53 Fri 9:30 Poster E

Protective Layer on Indexable Inserts — •Dustin Fischer, Mario Eschner, Jan Glühmann, Christine Lorenz, Andreas Neidhardt, Christel Reinhold, Ullrich Reinhold, Michael Schneeweiss, and Hans-Dieter Schnabel — Westsächsische Hochschule Zwickau, University of Applied Sciences, Leupold-Institut, 08056 Zwickau, Germany

The use of uncoated indexable inserts and micro tools is a common procedure for cutting metals. In order to achieve an effective removal of material, a uniform abrasion is required at the cutting edge of the tool. Despite great thermal resistance of the tool there is a high risk of oxidization at high temperatures so that the sealing of the inserts is indicated. An aluminium oxide (Al_2O_3) coating performed by Atomic Layer Deposition is a method to positively influence the cutting parameters as well as the wear and tear.

DS 44.54 Fri 9:30 Poster E

Optical Properties of Alucone Thin Films and Composite Materials — •Lilit Ghazaryan, Adriana Szeghalmi, Ernst-Bernhard Kley, and Andreas Tünnermann — Institute of Applied Physics, Friedrich Schiller University, Jena, Germany

Atomic layer deposition (ALD) is a powerful thin film coating technique that allows to precisely controlling the film thickness of inorganic coatings based on sequential self-limiting surface reactions. Similar to ALD, molecular layer deposition (MLD) enables growing completely organic or organic-inorganic hybrid polymer thin films typically using bi- or multifunctional monomers. One class of such hybrid polymers alucones had been recently grown with MLD using trimethylaluminium (TMA) as inorganic and ethylene glycol (EG) as organic constituent. In this contribution we have investigated the optical properties of alucone thin films prepared by MLD for possible applications as low refractive index optical coatings. The refractive index of the film can be precisely controlled through the composition of the coating. Using various bifunctional organic precursors it is possible to adjust the refractive index of the coating film in a controlled manner. Hybrid organic/inorganic nanolaminates have been deposited with ALD aluminium oxide and MLD alucone layers. By calcination of alucone layers at elevated temperatures it is possible to tune the refractive index of the coating to desired value. These films may find application in graded refractive index optical elements.

DS 44.55 Fri 9:30 Poster E

Optical Properties of Alucone Thin Films and Composite Materials — •Lilit Ghazaryan, Adriana Szeghalmi, Ernst-Bernhard Kley, and Andreas Tünnermann — Institute of Applied Physics, Friedrich Schiller University, Jena, Germany

Atomic layer deposition (ALD) is a powerful thin film coating technique that allows to precisely controlling the film thickness of inorganic coatings based on sequential self-limiting surface reactions. Similar to ALD, molecular layer deposition (MLD) enables growing completely organic or organic-inorganic hybrid polymer thin films typically using bi- or multifunctional monomers. One class of such hybrid polymers alucones had been recently grown with MLD using trimethylaluminium (TMA) as inorganic and ethylene glycol (EG) as organic constituent. In this contribution we have investigated the optical properties of alucone thin films prepared by MLD for possible applications as low refractive index optical coatings. The refractive index of the film can be precisely controlled through the composition of the coating. Using various bifunctional organic precursors it is possible to adjust the refractive index of the coating film in a controlled manner. Hybrid organic/inorganic nanolaminates have been deposited with ALD aluminium oxide and MLD alucone layers. By calcination of alucone layers at elevated temperatures it is possible to tune the refractive index of the coating to desired value. These films may find application in graded refractive index optical elements.

DS 44.56 Fri 9:30 Poster E

Guided mode resonance sensors for monitoring film nucleation in atomic layer deposition — •Adriana Szeghalmi, Haiyue Yang, Ernst Bernhard Kley, and Andreas Tünnermann — Institute of Applied Physics, Friedrich Schiller University, Jena, Germany

Thin films produced by atomic layer deposition (ALD) have interesting electrical, optical, catalytic applications. It is well known that the film growth rate in the ALD process is constant, and the ALD film thickness can be precisely controlled through the number of ALD cycles. However, the effect of the substrate surface on the nucleation of the ALD layers is generally unexplored. The surface chemistry will influence the adsorption of the precursors. Depending on the surface material, the film growth might be constant, substrate-inhibited, or substrate-enhanced. The main challenge in the study of ALD film nucleation is the development of in situ detection methods with atomic sensitivity to trace very small amounts of film growing on the substrate surface. Here, we developed guided mode resonance grating (GMRG) sensors for the in situ detection of sub-nm thin coatings. The nucleation of TiO2 on Al2O3 surface has been monitored. The GMRG sensor indicates the formation of ca. 4 Angstrom titania on the alumina surface after two cycles, and a constant growth rate (ca. 0.4 Angstrom/cycle) afterwards. Hence, the number of reactive sites on the Al2O3 surface (OH groups) is much larger than on TiO2. The coverage of alumina with titania is rapidly completed within the first two cycles. The titania layer is already continuous at a film thickness of 4 Angstrom.

DS 44.57 Fri 9:30 Poster E

Atomic Layer Deposition of Strontium Titanate using TDMAT and AbsoluteSr — •Solveig Rentrop, Theresa Moebus, Barbara Abendroth, and Dirk C. Meyer — TU Bergakademie Freiberg, Institut für Experimentelle Physik, Leipziger Straße 23, 09596 Freiberg

Atomic layer deposition (ALD) is a well-known technique used for binary systems in industry. Tenary oxides are desirable for high-k-dielectrics und resistive switching memories. Here we present preliminary studies on deposition of SrTiO3 as a model system for ternary oxides. The used precursors in the ALD system are TDMAT, AbsoluteSr and H2O. At this we have succeeded optimized TiO2 layers in a temperature range from 323K up to a maximum temperature of 593 K, whereby the purge time for a deposition at 593 K has to be a little higher. At time we are going to optimize SrO layers. Because of the TDMAT temperature limit and the fact that AbsoluteSr is only reactive from 573 K, the precursors merely overlap in this range. Febrication of SrTiO3 may be facilitated by using StarTi as a precursor since it has an ALD window with temperatures better comparable to AbsoluteSr.

DS 44.58 Fri 9:30 Poster E

Variation of the growth behavior of copper oxide deposited via ALD on thermally pretreated CNTs — •Marcel Melzer[1], Thomas Waechtler[1,2], Steve Mueller[2], Holger Fiedler[2], Sascha Hermann[1,2], Raul D. Rodriguez[3], Alexander Villabona[3], Andrea Sendzik[3], Robert Mothes[4], Stefan E. Schulz[1,2], Thomas Gessner[1,2], Dietrisch R.T. Zahn[3], Michael Hietschold[3], and Heinrich Lang[4] — [1]Fraunhofer Institute for Electronic Nano Systems (ENAS), Technologie-Campus 3, D-09126 Chemnitz, Germany — [2]Center for Microtechnologies, Chemnitz University of Technology, D-09107 Chemnitz, Germany — [3]Institute of Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany — [4]Institute of Chemistry, Chemnitz University of Technology, D-09107 Chemnitz, Germany

For a number of applications, carbon nanotubes (CNTs) need to be functionalized by metallic or metal oxide thin films or nanoparticles. The current work is therefore considered with the thermal atomic layer deposition (ALD) of Cu_xO from the liquid Cu(I) β-diketonate $[({}^n\mathrm{Bu}_3\mathrm{P})^2\mathrm{Cu(acac)}]$ and wet oxygen at 135°C on carbon nanotubes. Since high quality CNT surfaces are chemically inert, a pretreatment is required. For this reason the influence of different thermal oxidations onto the subsequent Cu_xO ALD was investigated. Depending on the oxidation either the growth of particles or a rather layer like growth was observed. The Cu/C ratio measured via EDX reaches its maximal values for a pretreatment with oxygen. This suggests that the used precursor couples to oxygen surface groups.

DS 44.59 Fri 9:30 Poster E

Investigation of Linear Dichroism in ALD layers of TiO_2 — •Chittaranjan Das, Matthias Städter, Massimo Tallarida, and Dieter Schmeisser — Brandenburgische Technische Universität, Konrad Wachsmann Allee, 17, 03046, Cottbus, Germany

Titanium dioxide is on the most studied material due to its wide range of applications in various fields such as self cleaning, photocatalysis, solar cell, water splitting, bio-implants, etc. In order to increase its efficiency in water splitting and solar cell, it is necessary to understand the crystal structure and electronic properties in thin films. In our approach we are investigating the X-ray linear dichroism (XLD) of thin layers of TiO_2. XLD studies have been done in multiferroics, antiferromagnetic, and ferromagnetic materials, but a very less amount of work have been done in studying XLD effect of TiO_2 thin films. These layers are grown by in-situ atomic layer deposition (ALD) system and are investigated with X-ray absorption spectroscopy (XAS) at BESSY II, Berlin. ALD is a promising technique to grow thin films on different substrates conveniently due to its uniform deposition property. XAS study will also help us to better understand the interfacial electronic properties of thin films of TiO_2.

DS 44.60 Fri 9:30 Poster E

Atomlagenabscheidung von Antimonoxid — •Bodo Kalkofen[1], Max Klingsporn[2], Bernd Garke[3] und Edmund Burte[1] — [1]IMOS, Otto-von-Guericke-Universität Magdeburg — [2]IHP, Frankfurt (Oder) — [3]IEP, Universität Magdeburg

Dünne Schichten aus Antimonoxid wurden mittels Atomlagenabscheidung (ALD) auf Silicium aufgewachsen. Antimonoxid dient als Dotierstoff für Zinnoxid-Halbleiter, besitzt einen hohen optischen Brechungsindex und wird als Katalysator eingesetzt. Als Ausgangsstoffe für die Abscheidung wurden Triethylantimon (SbEt3) und Ozon eingesetzt. Typische Prozessparameter waren: SbEt3: 15ms/5s/8s (Puls-/Einwirk-/Spülzeit), O3: 3s/1s/13s; die Abscheidetemperaturen lagen im Bereich von 50°C bis 250°C. Die Schichtdicken und optischen Parameter wurden mittels spektroskopischer Ellipsometrie bestimmt. Die Schichten wurden weiterhin durch XPS, ToF-SIMS, SEM und HR-TEM analysiert, und die Stabilität der Schichten gegenüber Säureeinwirkung und bei Hochtemperaturprozessen wurde untersucht. Schichtwachstum wurde ab einer Temperatur von 100°C beobachtet. Im Bereich von 100°C bis 250°C stieg das Wachstum pro Zyklus linear mit T an und lag bei 250°C bei 0,65Å. Dabei konnten sehr homogene Schichten abgeschieden werden (1,6Å Min/Max-Variation bei 7,5nm Schichtdicke auf 150mm-Substrat). Die Analysen zeigten ein Interface von ca. 1,5nm SiO2 auf dem eingangs mit HF gereinigten Silicium unter den Schichten, die polykristalline Bereiche trotz der geringen Wachstumstemperaturen aufwiesen, was die gefundene hohe chemische Beständigkeit der Schichten gegenüber verschiedenen Säuren erklären kann.