Thin Films Division
Fachverband Dünne Schichten (DS)

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Overview of Invited Talks and Sessions

(lecture rooms GER 37 and GER 38; Poster P1 and P2)

Gaede Prize

DS 29.1	Wed	14:00–14:45	TRE Phy	**Spin-split metallic surface states on semimetals and topological insulators** — •Philip Hofmann

Invited Talks

DS 1.1	Mon	10:15–11:00	GER 37	**High-performance liquid- and vacuum-processed CZTSSe photovoltaic devices** — •David B. Mitzi, Oki Gunawan, Teodor K. Todorov, Aaron R. Barkhouse, Kejia Wang, Byungha Shin, Richard Haight, Supratik Guha, Kathleen B. Reuter, Thomas Goislard de Monsabert, S. Jay Chey, Andrew J. Kellock
DS 4.1	Mon	14:00–14:45	GER 37	**Low temperature grown high efficiency Cu(In,Ga)Se2 and CdTe flexible solar cells** — •Ayodhya Tiwari, Adrian Chirila, Patrick Bloesch, Julian Perrenoud, Krenz Lukas, Sighrad Seyrling, Fabian Pianezzi, Rajneesh Verma, Shioro Nishiwaki, Stephan Buecheler, Yaroslav Romanyuk
DS 17.1	Tue	10:15–11:00	GER 37	**Chemical Nanolithography** — •Michael Grunze, Michael Zharnikov
DS 19.1	Tue	14:00–14:45	GER 37	**Laser micro- and nanoprocessing** — •Boris Chichkov
DS 27.1	Wed	10:15–11:00	GER 37	**Stochastic approach to electronic and spin thermal transport** — •Roberto D'Agosta
DS 30.1	Wed	15:00–15:45	GER 37	**Electrical spin injection in a hybrid organic/inorganic spin-polarized light emitting diode (spin-LED)** — •Ezekiel Johnston-Halperin
DS 44.1	Thu	10:15–11:00	GER 37	**Electronic Properties of Metal Nanoclusters Measured by Low Energy Ion-Surface Charge Exchange** — •Jory Yarmoff
DS 46.1	Thu	14:00–14:45	GER 37	**Structuring Graphene with He Ions** — •David C. Bell
DS 58.1	Fri	10:15–11:00	GER 37	**Development of Highly Efficient IV-VI Thermoelectric Materials** — •Yaniv Gelbstein

Invited talks of the joint symposium SKM-SYOP

See SKM-SYOP for the full program of the symposium.

SKM-SYOP 1.1	Mon	10:30–11:00	TRE Ma	**Charge separation in organic solar cells and the principle of detailed balance** — •Uwe Rau, Thomas Kirchartz
SKM-SYOP 1.2	Mon	11:00–11:30	TRE Ma	**Three-Dimensional Nanoscale Organization of Bulk Heterojunction Polymer Solar Cells** — •Joachim Loos
SKM-SYOP 1.3	Mon	11:30–12:00	TRE Ma	**Reliable prediction of charge transfer excitations using optimally tuned range-separated hybrid functionals** — •Leeor Kronik
SKM-SYOP 1.4	Mon	12:00–12:30	TRE Ma	**Charge separation and recombination in organic solar cells** — •James Durrant

SKM-SYOP 1.5	Mon	12:30–13:00	TRE Ma	**Efficient and stable organic vacuum deposited p-i-n-type tandem solar cells** — •Martin Pfeiffer

Invited talks of the joint symposium SKM-SYNP

See SKM-SYNP for the full program of the symposium.

SKM-SYNP 1.1	Wed	14:30–15:00	TRE Ma	**Quantum Optics on Photonic Chips** — •Dirk Englund, Brendan Shields, Hongkun Park, Mikhail Lukin, Kelley Rivoire, Jelena Vuckovic, Fariba Hatami
SKM-SYNP 1.2	Wed	15:00–15:30	TRE Ma	**Two-photon Interference from Separate Quantum Dots** — Edward Flagg, Andreas Muller, Sergey Polyakov, Alexander Ling, Alan Migdall, •Glenn S. Solomon
SKM-SYNP 1.3	Wed	15:30–16:00	TRE Ma	**Coherent optoelectronic control of a single exciton qubit** — •Artur Zrenner, Steffen Michaelis de Vasconcellos, Simon Gordon, Dirk Mantei, Wadim Quiring, Mohannad Al-Hmoud, Torsten Meier, Max Bichler, Andreas D. Wieck, Dirk Reuter
SKM-SYNP 1.4	Wed	16:15–16:45	TRE Ma	**Generation of non-classical states of light with site- and potential-controlled pyramidal quantum dots** — •Eli Kapon
SKM-SYNP 1.5	Wed	16:45–17:15	TRE Ma	**Semiconductor Devices for Quantum Photonics** — •Andrew Shields, Anthony Bennett, Mark Stevenson, Cameron Salter, Raj Patel, Ian Farrer, Christine Nicoll, David Ritchie

Invited talks of the joint symposium SKM-SYMF

See SKM-SYMF for the full program of the symposium.

SKM-SYMF 1.1	Thu	14:30–15:00	TRE Ma	**Visualizing the structural solid-liquid transition with colloidal suspensions** — •Peter Schall
SKM-SYMF 1.2	Thu	15:00–15:30	TRE Ma	**Crystallization process in suspensions of hard spheres** — •Tanja Schilling, Hans-Joachim Schoepe, Martin Oettel, George Opletal, Ian Snook
SKM-SYMF 1.3	Thu	15:30–16:00	TRE Ma	**Homogeneous bulk, surface, and edge nucleation in crystalline nanodroplets** — •Kari Dalnoki-Veress, Jessica Carvalho
SKM-SYMF 1.4	Thu	16:00–16:30	TRE Ma	**Polymer Crystallization: Ordered Structures in Complex Systems** — •Jens-Uwe Sommer
SKM-SYMF 1.5	Thu	16:30–17:00	TRE Ma	**Phase formation and microstructure development in multicomponent alloys** — •Jürgen Eckert

Topical Talks

DS 2.1	Mon	11:00–11:30	GER 37	**Cu(In,Ga)Se_2 solar cells: the importance of lateral variations of the absorber quality** — •Susanne Siebentritt
DS 2.2	Mon	11:30–12:00	GER 37	**Efficient Photovoltaic Devices using Multinary Chalcogenide Semiconductors** — •Hans-Werner Schock, Thomas Unold
DS 2.3	Mon	12:00–12:30	GER 37	**From Micro Meter to Mega Watt: Pentanary Chalcopyrite Thin film Solar Cells** — Joerg Palm, Alejandro Avellan, •Thomas Dalibor, Stefan Jost, Helmut Vogt, Thomas Niesen, Paul Mogensen, Franz Karg
DS 2.4	Mon	12:30–13:00	GER 37	**Electrical Characterization of Cu(In,Ga)(Se,S)$_2$ -Based Solar Cells at Low Temperatures** — •Udo Reislöhner
DS 5.1	Mon	14:45–15:15	GER 37	**Dünnschicht-Chalkogenid-Solarzellen: Überblick und Forschungsfelder** — •Michael Powalla
DS 18.1	Tue	11:00–11:30	GER 37	**Microcontact chemistry: surface reactions in nanoscale confinement** — •Bart Jan Ravoo
DS 18.2	Tue	11:30–12:00	GER 37	**Electrochemical Microstructuring** — Xinzhou Ma, Vadym Halka, •Rolf Schuster

DS 18.3	Tue	12:00–12:30	GER 37	**Electrochemical Oxidation and Anodization Lithography on Self-Assembled Monolayers** — •Stephanie Hoeppener
DS 18.4	Tue	12:30–13:00	GER 37	**Surface Structuring by Single Pulse Laser Interference: Principles and Applications** — •Johannes Boneberg
DS 28.1	Wed	11:00–11:30	GER 37	**Selective spin-blockade in interacting molecular interferometers** — •Milena Grifoni, Andrea Donarini, Georg Begemann
DS 28.2	Wed	11:30–12:00	GER 37	**Charge and Spin Transport through Single-Atom and Single-Molecule Junctions** — •Jörg Kröger
DS 28.3	Wed	12:00–12:30	GER 37	**The strange life of a molecular spin observed under a microscope** — •Germar Hoffmann
DS 31.1	Wed	15:45–16:15	GER 37	**Organic spintronics and the great potential of ferromagnetic metal-organic interfaces** — •Martin Aeschlimann
DS 45.2	Thu	11:15–11:45	GER 37	**Energy dissipation in the scattering of N_2 from W(110)** — •J. Inaki Juaristi
DS 47.1	Thu	14:45–15:15	GER 37	**Trails of kilovolt ions created by subsurface channeling** — •Thomas Michely, Alex Redinger, Sebastian Standop, Yudi Rosandi, Herbert Urbassek
DS 47.2	Thu	15:15–15:45	GER 37	**The impact of fast ions in pulsed laser deposition** — •Michael Schmid
DS 48.1	Thu	16:00–16:30	GER 37	**Ion beam doping of semiconductor nanowires** — •Carsten Ronning
DS 49.1	Thu	17:45–18:15	GER 37	**Nano-scale surface modifications produced by highly charged ion impact** — •Friedrich Aumayr
DS 59.1	Fri	11:00–11:30	GER 37	**Nanocrystalline silicon for thermoelectricity** — •Gabi Schierning
DS 59.2	Fri	11:30–12:00	GER 37	**Nanoscale Thermoelectrics** — •Jan D. König
DS 59.3	Fri	12:00–12:30	GER 37	**Thermal transport and thermoelectric effect in thin semiconductor membranes** — •Matthias Schmidt, Thorben Bartsch, Christian Heyn, Wolfgang Hansen
DS 59.4	Fri	12:30–13:00	GER 37	**Theoretical studies of electrical cross-plane transport in semiconductor multilayer heterostructures** — •Peter Kratzer, Vladimir M. Fomin

Sessions

DS 1.1–1.1	Mon	10:15–11:00	GER 37	**Invited – Mitzi**
DS 2.1–2.4	Mon	11:00–13:00	GER 37	**Thin Film Chalcogenide Photovoltaics I (Focused Session – Organiser: Ronning)**
DS 3.1–3.1	Mon	13:00–13:30	POT 06	**Invited – Böer**
DS 4.1–4.1	Mon	14:00–14:45	GER 37	**Invited – Tiwari**
DS 5.1–5.3	Mon	14:45–15:45	GER 37	**Thin Film Chalcogenide Photovoltaics II (Focused Session – Organiser: Ronning)**
DS 6.1–6.6	Mon	16:00–17:30	GER 37	**Thin Film Chalcogenide Photovoltaics III (Focused Session – Organiser: Ronning)**
DS 7.1–7.7	Mon	17:45–19:30	GER 37	**Layer Properties: Electrical, Optical and Mechanical Properties**
DS 8.1–8.6	Mon	10:15–11:45	GER 38	**Thin Film Characterisation: Structure Analysis and Composition (XRD, TEM, XPS, SIMS, RBS, ...) I**
DS 9.1–9.4	Mon	12:00–13:00	GER 38	**Thin Film Characterisation: Structure Analysis and Composition (XRD, TEM, XPS, SIMS, RBS, ...) II**
DS 10.1–10.6	Mon	14:00–15:30	GER 38	**Thin Film Characterisation: Structure Analysis and Composition (XRD, TEM, XPS, SIMS, RBS, ...) III**
DS 11.1–11.5	Mon	15:45–17:00	GER 38	**Thin Film Characterisation: Structure Analysis and Composition (XRD, TEM, XPS, SIMS, RBS, ...) IV**
DS 12.1–12.5	Mon	17:15–18:30	GER 38	**Layer Deposition Processes**
DS 13.1–13.12	Mon	14:00–17:30	ZEU 222	**Organic Electronics and Photovoltaics CPP-I (jointly with CPP, HL, and O)**
DS 14.1–14.4	Mon	17:45–18:45	FOE Anorg	**Organic Electronics and Photovoltaics HL-I (jointly with CPP, HL, and O)**
DS 15.1–15.8	Mon	15:00–17:00	PHY C213	**Plasmonics and Nanophotonics O-I (jointly with HL and O)**
DS 16.1–16.8	Mon	17:15–19:15	PHY C213	**Plasmonics and Nanophotonics O-II (jointly with HL and O)**

DS 17.1–17.1	Tue	10:15–11:00	GER 37	**Invited – Grunze**
DS 18.1–18.4	Tue	11:00–13:00	GER 37	**Progress in Micro- and Nanopatterning: Techniques and Applications I (Focused Session, jointly with O – Organisers: Graaf, Hartmann)**
DS 19.1–19.1	Tue	14:00–14:45	GER 37	**Invited – Chichkov**
DS 20.1–20.8	Tue	10:15–12:15	GER 38	**Application of Thin Films**
DS 21.1–21.6	Tue	13:45–15:15	GER 38	**High-k and Low-k Dielectrics (jointly with DF)**
DS 22.1–22.6	Tue	10:15–13:00	POT 151	**Focussed Session: Inorganic/Organic Semiconductor Hybrid Structures I (jointly with HL and O)**
DS 23.1–23.2	Tue	14:15–15:15	POT 151	**Focussed Session: Inorganic/Organic Semiconductor Hybrid Structures II (jointly with HL and O)**
DS 24.1–24.9	Tue	10:30–13:00	ZEU 222	**Organic Electronics and Photovoltaics CPP-II (jointly with CPP, HL, and O)**
DS 25.1–25.5	Tue	14:00–15:15	ZEU 222	**Organic Electronics and Photovoltaics CPP-III (jointly with CPP, HL, and O)**
DS 26.1–26.7	Tue	11:15–13:00	WIL A317	**Plasmonics and Nanophotonics O-III (jointly with HL and O)**
DS 27.1–27.1	Wed	10:15–11:00	GER 37	**Invited – D'Agosta**
DS 28.1–28.5	Wed	11:00–13:00	GER 37	**Spins in Organic Materials I (Focused Session, jointly with MA – Organisers: Salvan, Hess, Timm)**
DS 29.1–29.1	Wed	14:00–14:45	TRE Phy	**Gaede Prize Talk – Philip Hofmann**
DS 30.1–30.1	Wed	15:00–15:45	GER 37	**Invited – Johnston-Halperin**
DS 31.1–31.3	Wed	15:45–16:45	GER 37	**Spins in Organic Materials II (Focused Session, jointly with MA – Organisers: Salvan, Hess, Timm)**
DS 32.1–32.6	Wed	17:00–18:30	GER 37	**Spins in Organic Materials III (Focused Session, jointly with MA – Organisers: Salvan, Hess, Timm)**
DS 33.1–33.8	Wed	11:00–13:00	GER 38	**Progress in Micro- and Nanopatterning: Techniques and Applications II (Focused Session, jointly with O – Organisers: Graaf, Hartmann)**
DS 34.1–34.8	Wed	15:00–17:00	GER 38	**Progress in Micro- and Nanopatterning: Techniques and Applications III (Focused Session, jointly with O – Organisers: Graaf, Hartmann)**
DS 35.1–35.8	Wed	17:15–19:15	GER 38	**Plasmonics and Nanophotonics (jointly with HL and O)**
DS 36.1–36.8	Wed	10:15–12:15	POT 251	**Plasmonics and Nanophotonics HL-I (jointly with HL and O)**
DS 37.1–37.7	Wed	11:15–13:00	WIL A317	**Plasmonics and Nanophotonics O-IV (jointly with HL and O)**
DS 38.1–38.8	Wed	15:00–17:00	WIL A317	**Plasmonics and Nanophotonics O-V (jointly with HL and O)**
DS 39.1–39.10	Wed	14:00–17:00	ZEU 222	**Organic Electronics and Photovoltaics CPP-IV (jointly with CPP, HL, and O)**
DS 40.1–40.12	Wed	10:15–13:30	FOE Anorg	**Organic Electronics and Photovoltaics HL-II (jointly with CPP, HL, and O)**
DS 41.1–41.6	Wed	18:00–19:30	FOE Anorg	**Organic Electronics and Photovoltaics HL-III (jointly with CPP, HL, and O)**
DS 42.1–42.125	Wed	15:00–17:30	P1	**Poster I: Progress in Micro- and Nanopatterning: Techniques and Applications (jointly with O); Spins in Organic Materials; Ion Interactions with Nano Scale Materials; Organic Electronics and Photovoltaics; Plasmonics and Nanophotonics (jointly with HL and O); High-k and Low-k Dielectrics (jointly with DF); Organic Thin Films; Nanoengineered Thin Films; Layer Deposition Processes; Layer Properties: Electrical, Optical, and Mechanical Properties; Thin Film Characterisation: Structure Analysis and Composition; Application of Thin Films**
DS 43.1–43.18	Wed	15:00–17:30	P2	**Poster II: Thin Film Chalcogenide Photovoltaics; Thermoelectric Materials, Thin Films, and Nanostructures**
DS 44.1–44.1	Thu	10:15–11:00	GER 37	**Invited – Yarmoff**
DS 45.1–45.7	Thu	11:00–13:00	GER 37	**Ion Interactions with Nano Scale Materials I (Focused Session – Organisers: Diesing, Facsko)**
DS 46.1–46.1	Thu	14:00–14:45	GER 37	**Invited – Bell**

DS 47.1–47.2	Thu	14:45–15:45	GER 37	**Ion Interactions with Nano Scale Materials II (Focused Session – Organisers: Diesing, Facsko)**
DS 48.1–48.5	Thu	16:00–17:30	GER 37	**Ion Interactions with Nano Scale Materials III (Focused Session – Organisers: Diesing, Facsko)**
DS 49.1–49.5	Thu	17:45–19:15	GER 37	**Ion Interactions with Nano Scale Materials IV (Focused Session – Organisers: Diesing, Facsko)**
DS 50.1–50.6	Thu	10:15–11:45	GER 38	**Organic Electronics and Photovoltaics I (jointly with CPP, HL, and O)**
DS 51.1–51.4	Thu	12:00–13:00	GER 38	**Organic Electronics and Photovoltaics II (jointly with CPP, HL, and O)**
DS 52.1–52.8	Thu	14:00–16:00	GER 38	**Organic Electronics and Photovoltaics III (jointly with CPP, HL, and O)**
DS 53.1–53.6	Thu	16:15–17:45	GER 38	**Organic Electronics and Photovoltaics IV (jointly with CPP, HL, and O)**
DS 54.1–54.6	Thu	18:00–19:30	GER 38	**Nanoengineered Thin Films**
DS 55.1–55.5	Thu	14:30–17:15	POT 51	**Focused Session: Novel Green Laser Diodes (jointly with HL and O)**
DS 56.1–56.7	Thu	11:15–13:00	WIL A317	**Plasmonics and Nanophotonics O-VI (jointly with HL and O)**
DS 57.1–57.5	Thu	15:00–16:15	WIL A317	**Plasmonics and Nanophotonics O-VII (jointly with HL and O)**
DS 58.1–58.1	Fri	10:15–11:00	GER 37	**Invited – Gelbstein**
DS 59.1–59.4	Fri	11:00–13:00	GER 37	**Thermoelectric Materials, Thin Films, and Nanostructures I (Focused Session – Organisers: Nielsch, Rastelli, Balke)**
DS 60.1–60.7	Fri	14:00–15:45	GER 37	**Thermoelectric Materials, Thin Films, and Nanostructures II (Focused Session – Organisers: Nielsch, Rastelli, Balke)**
DS 61.1–61.6	Fri	16:00–17:30	GER 37	**Thermoelectric Materials, Thin Films, and Nanostructures III (Focused Session – Organisers: Nielsch, Rastelli, Balke)**
DS 62.1–62.6	Fri	10:15–11:45	GER 38	**Organic Thin Films I**
DS 63.1–63.4	Fri	12:00–13:00	GER 38	**Organic Thin Films II**
DS 64.1–64.7	Fri	14:00–15:45	GER 38	**Organic Thin Films III**
DS 65.1–65.6	Fri	16:00–17:30	GER 38	**Organic Thin Films IV**
DS 66.1–66.5	Fri	11:15–12:30	WIL B122	**Organic Electronics and Photovoltaics O-I (jointly with CPP, HL, and O)**

Annual General Meeting: German Vacuum Society (DVG)

Monday 18:45–19:15 GER 38

Annual General Meeting: Thin Films Division (DS)

Monday 19:15–19:45 GER 38

DS 1: Invited – Mitzi

Time: Monday 10:15–11:00 Location: GER 37

Invited Talk DS 1.1 Mon 10:15 GER 37

High-performance liquid- and vacuum-processed CZTSSe photovoltaic devices — •David B. Mitzi[1], Oki Gunawan[1], Teodor K. Todorov[1], Aaron R. Barkhouse[1], Kejia Wang[1], Byungha Shin[1], Richard Haight[1], Supratik Guha[1], Kathleen B. Reuter[1], Thomas Goislard de Monsabert[1], S. Jay Chey[1], and Andrew J. Kellock[2] — [1]IBM T. J. Watson Research Center, Yorktown Heights, NY, USA — [2]IBM Almaden Research Center, San Jose, CA, USA

While thin-film CdTe and CIGS (Cu-In-Ga-Se) photovoltaic technologies are increasing market share due to their cost competitiveness and high performance, reliance on the expensive and/or scarce elements Ga, In and Te, or the heavy metal Cd, has presented a potential obstacle to the target of terawatt deployment using these materials. The kesterites, $Cu_2ZnSnS_{4-y}Se_y$ (CZTSSe), are considered a promising alternative because of similar electronic properties to the two leading technologies and low-cost, readily-available constituents. This talk will focus on recent developments in fabricating high-performance CZTSSe devices. First, a simple particle-based liquid approach has been employed to prepare photovoltaic devices with a glass/Mo/CZTSSe ($y > 2$)/CdS/i-ZnO/ITO structure and with power conversion efficiencies of $> 9.5\,\%$, a record for the kesterites. Using a vacuum-based coevaporation approach, power conversion efficiencies of as high as 7

DS 2: Thin Film Chalcogenide Photovoltaics I (Focused Session – Organiser: Ronning)

Time: Monday 11:00–13:00 Location: GER 37

Topical Talk DS 2.1 Mon 11:00 GER 37

Cu(In,Ga)Se$_2$ solar cells: the importance of lateral variations of the absorber quality — •Susanne Siebentritt — University of Luxembourg, Laboratory for Photovoltaics, Belvaux, Luxembourg

Thin film solar cells are considered the second generation of photovoltaic technologies, because of their considerable cost reduction based on the small amounts of material and energy used in production. Among these technologies solar cells based on Cu(In,Ga)Se$_2$ show the highest efficiencies in the lab as well as in industry. Record efficiencies above 20 % have been reached with these polycrystalline solar cells.

It becomes more and more evident that lateral inhomogeneities, most prominently grain boundaries, limit the efficiency. Electrostatic band bending at grain boundaries appear a major obstacle for higher open circuit voltages. Fluctuations of the band gap and the quasi-Fermi level splitting have been determined by laterally resolved photoluminescence. Some of these variations can be related to lateral changes of the Cu supply during growth - with far reaching consequences for the design of preparation processes.

Topical Talk DS 2.2 Mon 11:30 GER 37

Efficient Photovoltaic Devices using Multinary Chalcogenide Semiconductors — •Hans-Werner Schock and Thomas Unold — Helmholtz Zentrum Berlin für Materialien und Energie, Hahn-Meitner Platz 1, 14109 Berlin, Germany

Multinary compounds like Cu(In,Ga)S,Se$_2$ are very promising materials for thin film solar cells currently reaching photoconversion efficiencies beyond 20 % for small device areas. The tolerance of chalcopyrite semiconductors regarding grain structure and defects allows to fabricate Cu(In,Ga)Se$_2$ thin films with a variety of deposition technologies and significant differences in the growth parameters and composition. In the long term, modifications of materials and devices are needed in order to overcome limitations by the use of rare elements e.g replacing indium by the combination of a group II and a group IV element to form the kesterite compound Cu_2ZnSnS_4. Advanced methods for film characterisation facilitate the analysis of such new materials, also in-situ during film growth. The combination of analytical methods based on x-ray methods, electron beams and optical and electrical spectroscopy give insights in the microstructure and related electronic properties of the absorber films. Due to the large degrees of freedom in multinary materials, analysis and control of structural and electronic inhomogeneities is essential to reach efficient photoconversion.

Topical Talk DS 2.3 Mon 12:00 GER 37

From Micro Meter to Mega Watt: Pentanary Chalcopyrite Thin film Solar Cells — Joerg Palm, Alejandro Avellan, •Thomas Dalibor, Stefan Jost, Helmut Vogt, Thomas Niesen, Paul Mogensen, and Franz Karg — AVANCIS GmbH & Co KG, Otto-Hahn Ring 6, 81739 München

CIS based thin film solar cells and modules are currently entering the phase of mass production with hundreds of megawatts capacity per year. This presentation illustrates how materials and device research in cooperation between industrial R&D and university groups significantly support the development of highly efficient solar cells. The pentanary chalcopyrite absorber film based on Cu, In, Ga, Se and S is preferably formed in a two stage process by chalcogenization of metal precursor films. The understanding of the reaction paths from metals via binaries to the pentanary phase has been deepened by X-ray diffraction studies. The chalcopyrite/II-VI hetero-junction is a complex interface between absorber surface region, buffer layers and the transparent conducting oxide. Several heterojunction partners are being investigated in terms of device efficiency, band alignment and interface structure. The physical processes involved in layer removal for monolithic interconnection completely change while going from mechanical patterning via nanosecond pulsed laser to ultrashort laser pulses. Device simulation helps identifying loss mechanisms in the solar cell structure. In the AVANCIS pilotline modules of size 30cm x30cm are processed with a record efficiency well above 15%. We finally present the realization of a mass production process at AVANCIS.

Topical Talk DS 2.4 Mon 12:30 GER 37

Electrical Characterization of Cu(In,Ga)(Se,S)$_2$ -Based Solar Cells at Low Temperatures — •Udo Reislöhner — Friedrich-Schiller-Universität Jena, Physikalisch-Astronomische Fakultät, Institut für Festkörperphysik, Max-Wien-Platz 1, D-07743 Jena, Germany

Thin-film solar cells based on Cu(In,Ga)(Se,S)$_2$-absorbers are industrially produced as mass product on a high level of quality. Due to rising production capacities and promising non-vacuum processes like chemical deposition or printing techniques a further cost reduction is expected. But contrary to the great success in production is the peculiar lack of comprehension concerning basic electrical spectroscopy of band-gap levels in this material system. A prominent example is the so called N1-defect observed by capacitance based methods like thermal admittance spectroscopy (TAS) and DLTS. It has unusual properties, e.g. a continuous shift of its band-gap level after moderate annealing, and has been controversially discussed for longer than a decade. However, these measurements extend to temperatures well below 200K and thereby overlap with the temperature domain where charge carrier transport by hopping is expected in the absorber. By consequently considering the impact of hopping transport on the capacitance measurement a hitherto undiscovered reason for a TAS-signal is found and the N1-signal is shown not to be correlated with a defect. Instead, this signal is generated by the freezing-out of carrier mobility with decreasing temperature when hopping conduction prevails. The consequence of this finding on electrical measurements and defect spectroscopy at Cu(In,Ga)(Se,S)$_2$-based solar cells will be discussed.

DS 3: Invited – Böer

Time: Monday 13:00–13:30 Location: POT 06

Invited Talk DS 3.1 Mon 13:00 POT 06
Why does a thin Layer of CdS on top of CdTe, and other thin-film solar cells improve their efficiency dramatically — •Karl W. Boer — Physics and Astronomy, Newark DE 19716

Karl W. Boer, University of Delaware When changing the bias from forward to Voc , the field at the CdS side of the CdS/CdTe junction increases. When it reaches the threshold of field-quenching the hole density increases while the electron density decreases, and the electron conductivity in CdS decreases with further shifting bias, i.e. with the increasing field. For reasons of the minimum entropy principle, a high-field domain must appear and absorbs the additional voltage drop. This limits the field at the junction interface to * 50 kV/cm, that is below the tunneling field. It thereby reduces junction leaking. With field quenching, the Fermi level moves further away from the conduction band, and this band must disconnect at the interface from the conduction band of the CdTe. This requires a change in the electron affinity as a function of bias. A similar change of the work function from a blocking contact of CdS as function of the conductivity has been observed, supporting this assumption. In forward bias the two conduction bands seem to be connected, easing the electron flux from CdS into CdTe. With reduced leakage Voc and FF is increased, explaining the observed improvement of the efficiency of the CdS/CdTe solar cell.

DS 4: Invited – Tiwari

Time: Monday 14:00–14:45 Location: GER 37

Invited Talk DS 4.1 Mon 14:00 GER 37
Low temperature grown high efficiency Cu(In,Ga)Se2 and CdTe flexible solar cells — •Ayodhya Tiwari, Adrian Chirila, Patrick Bloesch, Julian Perrenoud, Krenz Lukas, Sighrad Seyrling, Fabian Pianezzi, Rajneesh Verma, Shioro Nishiwaki, Stephan Buecheler, and Yaroslav Romanyuk — , Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland

CdTe solar cells of 15.6% efficiency have been developed on glass substrates using evaporated CdS/CdTe layers and keeping the overall processing temperature to below 450 °C. This process has been applied to develop up to 12.4% efficiency flexible solar cells and a laser patterning technology has been used for the development of monolithically interconnected flexible modules. Effects of various layers, processes and parametric optimization for achieving high efficiency will be presented. Properties of layers and interfaces will be correlated with the photovoltaic properties of solar cells.

CIGS solar cells are developed with co-evaporation of elements Cu, In, Ga, Se, in a specific manner that gives compositionally graded layer where Ga grading changes along the layer thickness. The composition gradient and structural characteristics of the CIGS absorber depend on the substrate temperature, NaF, and evaporation flux profiles. Properties of CIGS layers and NaF incorporation are optimised for flexible CIGS solar cells on polymer and stainless steel foils with efficiencies exceeding 18%.

DS 5: Thin Film Chalcogenide Photovoltaics II (Focused Session – Organiser: Ronning)

Time: Monday 14:45–15:45 Location: GER 37

Topical Talk DS 5.1 Mon 14:45 GER 37
Dünnschicht-Chalkogenid-Solarzellen: Überblick und Forschungsfelder — •Michael Powalla — Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg

Unter allen Dünnschichtsolarzellenkonzepten bietet die sogenannte CIGS-Technologie (Copper, Indium, Gallium, Selenium, Sulfur) das höchste Kostenreduktionspotenzial in der industriellen Fertigung. Dies ist begründet in dem im Labor nachgewiesenen hohen Wirkungsgradpotenzial, welches vergleichbar mit Solarzellen aus polykristallinem Silizium ist.

Der Vortrag gibt einen Überblick über den Stand der Entwicklung der CIGS-Solarzellen und -module in der Industrie und der Forschung. Ein Fokus liegt dabei auf der Licht absorbierenden, p-halbleitenden CIGS-Schicht, der Grenzfläche und dem n-leitenden Heterokontaktpartner. Die CIGS-Schicht wird mittels thermischer Koverdampfung oder in einem sequentiellen Verfahren hergestellt. Für den n-leitenden Frontkontakt werden unterschiedliche II/VI-Materialien verwendet, die sowohl im chemischen Bad als auch von der Gasphase abgeschieden werden können.

Am ZSW wird eine Kleinzellenlinie sowie eine Modullinie (Glassubstrate bis 30 cm x 30 cm) zur Herstellung von CIGS-Solarzellen betrieben. Speziell für flexible Substratträger (Polyimid, Metallfolien) werden Beschichtungen auf einer Rolle-zu-Rolle-Beschichtungsanlage durchgeführt. Aktuelle Forschungsergebnisse wie z. B. die Erreichung des weltbesten Wirkungsgrades für Dünnschichtsolarzellen von 20,3 % mit einer CIGS/CdS-Diode werden präsentiert.

DS 5.2 Mon 15:15 GER 37
Thin film solar cells based on the ternary compound Cu_2SnS_3 — •Dominik M. Berg, Phillip J. Dale, and Susanne Siebentritt — University of Luxembourg, Laboratory for Photovoltaics, 41 rue du Brill, L-4422 Belvaux, Luxembourg

Thin films of kesterite ($Cu_2ZnSn(S/Se)_4$) semiconductors are considered promising absorber layer materials for low cost thin film photovoltaic devices. Experimental and theoretical investigations show, however, that the existence region of a single phase kesterite is relatively small making it difficult to grow single phase absorbers. The semiconducting compound Cu_2SnS_3 is a common secondary phase that forms in Cu and Sn rich kesterite thin films during growth. Its appearance in a kesterite device would limit the V_{OC} due to its smaller band gap. However, the band gap of about 1 eV, reported hole concentrations of 10^{18} cm^{-3}, and an absorption coefficient in the visible region of 10^5 cm^{-1} make the Cu_2SnS_3 compound itself a promising candidate for low cost photovoltaic applications.

In this report we demonstrate the successful fabrication of a thin film solar cell based on Cu_2SnS_3 via a precursor annealing process. The precursor is prepared by low cost electrodeposition. A maximum external quantum efficiency of about 60% at 800 nm and a band gap of 1.0 eV could be measured. To the best of our knowledge, there have been no other reports on the fabrication of Cu_2SnS_3 based solar cell devices so far. Loss mechanisms and ways to increase efficiency will be discussed.

DS 5.3 Mon 15:30 GER 37
Investigation of lattice defects and compositional gradients in $Cu(In,Ga)Se_2$ thin films for solar cells — •Jens Dietrich[1], Daniel Abou-Ras[2], Thorsten Rissom[2], Thomas Unold[2], Hans-Werner Schock[2], and Christian Boit[1] — [1]Department of Semiconductor Devices, Berlin University of Technology, Einsteinufer 19, 10587 Berlin — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin

$Cu(In,Ga)Se_2$ absorber layers used in thin-film solar cells exhibit, when grown in a multi-stage process, compositional gradients of gallium and indium, dependent on process parameters such as the Ga content. The high lateral resolution of transmission electron microscopy (TEM) imaging and energy-dispersive X-ray spectroscopy (EDX) allows the determination of lattice defects and the elemental concentrations at identical sample positions. Cross-sectional TEM samples of ZnO/CdS/Cu(In,Ga)Se_2/Mo/glass stacks were prepared with varying [Ga]/([In]+[Ga]) ratio in the absorber. The shape of the Ga distribution was measured by means of EDX and differs for the various [Ga]/([In]+[Ga]) ratios. Linear (dislocations) and planar defects (stacking faults, microtwins) were studied by means of TEM bright field and dark field images along the lengths of the Cu(In,Ga)Se_2 layers. Strong Ga compositional gradients were found even within individual grains. It appears that these Ga gradients correlate with the occurrence of dislocation networks in large grains (diameter $> 1\,\mu$m). We assume that these dislocations compensate for lattice mismatch due to the change in composition in this area of the lattice.

DS 6: Thin Film Chalcogenide Photovoltaics III (Focused Session – Organiser: Ronning)

Time: Monday 16:00–17:30 Location: GER 37

DS 6.1 Mon 16:00 GER 37

Time dependent capacitance voltage measurements on Cu(In,Ga)Se_2 Solar Cells — •Tobias Adler[1], Wolfram Witte[2], Dimitrios Hariskos[2], and Andreas Klein[1] — [1]Darmstadt University of Technology, Institute of Materials Science, Petersenstrasse 32, D-64287 Darmstadt, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), Industriestrasse 6, D-70565 Stuttgart, Germany

Capacitance Voltage (C-V) measurements are widely used to determine the doping density of semiconductor interfaces in dependence on the width of the space charge layer. In Cu(In,Ga)Se_2 (CIGS) solar cells we observe a time dependent capacitance signal, which can be explained by different models like filling and emptying of electronic (metastable) defect states or by the diffusion of copper ions. The observed capacitance transients are compared to the different models.

DS 6.2 Mon 16:15 GER 37

Charakterisierung der elektrischen Eigenschaften von Korngrenzen an polykristallinen Chalkopyriten — •Sebastian Linke, Thorsten Rissom, Daniel Abou-Ras, Martha Ch. Lux-Steiner und Sascha Sadewasser — Helmholtz-Zentrum für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin

Polykristalline $CuIn_{1-x}Ga_xSe_2$ (CIGSe) Absorberschichten bilden die Grundlage der Dünnschicht-Solarzellen mit dem momentan höchsten Wirkungsgrad. Eine Besonderheit ist, dass polykristalline CIGSe Solarzellen, im Gegensatz zu Dünnschichtzellen auf Siliziumbasis, höhere Wirkungsgrade als die monokristallinen Pendants erzielen. Die Gründe dafür sind Gegenstand aktueller Forschung. Der Einfluß der Korngrenzen auf den Ladungstransport, insbesondere in Abhängigkeit vom [Ga]/[Ga+In]-Verhältnis, ist hierbei von großem Interesse. Die Charakterisierung der elektrischen Eigenschaften der Korngrenzen ist Voraussetzung, um ein besseres Verständnis der hohen Wirkungsgrade (> 20%) polykristalliner Absorber zu erhalten. Wir präsentieren Untersuchungen polykristalliner $CuInSe_2$ sowie $CuIn_{0.67}Ga_{0.33}Se_2$ Absorberschichten mittels Rastertunnelspektroskopie (STS) im Ultrahochvakuum bei Raumtemperatur, sowohl im Dunkeln als auch unter Beleuchtung. Bestimmte Korngrenzen zeigen im Vergleich zu ihrer direkten Umgebung eine reduzierte Dichte an Defektzuständen innerhalb der Bandlücke. Dies ist eine mögliche Erklärung für die herausragende Effizienz polykristalliner CIGSe Solarzellen. Unter Beleuchtung nimmt die differentielle Leitfähigkeit ab. Desweiteren wurden Strukturuntersuchungen mittels Elektronenbeugung (EBSD) durchgeführt.

DS 6.3 Mon 16:30 GER 37

Analysis of $Cu_2ZnSn(S/Se)_4$ by Photoluminescence and Raman — •Rabie Djemour, Levent Gütay, and Susanne Siebentritt — Laboratory for Photovoltaics, University of Luxembourg

Kesterites $Cu_2ZnSn(S/Se)_4$ are promising absorber materials for low cost thin film photovoltaic devices, since they are composed of cheap, abundant, and non toxic materials. However, growing single phase $Cu_2ZnSn(S/Se)_4$, turns out to be a difficult task because of the very small existence region, as shown experimentally and theoretically. Thus, for proper optimization of the growth process of kesterites it is essential to detect the occurrence of any secondary phase. Since conventional X-ray diffraction and energy dispersive X-ray analysis are lacking unambiguous phase resolution, we perform photoluminsecence (PL) and Raman measurements, which allow for non-ambiguous identification of the kesterite and co-existing secondary phases. We present a homebuilt system that allows PL and Raman measurements at the same spot with a spatial resolution in the one micron range. We show and discuss characteristic PL spectra for kesterites of different composition and varying crystal quality and demonstrate that even single crystals show compositional and opto-electronic inhomogeneities.

DS 6.4 Mon 16:45 GER 37

Influence of band-gap grading on luminescence properties of Cu(In,Ga)Se_2 — •Jakob Haarstrich[1], Heiner Metzner[1], Carsten Ronning[1], Thorsten Rissom[2], Christian A. Kaufmann[2], Hans-Werner Schock[2], and Andreas Undisz[3] — [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 — [3]Institute for Material Science and Technology, Metallic Materials, Friedrich-Schiller-University Jena, Loebdergraben 32, 07743 Jena, Germany

Cathodoluminescence (CL) has been measured on Cu(In,Ga)Se_2 with Ga-grading as it is used in high-efficiency thin-film solar cells at 10 K in both cross-section and plain view configuration. In cross-section geometry, we show that the vertical profile of the emission energy represents the Ga-profile in the film and, thus, we are able to measure the band-gap grading present by means of CL methods. At the same time, we observe a strong drift of excited charge carriers towards the minimum of the band-gap which can be explained by the Ga-grading. It is shown by voltage-dependent CL, how these results directly influence the interpretation of luminescence spectra obtained on Ga-graded Cu(In,Ga)Se_2 and, thus, they will have to be considered as a basis for all forthcoming investigations on this topic.

DS 6.5 Mon 17:00 GER 37

Pump-probe investigations on thin film ablation with ultrashort laser pulses — •Matthias Domke, Gerhard Heise, and Heinz Huber — Hochschule München

Laser lift-off processes have been observed during structuring CIGS thin film solar cells. To get a deeper insight in the underlying physical processes a pump-probe setup is used for spatial and temporal investigation of the interaction of ultra-short laser pulses with thin films. The setup consists of a 10 ps-laser pulse at a wavelength of 1064 nm that is split up into a pump and a probe beam. The pump beam is used to ablate thin films with single or multiple pulses. The probe beam illuminates the ablation area after an optically or electronically defined delay. A CCD Camera behind a microscope objective captures an image of the ultra-short exposed region. The probe beam is frequency doubled so that the pump light may be filtered out at the camera. Thus, the development of multiple pulse ablation is investigated in situ by taking pictures after each single pulse. Furthermore, a series of pictures can be taken on a picosecond time-scale by increasing the temporal delay of pump and probe beam. Consequently, the temporal evolution of direct and indirect (lift off) laser ablation of thin films can be studied.

DS 6.6 Mon 17:15 GER 37

Spectroscopic Imaging ellipsometry on arsenic sulphide fibers with a lateral resolution down to one micrometer — •Peter H Thiesen and Christian Röling — Accurion GmbH, Stresemannstr. 30, 37079 Göttingen

The cross section of three different arsenic sulphide fibers with different core diameters and different core/clad ratios were characterized. Ellipsometric contrast micrographs were recorded; wavelength spectra between 360 and 1000 nm at different regions of interest (ROI) and maps with a lateral resolution down to 1 micrometer of Delta and Psi were measured. The optical dispersion of the samples was described by a layer stack including an arsenic sulphide substrate, a roughness layer and air as ambient. The optical dispersion of arsenic sulphide was expressed by a Tauc-Lorentz function and the roughness layer by an effective medium approach. For the transformation of Delta and Psi maps to maps of thickness of roughness layers and maps of refractive index, the Tauc-Lorentz function was substituted by n and k as fitting parameters. Maps of refractive index and of thickness of roughness layer were obtained. Position dependent optical properties of cross sections of arsenic sulphide fibres, with core diameters down to few micrometers, can be characterized by spectroscopic imaging ellipsometry. Refractive index maps were obtained for selected wavelengths with a lateral resolution better than one micrometer.

DS 7: Layer Properties: Electrical, Optical and Mechanical Properties

Time: Monday 17:45–19:30 Location: GER 37

DS 7.1 Mon 17:45 GER 37

Ink-jet printing of silver tracks on porous surfaces and improvement of conductivity

— •Anna Schuppert[1], Joachim Wollschläger[2], Lorentz Walder[3], and Wolfgang Schmidt[4] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf — [2]Fachbereich Physik, Universität Osnabrück — [3]Fachbereich Chemie, Universität Osnabrück — [4]Felix Schoeller Service GmbH und Co. KG, Osnabrück

Different porous coatings on polyethylene treated paper were checked as a support for ink-jet printed silver tracks. The goal of this work, was to achieve a good conductivity at short post processing and low temperatures. This was achieved by a presintering initialised by the surface.

For this purpose thin films of Al_2O_3 particles on PE-sealed paper were prepared and the pore size distribution was measured with Hg-Porosimetry. Using a Dimatix Materials Printer silver tracks were printed on these substrates. The resistance was measured with a four point probe and analysed as a function of the pore size.

It was found that smaller pore sizes yield higher conductivity, which is interpreted as a destabilisation of the ink immediately after printing. The initial conductivity can be improved by sintering for some minutes at 70 °C or 100 °C. Other important parameters influencing the conductivity found in this study are roughness, pH and added salts.

DS 7.2 Mon 18:00 GER 37

Statistical Analysis of Computer-simulated On-Chip Interconnect Electromigration Lifetimes under the Influence of Microstructure and Strengthened Top Interface

— •Matthias Kraatz[1], Lijuan Zhang[2], Dieter Schmeisser[1], Ehrenfried Zschech[3], and Paul S. Ho[2] — [1]BTU Cottbus, Germany — [2]The University of Texas at Austin, USA — [3]Fraunhofer Institute for Non-Destructive Testing IZFP, Dresden, Germany

We are investigating the statistics of computer-simulated interconnect electromigration (EM) lifetimes with regard to the effects of microstructure and a strengthened top interface. The degradation process of EM once threatened the entire existence of integrated circuit industry in the 1960s and has remained a major reliability concern. Ongoing miniaturization and the introduction of new materials further complicate the task of EM-resistant chip manufacturing. We have developed a simple two-dimensional finite difference simulation that models the mass transport by electromigration along the grain boundaries and the top interface of interconnect segments that allows us to do calculations of void nucleation and growth. A parallel computer simulates hundreds of interconnects simultaneously and statistical analysis becomes feasible. A Monte Carlo grain growth algorithm (a modified Potts version) is applied to model the grain structure of the interconnect segments. We will show that the simulation can be used to compare simulation and experiment qualitatively. Four cases have been studied: interconnect segments with small/large grains and weak/strong top interface.

DS 7.3 Mon 18:15 GER 37

Entwicklung eines Messverfahrens zur Bestimmung der elektrostriktiven Konstante von dünnen Polymerschichten

— •Christian Schirrmann, Kirstin Bornhorst und Florenta Costache — Fraunhofer-Institut für Photonische Mikrosysteme IPMS, Maria-Reiche-Str. 2, Dresden, Deutschland

Polymeraktoren sind aufgrund ihrer großen elektromechanischen Verformung sehr vielversprechend für den Einsatz in aktiven mikro-opto-elektro-mechanischen Systemen (MOEMS).

Es wurde ein Messverfahren für dünne elektrostriktive Polymerschichten entwickelt, welches es ermöglicht, die Verformung, hervorgerufen durch die dielektrische Anziehung der Elektrode und die im Material auftretende Elektrostriktion, zu unterscheiden. Dabei wurde die kombinierte dielektrisch-elektrostriktive Verformung interferometrisch gemessen. Der elastische Modulus wurde für dünne, elastische und transparente Schichten mittels eines optimierten interferometrischem Bulge-Test ermittelt. Weiterhin wurde die relative Permittivität mittels Impedanzspektroskopie bestimmt.

Anhand der gewonnen Materialkonstanten wurde das mechanische Verhalten eines elektrostriktiven Bimorphs mittels dreidimensionaler Finite-Elemente-Methode simuliert und mit auftretenden Deformationen eines mikromechanisch gefertigten Multilayerstacks verglichen.

DS 7.4 Mon 18:30 GER 37

Charging of internal interfaces in metal-insulator-metal heterosystems by low energy electron beams

— •Johannes Hopster[1], Marika Schleberger[1], Andreas Wucher[1], and Detlef Diesing[2] — [1]Fakultät für Experimentalphysik, Universität Duisburg-Essen — [2]Fakultät für Physikalische Chemie, Universität Duisburg-Essen

Metal-insulator-metal (MIM) and metal-semiconductor (MS) heterosystems can be used to detect low energy electrons, which are for example released by a surface chemical reaction. These electrons usually do not have sufficient excess energy to overcome the work function of the metal film. But these electrons can overcome the internal barrier of the heterosystems since the internal barrier is usually 1-2 eV lower than the workfunction of the metal film. The transmission of electrons over the internal barrier is determined by its height and thickness. By exposing these heterosystems to a low energy electron beam in ultra high vacuum we studied the electron transmission. The barrier properties and the transmission of the device remain unchanged for small currents impinging on the device (< 1 nA). For primary electron currents > 100 nA the internal barrier can be reversibly changed. The barrier returns to its ground level state within some 10s following an exponential time law. The time constant depends clearly on the field strength in the device. A model considering charge exchange processes between the two interfaces of the device is presented to explain the beam induced barrier changes.

DS 7.5 Mon 18:45 GER 37

Mapping of internal photoemission in metal–insulator–metal heterosystems

— Dominik Differt[1], Walter Pfeiffer[1], and •Detlef Diesing[2] — [1]Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany — [2]Fakultät für Chemie, Universität Duisburg-Essen, D-45117 Essen, Germany

Internal **p**hoto**e**mission (IPE) in heterosystems is determined by light absorption and **e**lectron **h**ole (e-h) pair generation in the layers of the systems. Lateral inhomogeneities of the dielectrical properties, layer thickness variations or local defects can for example cause lateral variations in the IPE signal. With photon energies smaller than the band gap of the insulator one can selectively probe e-h pair generation in the back and top metal layers. For the lateral mapping of IPE a Ag-TaO-Ta heterosystem is raster scanned across the focus of a Schwarzschild objective (NA=0.4). The illumination with 400 nm laser radiation results in a focus diameter of $7\mu m$ limiting the spatial resolution of the IPE microscopy. Mapping across the $70\mu m$ wide edge of the top metal film shows transport effects in the top silver electrode as well as the increasing excitation of carriers in the tantalum backelectrode with decrasing top electrode thickness. The variation of the top electrode thickness and comparison to simulated excitation profiles allows the investigation of excited electron transport in the metal-insulator-metal junction.

DS 7.6 Mon 19:00 GER 37

Determination of the electrically active Al fraction in Al doped ZnO grown by pulsed reactive magnetron sputtering

— •Steffen Cornelius, Mykola Vinnichenko, Frans Munnik, René Heller, Andreas Kolitsch, and Wolfhard Möller — Helmholtz Zentrum Dresden-Rossendorf, Dresden, Germany

Al-doped ZnO (AZO) films which combine maximum carrier mobility, moderate free electron densities and high surface roughness are of special interest for application as transparent front electrode in thin film solar cells. They posses high transmission in the near infrared spectral range, close to the bandgap energy of absorber materials like Si (Eg=1.11 eV), and enable a superior light trapping behaviour. A key to tailor AZO film properties is understanding the mechanisms and effects of the Al-dopant incorporation into the ZnO matrix. It is well accepted that the mobilities in degenerately doped AZO are limited by ionized impurity scattering. A way to overcome this limitation would be to reduce the density of ionized impurities which either do not donate electrons themselves or compensate the Al donor. This is equivalent to increasing the fraction of electrically active Al in the ZnO host material. Systematic and quantitative information on this topic is still missing in literature. Therefore this work focuses on quantification of the Al concentration by ion beam analysis methods in conjuction with Hall-effect measurements for AZO films grown by reactive pulsed magnetron sputtering. The influence of parameters like target composition and substrate temperature on the Al activation will be discussed.

DS 7.7 Mon 19:15 GER 37

Ellipsometric study of copper growth on silicon — •Francisc Haidu, Ovidiu D. Gordan, and Dietrich R. T. Zahn — Chemnitz University of Technology, Semiconductor Physics, 09107 Chemnitz, Germany

Thin copper films are of high interest for interconnect applications. However, optical studies, such as ellipsometry, of metallic thin films are still rare as the measurements are difficult to interpret due to the lack of a transparent range and often island-like growth at very low cowerages. We investigated by in situ Spectroscopic Ellipsometry the growth of thermally evaporated thin copper films on silicon substrates from 0.5 nm to more than 100 nm, a thickness for which bulk-like response is observed. A strong change in the optical response was observed for films thinner than 10 nm as a result of plasmonic effects. For the interpretation of the spectra Effective Medium Approximation theory was employed using the thicker films as reference. Furthermore, copper oxidation was also studied. Here a pronounced change in the optical response is observed within the first 10 minutes of oxidation. Thereafter the response changes at a slower rate without reaching saturation.

DS 8: Thin Film Characterisation: Structure Analysis and Composition (XRD, TEM, XPS, SIMS, RBS, ...) I

Time: Monday 10:15–11:45 Location: GER 38

DS 8.1 Mon 10:15 GER 38

Oberflächennahe Analytik mit Kleinwinkelröntgenstreuung im Labor — •Jörg Wiesmann[1], Peter Siffalovic[2], Jozef Keckes[3] und Günther Maier[3] — [1]Incoatec GmbH, Geesthacht, Deutschland — [2]Slovak Academy of Sciences, Bratislava, Slowakei — [3]Erich Schmid Institut für Materialwissensch., Leoben, Österreich

Kleinwinkelstreuung mit Röntgenstrahlung (SAXS) ermöglicht die Untersuchung von Materialien im Nanometermaßstab. Aussagen zu Teilchengrößen und -verteilung sind möglich. Die Eindringtiefe der Röntgenstrahlung ermöglicht zudem Informationen aus der Probentiefe ohne Zerstörung der Proben. In den letzten Jahren wurde SAXS vorwiegend am Synchrotron verwendet. Durch Entwicklung neuer Hochleistungsquellen können nun viele Fragestellungen auch im Labor gelöst werden. In unserem Beitrag stellen wir die hochbrillante Mikrofokus Röntgenquelle IμS vor, beschreiben ihre Verwendung in typischen Labor-SAXS Instrumenten und zeigen Messergebnisse an dünnen Multilayer-Strukturen und nanoskaligen Proben. Die IμS besteht aus einer 30W luftgekühlten Röhre, die charakteristische Ag, Cu, Cr, oder Mo Strahlung liefert. Sie wird verbunden mit 2D strahlformenden Multilayer-Röntgenoptiken. Dadurch entsteht ein kollimierter Strahl von <0.5mm mit einer Divergenz von 1mrad oder kleiner. In Kombination mit 2D Detektoren können damit im Labor Messungen durchgeführt werden wie sie sonst nur am Synchrotron möglich sind. Wir zeigen das Potential von Laborgeräten für SAXS und GISAXS (GI steht für streifenden Einfall) anhand von Beispielen aus der Dünnfilmtechnik (Multilayer als Röntgenoptiken).

DS 8.2 Mon 10:30 GER 38

BioRef - a versatile time-of-flight reflectometer for soft matter applications at Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin — •Markus Strobl[1], Roland Steitz[1], Martin Kreuzer[1,2], Reiner Dahint[2], and Michael Grunze[2] — [1]Helmholtz Zentrum Berlin für Materialien und Energie, Hahn-Meitner Platz 1, 14109 Berlin — [2]Universität Heidelberg, Im Neuenheimer Feld 229, 69120 Heidelberg

BioRef is a versatile novel time-of-flight (TOF) reflectometer at the reactor neutron source BER II of the Helmholtz Centre Berlin (HZB) featuring an infrared spectrometer for complementary in-situ ATR-FTIR measurements. The instrument has recently undergone commissioning and is now available for specular and off-specular neutron reflectivity measurements. BioRef is especially dedicated to the investigation of soft matter systems and studies at the solid liquid interface. Due to flexible resolution modes and variable utilized wavelength bands that allow for focusing onto a selected q-range BioRef enables a broad range of surface and interface investigations and even kinetic studies with sub-second time resolution. The instrumental conditions can be tailored to the specific requirements of a wide range of applications. The performance is demonstrated by several reference measurements and the unique option of in-situ on-board infrared spectroscopy is introduced by the example of a phase transition study in a lipid multilayer film.

DS 8.3 Mon 10:45 GER 38

Comparison of quantitative X-Ray Fluorescence Spectrometry under normal and grazing incidence condition by means of buried nanolayers — •Rainer Unterumsberger[1], Beatrix Pollakowski[1], Matthias Müller[1], Burkhard Beckhoff[1], Wolfgang Ensinger[2], Peter Hoffmann[2], Tobias Adler[2], and Andreas Klein[2] — [1]Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin, Germany — [2]Institute of Materials Science, Technische Universität Darmstadt, Petersenstr. 32, 64287 Darmstadt, Germany

Non-destructive thickness determination of nanolayer and thin films becomes more and more important. The quantitative X-Ray Fluorescence Spectrometry (XRF) with synchrotron radiation is a well-established method for thickness determination of thin layers. Under grazing incidence condition (GIXRF), due to total reflection of the incidence beam the x-ray standing wave (XSW) field occurs. That enables near surface quantification of lowest depositions and the possibility of buried nanolayer quantification. In this work quantitative XRF and GIXRF will be compared and the advantages and limits of both methods will be demonstrated. Within a project of the German Science Foundation (DFG), a special sample system was investigated. It consists of buried borcarbide nanolayers varying in thickness deposited on 10 nm titanium and covered with 2.5 nm silicon dioxide. All layered structures are deposited on silicon-wafers. The measurements were carried out in the PTB laboratory at BESSY II. The result of the buried nanolayer thicknesses matches in both methods.

DS 8.4 Mon 11:00 GER 38

X-ray Reflectivity and Grazing Incidence X-ray Diffraction — •Markus Meyl[1], Bogdan Szymański[2], Arno Ehresmann[1], and Feliks Stobiecki[2] — [1]University of Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany — [2]Institute of Molecular Physics, Polish Academy of Sciences, Mariana Smoluchowskiego 17, 60-179 Poznań, Poland

X-ray Reflectivity and Grazing Incidence X-ray Diffraction in Bragg-Brentano-Geometry and by the Guinier-Process for the investigation of thin films will be discussed. The Guinier-Process as compared to the Seemann-Bohlin-Geometry includes the use of a monochromator between the X-ray tube and the sample for achieving strictly monochromatic incident X-rays as well as its very small angle of incidence. As a result the diffraction spectra have less background signal and higher intensities. Furthermore the structural information which can be received by these methods will be mentioned. From the spectra measured with the Bragg-Brentano-Geometry the layer thicknesses, the interface roughness's and the densities of the thin films can be determined. In addition the diffraction spectrum obtained with the Guinier-Process provides e.g. information about the lattice parameter, the lattice type and the crystallite sizes. In the last part exemplary results of thin films on a silicon substrate will be presented.

DS 8.5 Mon 11:15 GER 38

Nucleation Mechanisms In High Energy Ion Beam Induced Dewetting — •Michael Haag, Daniel Garmatter, Redi Ferhati, Sankarakumar Amirthapandian, and Wolfgang Bolse — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart

Solid coatings, when heated above their melting points, often break up by forming small round holes, which then grow, coalesce and finally turn the initially contiguous film into a pattern of isolated droplets. Such dewetting has been intensively studied using thin polymer films on Si [1]. Three different hole nucleation mechanisms were discovered: homogeneous (spontaneous) nucleation, heterogeneous nucleation at defects, and spinodal dewetting by self-amplifying capillary waves. We have recently found that swift heavy ion (SHI) irradiation of thin oxide films on Si results in similar dewetting patterns, even though the films were kept far below their melting points [2]. Using our new in-situ SEM at the UNILAC accelerator of GSI [3], we were now able to identify the mechanisms behind this SHI induced dewetting phenomenon. By varying the film thickness and introducing defects at the interface, we can directly address the hole nucleation processes. Besides homogeneous and heterogeneous nucleation, we also found a process, which very much resembles the spinodal mechanism found for liquid polymers, although in the present case the instable wavy surface is not generated by capillary waves, but by ion beam induced stresses. [1] S. Herminghaus, et al., Science 282 (1998), [2] T. Bolse, et al., Nucl.Instr.Meth. 245 (2006), [3] S. Amirthapandian, et al., Rev.Sci.Instr. 81, (2010)

DS 8.6 Mon 11:30 GER 38

Sophisticated analysis of the PDA of thin praseodymia films at temperatures up to 300°C — •Sebastian Gevers[1], Daniel Bruns[1], Alessandro Giussani[2], Thomas Schröder[2], and Joachim Wollschläger[1] — [1]Fachbereich Physik, Universitaet Osnabrueck, Barbarastr. 7, 49069 Osnabrueck, Germany — [2]IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany

High quality praseodymia films are discussed as insulating buffer material, e.g. to form high-functional Germanium On Insulator (GeOI) heterostructures on the dominating Si wafer platform. For this purpose, thermal treatment of the oxide buffer layers is necessary to grow high quality Ge films with low defect densities. To control and to improve the quality of the GeOI structures, it is crucial to understand the behavior of preaseodymia films regarding structure and defect formation during these annealing processes.

Therefore, thin heteroepitaxial praseodymia films with fluorite structure on Si(111) were annealed under UHV conditions at temperatures up to 300°C. Afterwards, investigations by X-ray diffraction (XRD), grazing incidence X-ray diffraction (GIXRD) and X-ray reflectometry (XRR) were performed to obtain information about structural changes of the film during the annealing process. Analyzing the XRD measurements within the kinematic diffraction theory leads to a detailed view on structural changes of the oxide films, e.g. separation into different crystalline phases.

DS 9: Thin Film Characterisation: Structure Analysis and Composition (XRD, TEM, XPS, SIMS, RBS, ...) II

Time: Monday 12:00–13:00 Location: GER 38

DS 9.1 Mon 12:00 GER 38

The interface of epitaxial bixbyite-structured rare-earth sesquioxides on Si(111) — •Michael Niehle, Tatsuro Watahiki, and Achim Trampert — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin

Rare-earth oxides (RE_2O_3) are promising high-κ materials for replacement of SiO_2 as insulator in CMOS technology. They are required for further downscaling. Recently, the possibility to grow single domain RE_2O_3 in the cubic bixbyite structure on Si(111) with atomically smooth, chemically stable and crystalline interfaces has been demonstrated by molecular beam epitaxy. Understanding the interface's microstructure is necessary to optimize growth conditions and to estimate applicability in future devices. Binary Gd_2O_3 or an adequate ternary alloy like $(La,Lu)_2O_3$ allow for a nearly lattice matched epitaxial growth. High-resolution transmission electron microscopy (HRTEM) is used to demonstrate that a coherently grown heterostructure is feasable. Two models for the atomic configuration at the interface are proposed and incorporated in a supercell which serves as input for HRTEM image simulation applying the multi-slice algorithm. Results of the simulation are confirmed by comparison to experimental HRTEM-images of $(La_{1-x}Lu_x)_2O_3$ and $(Gd_{1-x}Lu_x)_2O_3$ with $x \approx 0.5$ and $x \approx 0$, respectively. Competing crystal structures to the bixbyite phase are excluded.

DS 9.2 Mon 12:15 GER 38

Structure of heteroepitaxial type-B oriented $CeO_2(111)$ on cubic- and hexagonal-Pr_2O_3/Si(111) supports — •Marvin Zoellner[1], Joachim Wollschläger[2], Marcus Bäumer[3], Michael Reichling[2], Peter Zaumseil[1], and Thomas Schroeder[1] — [1]IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany. — [2]Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany. — [3]Universität Bremen, Leobener Str. 2, 28359 Bremen, Germany.

Single crystalline epitaxial cerium oxide is of interest for model catalysis. Furthermore, a combination with praseodymium oxide exhibits an enhanced oxygen storage capability. Therefore, $CeO_2(111)$ thin films were grown on cub-$Pr_2O_3(111)$/Si(111) and hex-$Pr_2O_3(0001)$/Si(111) by molecular beam epitaxy (MBE). The cub-$CeO_2(111)$ lattice has an ABCABC... and the hex-$Pr_2O_3(0001)$ lattice an ABABAB... stacking sequence. In such oxide heterostructures stacking twins can occur, which influence catalytic activity. Reflection high energy electron diffraction (RHEED) was used for in-situ monitoring of the layer orientation. To gain a global and local insight of the heterostructures, X-ray diffraction (XRD) and transmission electron microscopy (TEM) were performed ex-situ. Finally, synchrotron radiation-grazing incidence X-ray diffraction (SR-GIXRD) gives a surface sensitive twin analysis. A twin-free, exclusively type-B oriented CeO_2[1-10]||Si[-110] epitaxial relationship of the $CeO_2(111)$ film on the cub- as well as on the hex-Pr_2O_3 was detected. Theoretical ab initio calculations were carried out to gain an understanding of the unexpected twin-free growth mechanism.

DS 9.3 Mon 12:30 GER 38

Epitaxial growth of GeTe on Si(111) and in-situ compositional analysis — •Karthick Perumal, Wolfgang Braun, and Raffaella Calarco — Paul Drude Institut für Festkörperelektronik, Berlin, Deutschland

GeTe is an important phase change material lying on one end of the pseudobinary line of Ge-Sb-Te alloys, with Sb_2Te_3 at the other end. The complex growth behaviour of ternary Ge-Sb-Te alloys requires better understanding of the binary component GeTe. Here, we report on the molecular beam epitaxy of GeTe on Si(111) substrates and the use of desorption mass spectroscopy as an in-situ technique for compositional analysis during the growth. The source fluxes of Ge and Te are kept at a ratio of 2:5. The GeTe samples grown at different substrate temperatures were continuously monitored by a quadrupole mass spectrometer and an algorithm was made to subtract the observed background pressure, thereby deducing the incorporation ratio of various atomic species. With the assumption that the sensitivity of the mass spectrometer is one, we calculate the Te to Ge ratio of incorporating atoms. The compositional results lie within 10% of the values confirmed by XRF measurements. X-ray diffraction analysis was performed on the grown samples and the crystal structure was found to be hexagonal. We find that the growth of GeTe is independent of Te as long as there is an excess tellurium flux, which shows that GeTe behaves like III-V materials: with higher Te flux, the growth is Ge limited.

DS 9.4 Mon 12:45 GER 38

Electron microscopy study of amorphous SiCN hard coatings — •Andrea Sendzik, Steffen Schulze, Marcus Günther, Frank Richter, and Michael Hietschold — Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz

The two-component systems Si-C, Si-N and C-N have been studied in terms of their mechanical, electrical and optical properties. The goal for the ternary amorphous SiCN compounds is to unite the positive properties of the binaries, such as chemical stability, hardness and large band gap. We have characterized thine layers by scanning electron microscopy (SEM) and transmission electron microscopy (TEM), through the studies of diffraction patterns and the analysis of electron energy loss spectra (EELS).The layers were produced by plasma enhanced chemical vapor deposition PECVD. For this a mixture of following gases was used: Ttrimethylsilane ($SiH(CH_3)_3$), N_2 and Ar. A series of samples has been prepared, differing in terms of gas composition and pressure. All SiCN films were deposited on silicon or on NaCl(100) substrates. By SEM the morphology of the layers were characterized. The atomic structure was investigated by TEM. By analyzing diffraction patterns and EELS-spectra findings about the short-range order of atoms, the atomic composition, and the chemical bonding were made. By comparing the experimentally obtained scattering curves with model distributions earlier structural ideas could be expanded and systematized in accordance with the deposition conditions. In addition the first results of mechanical tests are presented, such as E-Modul and stress values of the layer.

DS 10: Thin Film Characterisation: Structure Analysis and Composition (XRD, TEM, XPS, SIMS, RBS, ...) III

Time: Monday 14:00–15:30 Location: GER 38

DS 10.1 Mon 14:00 GER 38

Structure and stability of laser deposited ZrO_2/Ti and ZrO_2/MgO multilayers — •Sarah Hoffmann, Benedikt Ernst, Tobias Liese, and Hans-Ulrich Krebs — Institut für Materialphysik, University of Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen

ZrO_2/Ti and ZrO_2/MgO thin multilayer systems have important applications in X-ray optics, especially in the 'water window' regime (wavelength: 2.3 - 4.4 nm) as X-ray mirrors and multilayer Laue lenses [1]. For this purpose the knowledge of the thermal stability of these multilayer systems is necessary. Thus, in this contribution the structure and stability of ZrO_2/Ti and ZrO_2/MgO multilayers is presented. The films were prepared on Si substrates using pulsed laser deposition (PLD) in ultra high vacuum. During heating the phase transformations of the components were studied using in-situ X-ray reflectometry (XRR) and in-situ X-ray diffraction (XRD). Furthermore, the changes in the structure were observed by in-situ transmission electron microscopy (TEM). The observed results are discussed with respect to the processes occuring 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 10.2 Mon 14:15 GER 38

Establishment of a structure zone model for the growth of reactively sputtered Titania thin films — •Azza Amin, Dominik Köhl, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

TiO_2 thin films are applied in a wide range of applications e.g. in self-cleaning, antibacterial, antifogging or optical coatings. The physical properties exploited in these applications strongly depend on the crystal structure of the films. Crystalline TiO_2 thin films typically exhibit an anatase or a rutile phase. Therefore, it is desirable to develop a thorough understanding of the structure formation. This would allow it to tailor the film structure with the aim to improve the desired properties needed for a targeted application. Therefore, the structural evolution during growth of reactively sputtered TiO_2 films has been comprehensively investigated as a function of various parameters comprising oxygen partial pressure, energetic ion bombardment, target age and substrate temperature. Pronounced correlations have been found between the deposition conditions, the film thickness, the crystal structure and the morphology of the films. These correlations have been summarized in a structure zone model that explicitly links the basic characteristics of the deposition process with the properties of the films fabricated.

DS 10.3 Mon 14:30 GER 38

Non-destructive species depth profile of nanolayered systems — •Beatrix Pollakowski and Burkhard Beckhoff — Physikalisch-Technische Bundesanstalt, Berlin, Germany

Analyzing nanolayered samples with thicknesses larger than the mean free path of electrons, only spectroscopic methods based on photon detection may provide information without modifications of the specimens. The combination of X-ray absorption spectroscopy and X-ray fluorescence spectrometry under grazing incidence conditions (GIXRF-NEXAFS) has shown that a non-destructive analysis regarding the chemical bonds of deeply buried single layers is feasible [1]. Utilizing the intensity of x-ray standing wave (XSW) field, which is directly related to the grazing incidence, as a marker the penetration depth can be tuned to a certain depth.

The multilayer systems investigated consist of a titanium oxide and metallic titanium layer, separated from each other by a 2 nm C layer. For the respective experiment, well-characterized monochromatic synchrotron radiation of the electron storage ring BESSY II and calibrated instrumentation was employed. A species depth profile was derived by means of a differential approach. Two GIXRF-NEXAFS measurements at the Ti-$L_{iii,ii}$ absorption edges at different penetration depths are necessary to determine the entire system. The results demonstrate the high potential of the approach for analyzing novel materials and may provide access to interfaces.

[1] B. Pollakowski et al., Phys. Rev. B **77**, 235408 (2008)

DS 10.4 Mon 14:45 GER 38

Crystallization and Oxygen loading in pulsed laser deposited YSZ-Films — •Benedikt Ernst, Tobias Liese, Sarah Hoffmann, and Hans-Ulrich Krebs — Institut für Materialphysik, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Yttria-stabilized zirconium dioxide (YSZ) as an oxygen ion conductor is widely used in technical applications, for example as solid oxide fuel cells. Thus, it is important studying the film stability at higher temperatures. In this contribution, amorphous YSZ films prepared by Pulsed Laser Deposition (PLD) at room temperature and annealed in argon/vacuum or oxygen atmosphere are presented. In a first thermal treatment in high vacuum up to temperatures of 800°C a loss of oxygen and crystallization of the film is achieved. Further heating in oxygen atmosphere leads to a reversible reloading of oxygen in the film. At this, changing the heating time and temperature enables to obtain different levels of oxygen in the samples. The weight change during outgasing and reloading was measured by thermal gravimetric analysis (TGA). The structure of different oxygen states and dynamics of crystallization was characterized by in-situ x-ray diffraction (XRD) and ellipsometry. This work is supported by the SFB755.

DS 10.5 Mon 15:00 GER 38

Hard X-ray photoelectron spectroscopy studies of newly designed charge transfer salts at PETRA III. — •Andrei Gloskovskii[1], Katerina Medjanik[2], Sebastian Thiess[3], Heiko Schulz-Ritter[3], Wolfgang Drube[3], Dennis Chercka[4], Martin Baumgarten[4], Klaus Müllen[4], Claudia Felser[1], and Gerd Schönhense[2] — [1]Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, Mainz — [2]Institute of Physics, Johannes Gutenberg - University, Mainz — [3]Hasylab/DESY, Hamburg — [4]Max Planck Institute for Polymer Research, Mainz

The undulator beamline P09 of the PETRA III storage ring is in user operation since September 2010. The hard X-Ray photoelectron spectroscopy (HAXPES) end station is located 95 m from the source. Photoelectrons with up to 15 keV kinetic energy can be measured in different experimental geometries by means of a SPECS Phoibos 225 HV analyser. Thin films and microcrystals of the organic charge-transfer compounds tetra- /hexamethoxypyrene - tetracyanoquinodimethane (TMP$_x$/HMP$_x$-TCNQ$_y$ in different stoichiometries) have been studied by HAXPES. The spectra of the HMP$_x$-TCNQ$_y$ compounds reveal two bonding states of oxygen, one of which stays fixed, but varies strongly in intensity and the other one is broadened and changes its energy position for x:y=2:1 microcrystals. This is an indication of the higher degree of charge transfer. The results correlate with previous investigations of the same systems using UPS/STS and NEXAFS. Funded by BMBF 05K10UMA, DFG/TR49, Graduate School of Excellence MAINZ, Centre of Complex Materials COMATT.

DS 10.6 Mon 15:15 GER 38

Transmission of ballistic electrons through metal–insulator–metal heterosystems — Johannes Hopster[1], Marika Schleberger[1], Lars Breuer[1], Andreas Wucher[1], Alexander Bernhart[1], Mark Kaspers[1], Christian Bobisch[1], Rolf Möller[1], and •Detlef Diesing[2] — [1]Institut für Experimentalphysik, Universität Duisburg-Essen — [2]Institut für Physikalische Chemie, Universität Duisburg-Essen

The transport of electrons through metal-insulator-metal heterosystems is determined by scattering processes in the metal layers and transport over or through the barrier in the insulator. We use an experimental setup combining a low energy electron gun with adjustable kinetic energy and a **b**allistic **e**lectron **e**mission **m**icroscope (BEEM). Electrons with excess energies of up to 5 eV are injected by a STM tip in the silver top electrode of a tantalum/tantalum–oxide/silver tunnel junction. The ratio of detected electrons in the tantalum back electrode and electrons injected into the silver top electrode depends exponentially on the tip voltage and thus, on the excess energy of the electrons in a wide range from 1.7 to 4.2 V. In experiments with an electron gun the transmission with primary energies from 20 eV to 600 eV was studied. With energies up to 600 eV the yield shows a monotonous increase but the dependence on the energy turns from an exponential behavior to a linear behavior.

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

Time: Monday 15:45–17:00 Location: GER 38

DS 11.1 Mon 15:45 GER 38

Modeling of the relaxation kinetics of Phosphorus doped metastable tensile strained Si:C alloys — •Felix Ulomek[1], Ina Ostermay[2], Thorsten Kammler[2], and Volker Mohles[1] — [1]Institut für Metallkunde und Metallphysik, RWTH Aachen — [2]GLOBALFOUNDRIES Dresden Module One LLC & Co. KG, Wilschdorfer Landstraße 101, 01109 Dresden

In order to enhance the performance of CMOS transistors, embedded epitaxial layers of Si:C are of interest. In the present work, Si:C layers with Carbon contents up to 1.9 at-% and in-situ Phosphorus doping up to 4E20 At/cm3 have been investigated. Due to the low solubility of Carbon in Silicon (0.0004 at.-% at the melting point), all layers considered in this work are metastable and tend to relax. Since it is crucial to the application to retain the strain of those layers, the responsible mechanisms must be understood. The relaxation during thermal treatment was studied by high resolution x-ray diffraction and was found to behave differently, depending on Carbon content and Phosphorus doping concentration. We model the macroscopic relaxation behavior by statistical simulations and extrapolate the behaviors for different relaxation conditions. The resulting activation energies, which are fit parameters in this model, are compared to values of atomistic simulations.

DS 11.2 Mon 16:00 GER 38

XPS depth profiling on polymers using Ar, C$_{60}$, Coronene and Gas Cluster Ion Beam. — •Andrey Lyapin[1], Stefan Reichlmaier[1], John S. Hammond[2], John F. Moulder[2], Takuya Miyayama[3], Noriaki Sanada[3], Mineharu Suzuki[3], and Atsushi Takahara[4] — [1]Physical Electronics GmbH, 85737 Ismaning, Germany — [2]Physical Electronics USA, 18725 Lake Drive East, Chanhassen, MN. 55317 USA — [3]ULVAC-PHI, Inc., 370 Enzo, Chigasaki, Kanagawa, 253-8522 Japan — [4]Kyushu University, Motooka, Nishi-ku, Fukuoka 8190395 Japan

The use of cluster ion sputtering for depth profiling of polymers, organics, and biomaterials has opened an entirely new field of application for surface analytical methods and shown potential to analyze chemical bonding and molecular structures during sputtering into a sample surface. In this talk we present a comparison of the use of XPS depth profiling of thin polymer films with Ar, C$_{60}$, Coronene and Ar Gas Cluster Ion Beam (GCIB) sputter sources. The GCIB sputter source produces an Ar$_{2500}{}^{+}$ ion beam with user definable incident beam energy. Optimized conditions for the incident ion beam energy of the GCIB will be presented to provide minimal chemical state damage during the depth profiling. Results will also be presented showing that the GCIB source can be used to remove damaged layers from modified surfaces.

DS 11.3 Mon 16:15 GER 38

Structure of FePt thin films with copper addition — •Herbert Schletter, Christoph Brombacher, Manfred Albrecht, and Michael Hietschold — Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz

The continuous increase in storage density of magnetic hard disk drives creates a need for new concepts and new materials in this field. One approach is the use of highly anisotropic materials which allow for further reduction of bit sizes. One of these materials is the L1$_0$ phase of FePt. However, a thermal treatment of the material (either during or after the deposition) is necessary to (i) transform the material from cubic A1 to tetragonal L1$_0$ phase and (ii) create a (001)-textured film, for which the magnetic anisotropy axis is perpendicular to the film plane.

In our experiments, different amounts of Cu (up to 21 at.%) were added to 5 nm thick FePt layers to support the phase transformation as well as the texture evolution during rapid thermal annealing (RTA) [1]. The structure of these layers was investigated by means of TEM and electron diffraction combined with multislice simulations. It was found, that pure FePt layers consist of a mixture of untextured A1-FePt and (001)-textured L1$_0$-FePt after RTA to 600 °C for 30 s. In this case, the A1-phase is encountered in significantly smaller grains ($\approx$ 10 nm) than the L1$_0$-phase ($\approx$ 50 nm). However, the addition of $\geq$ 9 at.% Cu leads to pure L1$_0$-FePt:Cu films with the desired (001)-texture when applying the same annealing parameters.

[1] D. Makarov et al., Appl. Phys. Lett. 96, 062501 (2010)

DS 11.4 Mon 16:30 GER 38

Depth resolved Doppler broadening spectroscopy in thin metallic films — •Markus Reiner[1,2], Philip Pikart[1,2], and Christoph Hugenschmidt[1,2] — [1]ZWE FRM 2, Garching, Germany — [2]Technische Universität München, Physikdepartment E 21, Garching, Germany

Within this contribution the examination of thin metallic films by (C)DB ((coincident) Doppler broadening) measurements at different temperatures is presented. Systems with a gold or copper layer with a thickness between 20 and 500 nm were produced by evaporation deposition on silicon substrates. Doppler broadening and positronium fraction were examined in order to investigate annealing processes. In addition, theses samples as well as gold-copper-silicon systems were studied by depth resolved CDB measurements with the goal to obtain information about temperature dependent diffusion processes at the interface.

These measurements were performed by use of the highly intensive positron beam NEPOMUC. Depth resolved DB measurements are used for the determination of the positron diffusion length which is highly sensitive to defect concentration. At high temperatures the thermic desorption of positronium can be detected and additionally considered to determine the diffusion length. Depth resolved CDB measurements allow the detection of the chemical surrounding of defects in layered structures. Recently a new heatable sample holder has been set up in order to achieve a sample temperature up to 1000 K.

DS 11.5 Mon 16:45 GER 38

Neutron Reflectometry and GISANS studies of Thin

Films at Refsans — •Jean-François Moulin[1], Martin Haese-Seiller[1], Reinhard Kampmann[1,2], Matthias Pomm[1], and Andreas Schreyer[2] — [1]Helmoltz Zentrum Geesthacht, Institute of Materials Research, Instrument REFSANS Lichtenbergstr. 1 85747 Garching (Germany) — [2]Helmoltz Zentrum Geesthacht Institut für Werkstoffforschung Abteilung WPN,Max-Planck-Straße 1 21502 Geesthacht (Deutschland)

Neutron reflectometry (NR) and grazing incidence small angle neutron scattering (GISANS) are two complementary techniques which enable to study the structure of thin films in a non destructive/non invasive manner. Given the sensitivity of neutron scattering to the isotopic composition of the system under investigation, contrast enhancement can be used to acces information that would otherwise remain masked e.g to conventional X-Ray methods.

The characteristics and operation modes of the neutron reflectomer REFSANS (which is operated at the FRM2 reactor near Munich) will be presented stressing how this versatile instrument can help elucidating the structure of different classes of materials. On one hand, examples of out of plane structure resolution via NR experiments performed on polymers, biological systems and metallic multilayers will be presented. On the other hand, the TOF-GISANS method will be introduced and it will be shown how it enables to resolve the lateral structure of thin films. Here too, examples from different fields of material physics will be shown.

DS 12: Layer Deposition Processes

Time: Monday 17:15–18:30 Location: GER 38

DS 12.1 Mon 17:15 GER 38

A growth model for the HfO_2 ALD process — •Marcel Michling, Massimo Tallarida, Krzysztof Kolanek, and Dieter Schmeisser — Brandenburgische Technische Universität Cottbus, Angewandte Physik / Sensorik, K.-Wachsmann-Allee 1, 03046 Cottbus

In this contribution we report on our in-situ^2 cycle-by-cycle (up to the 25 cycles) investigation of the HfO_2 atomic layer deposition (ALD) process using the method of x-ray photoelectron spectroscopy (XPS) and electron energy loss spectroscopy (EELS). We used Tetrakis-Dimethyl-Amino-Hafnium (TDMA-Hf) and H_2O as precursors and p-type Si wafer with native oxide as a substrate. The XPS measurements were carried out at BESSY II in Berlin with primary energies of 150 eV and 640 eV and the EELS measurements were done with a primary energy of 50 eV. We measured the O1s, Si2p core level and the valence band including the Hf 4f core level. From the Hf4f to Si2p ratios taken at each energy we developed a growth model for the first monolayer and for the following layers too. From our data we conclude, that in the first monolayer up to the fourth ALD cycle an island growth occurs. The height of these islands is about 0,5nm. After the first monolayer is completed, a layer- by-layer growth can be expected. In order to proof this observation we have simulated the Hf/Si ratio for different excitation energies and found a very good agreement with our measurement data. The EELS data especially the evaluation of the loss function onset confirm our growth model.

DS 12.2 Mon 17:30 GER 38

Atomic layer deposition of TiO_2 — •Massimo Tallarida, Nils Dessmann, Matthias Städter, Daniel Friedrich, Marcel Michling, and Dieter Schmeisser — BTU-Cottbus, Konrad-Wachsmann-Allee 17, 03046 Cottbus, Germany

We present a study of the initial growth of TiO_2 on Si(111) by *atomic layer deposition* (ALD). The Si substrate was etched with NH_4F before ALD to remove the native oxide film and to produce a Si-H termination. $In-situ$ experiments by means of photoemission and X-ray absorption spectroscopy were conducted with synchrotron radiation on Ti-oxide films produced using Ti-tetra-iso-propoxide (TTIP) and water as precursors. O1s, Ti2p, C1s, and Si2p core level, and O1s and Ti2p absorption edges show the transition of the Ti-oxide properties during the first layers. The growth starts with a very small growth rate (0.03nm/cycle) due to the growth inhibition of the Si-H termination and proceeds with higher growth rate (0.1nm/cycle) after 1.5nm Ti-oxide has been deposited.

DS 12.3 Mon 17:45 GER 38

Deposition and growth of antibacterial Ti-Cu films — •Vitezslav Stranak[1], Harm Wulff[1], Steffen Drache[1], Robert Bogdanowicz[1], Zdenek Hubicka[2], Carmen Zietz[3], Kathleen Arndt[4], Rainer Bader[3], Andreas Podbielski[4], and Rainer Hippler[1] — [1]University of Greifswald, Institute of Physik, Felix-Hausdorff-Str. 6, 17489 Greifswald, Germany — [2]Academy of Sciences of the Czech Rep., Institute of Physics, Na Slovance 2, 18221 Praha 8, Czech Republic — [3]University of Rostock, Department of Orthopaedics, Doberaner Str. 142, 18057 Rostock, Germany — [4]University of Rostock, Dept. of Med. Microbiol., Vir. and Hyg., Schillingallee 70, 18057 Rostock, Germany

Formation of Ti-Cu films prepared by advanced dual-magnetron sputtering techniques is presented. Three different methods of magnetron sputtering (dc, dual, and dual-HiPIMS) were employed to prepare intermetallic Ti-Cu films. Thin film properties were investigated by x-ray photoelectron spectroscopy and x-ray diagnostics. Preferential Cu crystallization is caused by a large density of Cu species in the discharge volume. The ion energy distribution in the substrate position (measured with a retarding field analyzer, RFA) corresponds with the crystallization process. The antimicrobial effect is caused by copper released from the Ti-Cu metallic structure; copper release was measured by atomic absorption spectroscopy. In vitro planktonic growth tests on Ti-Cu films prepared by dual-HiPIMS technique proved to kill bacteria efficiently.

DS 12.4 Mon 18:00 GER 38

Combination of ECR plasma and asymmetric bipolar pulsed bias voltage for deposition of hard a-C:H films — •Marcus Günther, Siegfried Peter, and Frank Richter — Technical University of Chemnitz, Institute of Physics, D-09107 Chemnitz, Germany

Thin hard layers of amorphous hydrogenated carbon a-C:H show a lot of special tribological, mechanical, electrical and optical properties. The commercial use of these films is mostly limited by the small deposition rate of usual deposition processes.

We have investigated a combination of magnetically supported microwave plasma and asymmetrical bipolar pulsed bias voltage in the mid-frequency region (100 kHz) which provides separate plasma generation and ion acceleration to the growing film. An electron cyclotron resonance (ECR) plasma source, operated at 400 W microwave power, generated a high density of film forming species (radicals and ions). A separate pulsed bias voltage of up to 550 V controlled the ion fluxes and as a consequence the layer properties.The a-C:H films were characterized with respect to hardness, deposition rate and surface topography. The chemical composition of the layers was analysed by ERDA and thermal desorption spectroscopy.

The deposition process was tested in mixtures of isobutene (C_4H_8) and argon at pressures below 2 Pa. The variation of the bias voltage allowed the deposition of both soft, hydrogen rich layers and hard a-C:H layers with less hydrogen. Thus, DLC films with a hardness of 25 GPa were deposited at high rates exceeding 10 μm/h.

DS 12.5 Mon 18:15 GER 38

Electrical and structural properties of magnetron sputtered hydrogenated amorphous Silicon films — •Frank Nobis, Hartmut Kupfer, Evelyn Breyer, Philipp Schäfer, Dietrich R. T. Zahn, and Frank Richter — Chemnitz University of Technology, Institute of Physics, 09107 Chemnitz, Germany

Magnetron sputtering could represent a valuable part of a low cost solar cell in line technology using amorphous silicon (a-Si) if a crucial problem could be overcome: In magnetron discharges, high energy particles are hitting the growing films. They cause a high defect density in the a-Si films, drastically reducing the efficiency of doping atoms.

We have investigated doped a-Si:H films sputtered by a pulsed DC magnetron discharge. The hydrogen content in the films was varied by changing the hydrogen partial pressure in the process gas. We found a saturation of the hydrogen content in the films at about 20 at.%. The electrical resistivity of the films was investigated at varied temperature to get information about the charge carrier transport. The results will be discussed in terms of different hopping conductivity mechanisms.

The investigations have shown that only a negligible fraction of the incorporated doping atoms are electrically active. Therefore, the goal of continued investigations is to increase dopant activation by changing the process parameters and by deposition at elevated substrate temperatures. Furthermore, the influence of substrate bias voltage and hydrogen partial pressure during deposition on the surface and structure of the film is reviewed.

DS 13: Organic Electronics and Photovoltaics CPP-I (jointly with CPP, HL, and O)

Time: Monday 14:00–17:30 Location: ZEU 222

Topical Talk DS 13.1 Mon 14:00 ZEU 222

Light harvesting in single polymer chains and inorganic nanostructures — •John M. Lupton — Institut für Experimentelle und Angewandte Physik, Universität Regensburg — Department of Physics and Astronomy, University of Utah, Salt Lake City

Optimization of materials for energy conversion applications requires an understanding of intermolecular heterogeneity to ultimately formulate synthetic approaches to maximizing the fraction of a particular subensemble. Single molecule spectroscopy can offer such insight as an exquisitely sensitive tool to unravel the underlying complexity of organic semiconductors. In the context of solar cells, for example, the technique can help to identify purely intramolecular exciton migration and charge separation processes.

Recently, we have explored the migration of excitons in single molecules as a function of the initial excitation energy, thus offering information on thermalization processes within the polymer chain. The approach allows a direct spectroscopic identification of the absorption of individual chromophores on the chain, whereas mere emission tends to provide information only on the lowest-energy unit in the intramolecular excitonic cascade [1].

The heterogeneity in light-harvesting characteristics is particularly pronounced in semiconductor nanostructures, where particle morphology directly influences the heterojunction band structure and the excitonic spectrum [2].

[1]Walter et al., Phys. Rev. Lett. 103, 167401 (2009).

[2]Borys et al., Science (in press).

DS 13.2 Mon 14:30 ZEU 222

Highly efficient vacuum processed BHJ solar cell based on merocyanines — •Vera Steinmann[1], Hannah Bürckstümmer[2], Nils M. Kronenberg[1], Martin R. Lenze[1], Dirk Hertel[1], Frank Würthner[2], and Klaus Meerholz[1] — [1]Department für Chemie, Universität Köln, Germany — [2]Institut für Organische Chemie and Röntgen Research Center for Complex Material Systems Universität Würzburg, Germany

Bulk heterojunction (BHJ) organic solar cells have attracted considerable interest due to their potential for large-scale, cost-effective and environmentally friendly power generation. Small molecules have been successfully introduced in solution- (SOL) as well as vacuum- (VAC) processed devices, reporting efficiencies (PCE) up to 4.4% and 5.7% respectively. For simple layer stack devices (2-3 layers) based on CuPc as electron donor and C60 as electron acceptor PCEs up to 5.0% have been achieved.

Recently, we presented a direct comparison of highly efficient SOL and VAC BHJ cells based on merocyanine dyes (MC) with a similarly simple layer stack as reported in the literature. Our most efficient devices exhibited PCEs up to 4.9%. Further optimizations on the VAC processed cells led to high PCEs exceeding 6% while keeping the same simple layer stack. In addition, these cells have demonstrated exceptional performance even at lower light intensities.

Due to the simple chemical variability of MC dyes, they are ideally suited for tandem solar cells. We will present first attempts in this direction.

DS 13.3 Mon 14:45 ZEU 222

Efficiency-Limiting Processes in Bulk Heterojunction Organic Solar Cells — Ian Howard, Ralf Mauer, Fabian Etzold, Valentin Kamm, Michael Meister, Hannah Mangold, and •Frédéric Laquai — Max Planck Research Group for Organic Optoelectronics, MPI for Polymer Research, Mainz, Germany

Despite significant study, the efficiency-limiting processes that govern the efficiency of bulk heterojunction photovoltaic devices still remain ambiguous. In particular the role of interfacial charge-transfer (CT) states as potential intermediates of free charge carriers is diversely debated. In this contribution we directly observe charge generation and recombination processes in state-of-the-art polymer:methanofullerene photovoltaic blends by transient absorption spectroscopy and compare polythiophene (P3HT) of varying regioregularity and low-bandgap polymers as electron donor materials. We observe a common feature of these blends is ultrafast (< 100 fs) exciton dissociation at the donor-acceptor interface. However, a certain fraction of excitons create CT states that predominantly recombine geminately within a few nanoseconds. On the other hand the fraction of free charge carriers recombines bimolecularly on a time scale competing with charge extraction and can thus be swept out of the device as photocurrent. The results demonstrate the importance of ultrafast free carrier generation and suppression of interfacial CT state formation to achieve high power conversion efficiencies in various material systems. [1] I.A. Howard, R. Mauer, M. Meister, F. Laquai, J. Am. Chem. Soc. 2010, 132, 14866. [2] I.A. Howard, F. Laquai, Macromol. Chem. Phys. 2010, 211, 2063.

DS 13.4 Mon 15:00 ZEU 222

Bias-Dependent Transient Absorption on Organic Solar Cells; Connection to Device Performance? — •Ian Howard, Ralf Mauer, Valentin Kam, Michael Meister, and Frédéric Laquai — Max Planck Forschungsgruppe für Organische Optoelektronik, Max-Planck-Institut für Polymerforschung, Mainz, Deutschland

We directly observe the bias dependence of charge-transfer state separation in organic bulk heterojunctions using in-situ transient absorption on operating organic solar cells. The effect of bias on charge-transfer state lifetime (< 2ns) is found to be minimal, however suppression of nongeminate recombination with bias on later timescales (>10 ns) is observed and explains the bias dependence of the photocurrent. The bias independence of charge-transfer state separation is directly applicable to interpreting organic solar cell performance under standard AM1.5 illumination. However, due to the differences in charge densities and dynamic versus steady-state behavior between pulsed measurements and standard operating conditions, the effects of bias on the suppression of nongeminate recombination are not simplistically transferable. We consider to what extent pulsed transient absorbtion techniques on devices can be used to reveal nongeminate recombination mechanisms in devices operating under standard illumination conditions.

DS 13.5 Mon 15:15 ZEU 222

Degradation effects related to the hole transport layer in organic solar cells — •Bernhard Ecker[1], Jairo Nolasco[2], Josep Pallarés[2], Lluis Marsal[2], Jörg Posdorfer[3], Jürgen Parisi[1], and Elizabeth von Hauff[1] — [1]Energy and Semiconductor Research Laboratory, Institute of Physics, Carl von Ossietzky University, 26111 Oldenburg (Germany) — [2]Departament d'Enginyeria Electrònica Elèctrica i Automàtica, Universitat Rovira i Virgili, Avda. Països Catalans 26, 43007 Tarragona (Spain) — [3]Enthone Nano Science Centre, Ormecon GmbH, Ferdinand-Harten-Str. 7, 22949, Ammersbek (Germany)

We discuss the influence of the hole transport layer on the device stability in organic bulk-heterojunction solar cells. Two water based hole transport layers, poly(3,4-ethylenedioxythiophene) : poly(styrene sulfonate) (PEDOT:PSS) and polyaniline : poly(styrene sulfonate) (PANI:PSS), and one isopropyl alcohol based PANI:PSS transport layer were investigated. Solar cells were prepared with the three different hole transport layers and degraded under illumination. Current-voltage, capacitance-voltage, and capacitance-frequency data were collected at varying light intensities over a period of 7 hours. Solar cell performance and stability were compared between non encapsulated and encapsulated samples to obtain understanding about degradation effects related to oxygen and water as well as degradation mechanisms related to the intrinsic instability of the solar cell materials and interfaces. We show that the properties of the hole transport layer can have a significant impact on the stability of organic solar cells.

15 min. break

DS 13.6 Mon 15:45 ZEU 222

Characterization of trap states in small-molecule organic solar cells by using Impedance Spectrocopy. — •Lorenzo Burtone, Debdutta Ray, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden Germany

In this work, we focus on the characterization of trap levels in the electronic gap of organic semiconductors used in solar cells. These states can modify the electric field inside the device, considerably affecting charge generation and transport and consequently the solar cell efficiency. A method to characterize traps by using impedance spectroscopy is presented. We propose a new equivalent circuit based on previously reported theoretical models and we apply it in the fitting procedure of the measured data. In particular, we measure the impedance spectra of two flat heterojunction small molecule solar cells, where one of them has doped electron and hole transport layers. We observe the contribution of trap states at low frequencies in the capacitance spectra for the devices with doped transport layers. The experimental results can be understood with the equivalent circuit proposed and the trap state contribution can be evaluated. From a fitting procedure, we estimate the density of trap states to be around $1\text{x}10^{17}\text{cm}^{-3}\text{eV}^{-1}$. Moreover we observe from the impedance analysis the presence of dopants in the intrisic layer with an estimated effective concentration of about $8.4\text{x}10^{17}\text{cm}^{-3}$. This value is in agreement with very low doping concentration and suggests the formation of a non-abrupt junction between intrinsic and doped layers.

DS 13.7 Mon 16:00 ZEU 222

The effect of energetic disorder on open-circuit voltage in organic photovoltaics — •James C Blakesley, Ilja Lange, and Dieter Neher — University of Potsdam, Germany

Open-circuit voltage (VOC) is one of the most important figures of merit describing the quality of organic photovoltaics (OPVs). Usually it is assumed that VOC depends on the energy difference between the highest occupied molecular orbital (HOMO) of the donor and the lowest unoccupied molecular orbital (LUMO) of the acceptor, but large deviations from this trend are often found. In reality, there is a distribution of energy levels within the components, and this should also be taken into account.

We simulate bulk heterojunction OPVs using a simulation that includes the effects of energetic disorder [1].We find that VOC depends on: 1) the nominal donor-HOMO to acceptor-LUMO energy gap; 2) the charge-carrier generation and recombination rates; 3) the electrodes; and 4) the amount of energetic disorder. While the first three of these points have been much discussed previously, the effect of the fourth has not been conclusively demonstrated. An increase in the amount of energetic disorder leads to a reduction in the VOC due to relaxation of the carriers into the lowest lying energy levels. We find an analytical expression that predicts well the modelled VOC, and suggest the use of an effective donor-acceptor energy gap that takes energetic disorder into account. Measurements of Fermi-level pinning might be useful for determining this effective energy gap. [1] J. C. Blakesley and N. C. Greenham, J. Appl. Phys. 106, 034507 (2009)

DS 13.8 Mon 16:15 ZEU 222

Modelling Temperature-Dependent Current-Voltage Curves of Organic Photovoltaic Devices — •Simon Züfle, Martin T. Neukom, Benjamin Perucco, Nils A. Reinke, and Beat Ruhstaller — ICP, ZHAW, Winterthur, Schweiz

Current-voltage curves allow to determine both fill-factor and efficiency of organic photovoltaic devices and are therefore a commonly used characterisation technique. Since analytical models for current-voltage curves fail in describing the fundamental processes of photogenerated current, more complex numerical calculations are mandatory for obtaining insight into the device physics. The analysis of multiple current-voltage curves at different temperatures calls for CPU-efficient algorithms combining state-of-the-art physical models and high calculation speed.

In order to model current-voltage curves simple drift-diffusion calculations with constant mobilities and thermionic emission as injection model are frequently used. In this study we investigate current-voltage curves measured at different temperatures with the help of a nonlinear least-square fitting algorithm in combination with a comprehensive physical model for charge carrier transport and injection. We evaluate the performance of different models for charge carrier transport, including the Gaussian Disorder Model, by simultaneously fitting multiple curves and discussing the mathematical quality of the fit. We employ an efficient algorithm for extracting material-specific parameters that allows modelling of measured current-voltage curves on a minute time-frame with a desktop PC.

DS 13.9 Mon 16:30 ZEU 222

Role of drift and diffusion in organic solar cells measured by transient photocurrents — •Wolfgang Tress, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, TU Dresden, Dresden, Germany

The role of the electric field and the contribution of diffusion to photocurrents are controversially discussed in the case of organic solar cells. We investigate flat heterojunction organic solar cells with systematically varied barriers at the contacts that are created by a HOMO offset between donor and hole transport layer. These barriers lead to S-kinks in the IV curve and to strong imbalanced and even reversed forces on charge carriers resulting from the field on the one hand and the concentration gradient on the other hand. By applying a rectangular illumination signal with varied light intensities, we observe in the photocurrent transients a pile-up of charge carriers at an extraction barrier. If an injection barrier is present, there exists a region in the IV curve where charges are extracted against the electric field by a strong diffusion gradient. These findings are based on the analysis of transient current data in the μs regime using electrical simulations based on a drift-diffusion model. The simulations show that observed overshoots in the photocurrent transients result from these imbalance effects and give new insights into the working principle of organic solar cells.

DS 13.10 Mon 16:45 ZEU 222

Charge extraction with linearly increasing voltage: A numerical model for parameter extraction — •Martin Neukom, Simon Züfle, Nils Reinke, and Beat Ruhstaller — Institute of Computational Physics, Technikumstr 9, 8401 Winterthur, Switzerland

Device characterisation is an essential part in the process of improving the performance and lifetime of organic solar cells. Most of the device and material parameters are not accessible by measurements therefore sophisticated measurement techniques in combination with numerical simulations are needed to extract these parameters. A frequently used method to determine material parameters like charge carrier mobilities and the recombination coefficient is the CELIV technique (charge extraction by linearly increasing voltage). In this technique a voltage ramp is applied to the device in order to extract free charge carriers inside the bulk. With a simple analytical formula the mobility is commonly estimated on the basis of the temporal position of the current peak. We simulate the CELIV experiment, transient and steady-state measurement techniques with a fully-coupled opto-electronic model. On the one hand we investigate the limitations of the analytical formulas for mobility determination. On the other hand we use our model to fit several experimental datasets simultaneously to obtain elementary material parameters like the electron and hole mobility, recombination coefficient, photon to charge conversion efficiency and injection barriers in both printed and spin-coated bulk heterojunction solar cells. We deduce the influence of these material parameters on the overall device performance.

DS 13.11 Mon 17:00 ZEU 222

Simulating electron transfer reactions in organic solar cell components — •Harald Oberhofer[1] and Jochen Blumberger[2] — [1]Department of Chemistry, University of Cambridge, UK — [2]Department of Physics and Astronomy, University College London, UK

Organic solar cells are envisaged as a promising alternative to silicon based solar cells. They are cheap and easy to produce, light and flexible, and easily deployed on walls or roofs. Unfortunately, these advantages currently come at the price of small photo-electric conversion efficiencies. To help overcome this deficiency we use advanced density functional theory (DFT) based methods to investigate the electron-conducting properties of modified Fullerene crystals which are commonly used as electron-conducting component in organic solar cells.

In our contribution we will briefly discuss the techniques used to estimate electron transfer rates from computer simulations. Then we present our calculations on modified Fullerene crystals. We studied $C_{61}H_2$—a commonly used test system—and [6,6]-phenyl-C61-butyricacid-methyl-ester (PCBM) for 3 different crystal lattices which are commonly found in experiments. In the crystal we estimated electron transfer rates between next- and next-nearest neighbours with and without the application of an external electric field. These results where then used to estimate the electron mobility for the different lattice types. These results can represent a starting point for the optimisation of electron conduction in next-generation organic solar cells.

DS 13.12 Mon 17:15 ZEU 222

Time resolved microwave conductivity reveals charge carrier dynamics in organic semiconductors — •Johannes Erben[1], Andreas Sperlich[1], Hannes Kraus[1], Tom J. Savenije[1,3], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — [2]ZAE Bayern, D-97074 Würzburg — [3]Department of Chemical Engineering, Delft University of Technology, NL-2628 BL Delft, The Netherlands

Understanding of the light induced charge carrier dynamics in organic semiconductors is essential to improve material properties and processing parameters, and, at long sight, device performance. Time Resolved Microwave Conductivity (TRMC) gives direct access to the microscopic transport properties, as the high frequency alternating electric field limits the drift of the charge carriers. After laser pulse excitation TRMC signal decays in P3HT:PCBM blends with varying PCBM content have been observed exhibiting a power law time dependence. The influence of morphology and temperature on the charge carrier recombination and mobility on a microscopic scale can thus be investigated.

DS 14: Organic Electronics and Photovoltaics HL-I (jointly with CPP, HL, and O)

Time: Monday 17:45–18:45 Location: FOE Anorg

DS 14.1 Mon 17:45 FOE Anorg

Band gap states of copper phthalocyanine thin films induced by nitrogen exposure — •Tomoki Sueyoshi[1,2], Haruya Kakuta[1], Masaki Ono[1], Kazuyuki Sakamoto[1], Satoshi Kera[1], and Nobuo Ueno[1] — [1]Graduate School of Advanced Integration Science, Chiba University, Chiba, Japan — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany and JARA-Fundamentals of Future Information Technology

Extensive experimental and theoretical investigations have demonstrated the strong correlation between electronic and structural properties of organic layers. Although understanding of this correlation is very crucial, the question whether the intrinsic or externally induced disorder in the molecular packing structure influences their electronic properties remains obscure.

Here we investigated impact of 1-atm N2 gas exposure on the electronic states of copper phthalocyanine thin films using ultrahigh-sensitivity ultraviolet photoelectron spectroscopy. The highest occupied molecular orbital band of the film showed a drastic reversible change in the bandwidth and band shape as well as in the energy position upon repeated cycles of N2 exposure and subsequent annealing. Furthermore, two types of gap-state densities with Gaussian and exponential distributions appeared after the exposure and disappeared due to the annealing. These changes are ascribed to a weak disorder in the molecular packing structure induced by N2 diffusion into the film.

DS 14.2 Mon 18:00 FOE Anorg

Influence of temperature and illumination on the photovoltage of organic solar cells — •Johannes Widmer, Wolfgang Tress, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, TU Dresden, George-Bähr-Straße 1, 01069 Dresden

Temperature plays an essential role in many processes in organic devices, including the current and voltage generation in organic solar cells. In this contribution, we focus on the open-circuit voltage of organic solar cells when varying illumination intensity and temperature in the range of 200K to 400K. Zinc phthalocyanine (ZnPc) and C60 are used as reference system and other materials are investigated in comparison to demonstrate the connection between the effective energy gap and the open-circuit voltage of a photovoltaic device. The use of doped transport layers in a p-i-n diode geometry allows to minimize the energetic losses between the active layers and the contacts and gives access to the quasi Fermi levels in the heterojunction. We can verify the dependence between the effective gap of a heterojunction and the open-circuit voltage. A substantial difference, however, is observed comparing the interplay of temperature and illumination intensity of bulk and flat heterojunction devices. Classic photo-diode like behaviour is observed for the open-circuit voltage of bulk heterojunction devices, as described by generation-recombination dynamics. In the case of a flat heterojunction, however, the influence of temperature and illumination become independent, which is not covered by the established theory. These findings can contribute to the understanding of the photo-voltage of organic devices.

DS 14.3 Mon 18:15 FOE Anorg

Open circuit voltage as function of mixing ratio in ZnPc:C60 bulk heterojunction organic solar cells — •Steffen Pfuetzner, Wolfgang Tress, Selina Olthof, Max Tietze, Jan Meiss, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01069 Dresden, Germany

We characterize organic solar cells composed of mixed layers of ZnPc:C_{60} as photoactive layer embedded between a p-doped hole transport (HTL) and an undoped electron transport layer. By varying the mixing ratio of the photoactive bulk heterojunction from 6:1 (ZnPc:C_{60}) to 1:6 by volume, we observe significant changes of V_{OC} from 0.54 to 0.63 V. To exclude that this increase with higher C_{60} content is caused by the increased contact area of C_{60} to the HTL, behaving as an additional exciton separating interface, *J(V)* measurements under spectral narrow red and blue illumination are performed. Independent of where absorption takes place (for red in ZnPc, for blue in C_{60}), V_{OC} is not affected significantly. Hence, we attribute the changes in V_{OC} not to an additional separating interface, but to an intrinsic blend layer effect. Further investigations using ultraviolet photoelectron spectroscopy measurements, absorption measurements, and HTL variations with different highest occupied molecular orbitals indicate as reason HOMO and LUMO shifts of C_{60} and ZnPc as a function of the mixing ratio.

DS 14.4 Mon 18:30 FOE Anorg

In-situ characterization of molecular semiconductor donor-acceptor-blends — Lena Kristin Cornelius, •Max Beu, and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email:schlettwein@uni-giessen.de

Blends of $F_{16}PcCu$ and $PcCu$ were prepared on glass by physical vapour deposition. The acquired thin films had a thickness of around 20nm. The co-evaporation of $PcCu$ and $F_{16}PcCu$ was varied to obtain different molecular mixtures. High admixture of $PcCu$ to $F_{16}PcCu$ as typically used in bulk-hetero-junctions were compared to very low admixtures typical for dopant interactions. The current-voltage characteristics were studied during evaporation (in-situ). High levels of $PcCu$ in $F_{16}PcCu$ (moderate per cent range) disturbed the charge flow in the films. Very little admixture of $PcCu$ in the low per mille range, however, led to an increased conductivity, indicating a successful dopant interaction. Optical transmission spectroscopy consequently showed the disturbance of the $F_{16}PcCu$ solid state structure. The dominant $\beta_{bilayer}$–structure of pure $F_{16}PcCu$ (highly conductive) was partly changed to the herringbone β–structure (less conductive). Consequences for photoconduction in the films will be discussed.

DS 15: Plasmonics and Nanophotonics O-I (jointly with HL and O)

Time: Monday 15:00–17:00 Location: PHY C213

DS 15.1 Mon 15:00 PHY C213

Quasistatic plasmon resonances in the visible spectral range of arbitrary shaped nano-grooves — •Camille Maxime[1,2], Aude Barbara[1,2], and Pascal Quemerais[1,3] — [1]Institut Néel, CNRS-UJF, Grenoble, France — [2]IAPP, TU Dresden, Germany — [3]MPI-PKS, Dresden, Germany

As we previously reported, plasmonic resonances inside rectangular nano-grooves periodically made on a silver surface present a cross-over between two physical regimes [1]: an optical one for groove widths w larger than 10 nm, and a quasistatic one for lower values. In that case, the grooves resonate in the visible range even for grooves height h of only a few nanometers (5-15 nm). A very strong light absorption occurs at the resonance together with an electric field intensity enhancement (EFIE) of about 400. These results were obtained with a method only available for rectangular shapes. To generalize, we have implemented a surface integral method [2] and adapted it to periodic profiles to avoid surface boundaries problems. As an example, the behaviour of Gaussian shaped grooves was studied. It fully confirms the transition to a quasistatic regime as the groove width decreases leading to unusual EFIE (up to about 10000) and a very strong light absorption. These original results are fundamental to explain surface enhanced Raman scattering (SERS) experiments such as the historical ones of Albano et al.[3].

[1] J. Le Perchec et al., *Phys. Rev. Lett.* **100**, 066408 (2008)

[2] A.A. Maradudin et al., *Ann. Phys.* **203**, 255 (1990)

[3] E.V. Albano et al., *Phys. Rev. Lett.* **51**, 2314 (1983)

DS 15.2 Mon 15:15 PHY C213

Coupled nanoantenna plasmon resonance spectra from two-photon laser excitation: longitudinal and transversal emission — •Matthias D. Wissert[1], Carola Moosmann[1], Konstantin S. Ilin[2], Michael Siegel[2], Uli Lemmer[1], and Hans-Jürgen Eisler[1] — [1]Light Technology Institute, DFG Heisenberg Group 'Nanoscale Science', Karlsruhe Institute of Technology, Germany — [2]Institute of Micro- and Nanoelectronic Systems, Karlsruhe Institute of Technology, Germany

We report on the plasmonic mode relaxation of coupled optical gold nanoantennas under two-photon laser excitation at 810 nm [1]. An oil immersion objective lens is used both for the excitation and detection channel. The plasmon emission intensity from single nanostructures is detected using a single-photon-counting avalanche photodiode, the response spectrum is observed with an EMCCD camera.

We show that the plasmon spectra are very similar to the well known scattering resonances [2] for such structures, albeit now obtained from single frequency excitation. We also show that not only the longitudinal, but also the transversal plasmon mode can be excited, using excitation light polarized exclusively along the long axis of the dipole antenna.

[1] M.D. Wissert, K.S. Ilin, M. Siegel, U. Lemmer, and H.-J. Eisler, Nano Letters **10**, 4161 (2010)

[2] M.D. Wissert, A.W. Schell, K.S. Ilin, M. Siegel, and H.-J. Eisler, Nanotechnology **20**, 425203 (2009)

DS 15.3 Mon 15:30 PHY C213

Metallic nanorod arrays: negative refraction and optical properties explained by retarded dipolar interactions — •René Kullock[1], Stefan Grafström[1], Paul R. Evans[2], Robert J. Pollard[2], and Lukas M. Eng[1] — [1]Institut für Angewandte Photophysik, TU Dresden, 01062 Dresden, Germany — [2]Centre for Nanostructured Media, IRCEP, The Queen's University of Belfast, Belfast BT7 1NN, UK

Two-dimensional (2D) arrays of metallic nanorods arranged perpendicular to a substrate exhibit novel optical features: a short-axis resonance, and several long-axis surface plasmon resonances (LSPRs) which appear for excitation with p-polarized light at specific angles of incidence [1]. Especially the first LSPR mode is very sensitive to both geometry and environment. In order to make it accessible for different applications, a fundamental physical understanding is indispensable.

Here, we theoretically treat such a 2D nanorod array by applying the retarded dipolar interaction model (DIM). First, we nicely follow the LSPR changes when extending our calculations from the single nanorod to a 2D array of nanorods [2]. Then, using the DIM model we are able to explain how the LSPR depends on several physically relevant parameters, such as the nanorod length, diameter, neighboring distance, material, and surroundings. Furthermore, the DIM also delivers conditions under which negative and extraordinary positive refraction in such metallic nanorod arrays will occur.

[1] R. Kullock et al., *Opt. Express 16, 21671 (2008)*

[2] R. Kullock et al., *J. Opt. Soc. Am. B 27, 1819 (2010).*

DS 15.4 Mon 15:45 PHY C213

Photoemission Microscopy on Surface Plasmon Polaritons in Ag Islands — Niemma Buckanie, Pierre Kirschbaum, Simon Sindermann, Michael Horn-von Hoegen, and •Frank Meyer zu Heringdorf — Universität Duisburg-Essen, Fakultät für Physik and Center for Nanointegration (CeNIDE), Lotharstrasse 1, 47057 Duisburg, Germany

The interaction of frequency doubled femtosecond laser pulses with Silver islands on Si in a photoemission electron microscope provides a fantastic toolbox to study the interaction of light with surface plasmon polaritons (SPP) in small Ag islands. In two photon photoemission microscopy (2PPE PEEM), SPPs are imaged as a time-integrated superposition of the electric field of the propagating SPP wave with the electric field of the exciting laser pulse that hits the surface under grazing incidence. A quantitative analysis of the experimentally observed moiré pattern allows studying of the SPP field strength and a determination of the propagation direction of the SPP. At the rear edge of the island the SPP wave can be converted back into light. The resulting superposition of the converted light with the incident laser pulse is manifested in an enhanced photoemission yield behind the island.

DS 15.5 Mon 16:00 PHY C213

Experimental observation of decoupled plasmon resonances in metallic nanoparticles — •Reto Giannini[1], Yasin Ekinci[1,2], and Jörg F. Löffler[1] — [1]Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, 8093 Zurich, Switzerland — [2]Laboratory for Micro and Nanotechnology, Paul Scherrer Institute, 5232 Villigen PSI, Switzerland

The optical response of designed metallic nanostructures is of high interest due to its importance in sensing applications, nanoantennas and nanooptics. With the aim to analyze the optical response of metallic nanostructures in the visible wavelength range, we produced metallic nanoparticles with the simple geometry of cylinders standing on a glass substrate by e-beam lithography. Additionally, a measurement set-up was established that allows the directional excitation of nanoparticles in three dimensions. Based on the analysis of the nanocylinders, we show experimental evidence that the overall optical response of such a system is the superposition of individually tunable plasmon resonances, i.e. normal modes. In the case of the cylinder, three normal modes associated with the main axes and therefore excitable by a polarization along these axes have been observed. Finally, these results are compared with FEM-based simulations.

DS 15.6 Mon 16:15 PHY C213

Modeling Metallic Nanostructures using a Discontinuous Galerkin Approach — •Jens Niegemann, Michael König, Christopher Prohm, Timo Köllner, and Kurt Busch — Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany

Over the past few years, the discontinuous Galerkin time-domain (DGTD) method has established itself as an extremely powerful and efficient numerical technique in the field of photonic. Due to its combination of an accurate spatial discretization with an explicit time-stepping scheme, the DGTD method is particularly well suited for studying ultra-short and/or plasmonic phenomena. Furthermore, the method is readily extended to also treat hydrodynamic equations, which allows us to also model the nonlocal and nonlinear properties of metallic nanostructures.

Here, we discuss our recent advances in using the DGTD method for the simulation of plasmonic devices. In particular, we present first results on a full hydrodynamical simulation of small metallic nanostructures.

DS 15.7 Mon 16:30 PHY C213

Mode imaging and selection in strongly coupled nanoantennas — Jer-Shing Huang[1], •Johannes Kern[1], Peter Geisler[1], Pia Weinmann[2], Martin Kamp[2], Alfred Forchel[2], Paolo Biagioni[3], and Bert Hecht[1] — [1]Experimental Physics 5, University of Würzburg, Germany — [2]Technische Physik, University of Würzburg, Germany — [3]CNISM, Politecnico di Milano, Italy

Plasmonic nanostructures consisting of gold nano-wire pairs offer a large variety of different modes, depending on their geometric arrangement, for which the optical near-fields can be strongly confined in nanometerscale gaps. Of particular interest are modes which couple only weakly to the radiation field, e.g. due to a quadrupolar charge distribution. For such modes, simulations predict that the corresponding resonances should exhibit comparatively large quality factors due to the absence or the reduction of radiation damping.

In order to demonstrate a correspondence between simulations and experiments, we strive to fabricate gold nanostructures that are free of defects and exhibit ultra-smooth surfaces. To achieve this goal, we apply top-down nanofabrication methods, which rely on focused-ion-beam milling of large, but ultrathin single-crystalline gold flakes.

We will discuss simulations and experimental investigations of strongly-coupled optical antennas selectively excited to their antibonding resonance.

DS 15.8 Mon 16:45 PHY C213

Size, gap, shape, and material dependence of third harmonic generation from bowtie nanoantenna arrays — •Mario Hentschel[1,2], Tobias Utikal[1,2], Markus Lippitz[1,2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, D-70569 Stuttgart, Germany — [2]Max-Planck-Institute for Solid State Research, Heisenbergstr. 1, D-70569 Stuttgart, Germany

We investigate third harmonic generation from gold bowtie nanoantenna arrays. We fabricated 9x11 arrays of 125x200 nanoantennas each, varying continuously the gap size as well as the bowtie size. Both structural parameters determine the resonance wavelength of these plasmonic dimers, leading to a wide range of resonance positions from 690 nm to 1020 nm. The linear transmittance spectra are measured by an FTIR microscope. 8 fs broadband laser pulses with a center wavelength of 820 nm are utilized to generate the third harmonic signal. We find that surprisingly the third harmonic signal does not scale with shrinking gap size as expected, but is rather a function of resonance energies in the hybridized plasmonic dimer. The third harmonic signal is strongest for maximum overlap of the extinction spectrum of the nanostructures and the laser spectrum, as well as when the plasmonic oscillator strength is largest. Furthermore we study variations of the nanoantenna system in order to gain further insight in the harmonic generation process. We are going to present resent results on the THG conversion efficiencies for different antenna designs, such as rod-, sphere-, and gap-antennas, as well as for different antenna materials.

DS 16: Plasmonics and Nanophotonics O-II (jointly with HL and O)

Time: Monday 17:15–19:15 Location: PHY C213

DS 16.1 Mon 17:15 PHY C213

Lithographically defined plasmonic waveguides on semiconductors for on-chip quantum optics applications — •Gregor Bracher, Konrad Schraml, Benedikt Mayer, Birgit Wiedemann, Simon Frédéric, Jonathan J. Finley, and Michael Kaniber — Walter Schottky Institut, Technische Universität München, Am Coulombwall 4, D-85748 Garching, Germany

We present optical investigations on lithographically defined plasmonic waveguides (WG). The metallic WGs are fabricated on GaAs substrates by electron beam lithography and subsequent metallisation. Structural properties are probed by atomic force microscopy and scanning electron microscopy revealing a surface roughness below 3 nm. For the optical characterisation we use a two axis confocal micro-photoluminescence setup that enables us to excite and detect plasmons perpendicular and parallel to the sample surface. First measurements show that Au WGs with a thickness of 100 nm and width of 4 μm exhibit a propagation length of 15 μm at $\lambda = 820\ nm$. We clearly observe strong localisation of the excitation at the wire end and the expected polarisation dependence along the WG axis. Using the same technique we prove that plasmons can be excited in lithographically defined Au nanowires with a cross section down to 100x100 nm^2. The deterministic control of the position and shape of the plasmonic nanostructures by means of electron beam lithography combined with near surface self-assembled InGaAs/GaAs quantum dots promises efficient on-chip generation and guiding of single plasmons for future applications in nanoscale quantum optics.

DS 16.2 Mon 17:30 PHY C213

Fabrication of high-quality large-area plasmonic oligomers — •Jun Zhao, Bettina Frank, and Harald Giessen — Universität Stuttgart

Plasmonic structures with a structure size of around 100nm are tremendously important for applications in the visible and near-IR range. Surface-enhanced Raman scattering substrates, localized surface plasmon resonance sensors, narrow resonances using plasmonic induced transparency, and local field concentration in oligomers to create hot spots are among those applications. Key issues in the design and manufacturing of such structures are small gaps in the range of sub-20nm, sharp edges, and narrow resonances. For applications, large fabrication areas in the range of cm^2 and low manufacturing costs are crucial. Here, we present a method that fulfils these requirements. Utilizing tilted-angle-rotation lithography with a polar and azimuthal rotation axis and shutter control together with monolayers of polystyrene spheres we create reproducibly homogeneous structures in 50nm to 200nm range with 10nm gaps over areas of cm^2. We fabricated triangular monomers, dimers, trimers, quadrumers, and pentamers, with open and closed gaps and with different size of nanospheres, and measured their transmittance spectra by FTIR microscopy. The spectra show well modulated resonances which depend sensitively on the incident polarization. We can attribute the various collective modes to the different features of the spectra and observe hybridization effects. This confirms the high quality of our fabrication method.

DS 16.3 Mon 17:45 PHY C213

Plasmonic nanostructures for strong light confinement fabricated using soft-lithography and plasma etching techniques — •Manuel Gonçalves[1], Tobias Paust[1], Fabian Enderle[2], Stefan Wiedemann[2], Alfred Plettl[2], Paul Ziemann[2], and Othmar Marti[1] — [1]Ulm University - Inst. of Experimental Physics, Albert-Einstein-Allee 11, 89069 Ulm, Germany — [2]Ulm University - Inst. of Solid State Physics, Albert-Einstein-Allee 11, 89069 Ulm, Germany

Nanosphere lithography has been commonly used for fabrication of plasmonic nanostructures. Small triangular particles of less than 100 nm size, with sharp corners, can be obtained at low cost. These structures have been used for plasmonic based sensing applications.

We show how nanosphere lithography can be extended for fabrication of more complex structures as arrays of holes on corrugated dielectrica and arrays of metal-dielectric pillars, using in combination soft-lithography and reactive ion-etching techniques (ICP-RIE). Surface plasmon modes can be easily excited on metal coated periodic dielectric structures using light. On the other hand, geometrical singularities lead to strong localized surface plasmons. The fabricated structures can be used for plasmonic effects as enhanced optical transmission, light confinement and surface enhanced Raman spectroscopy, due to their geometrical and optical properties. Confocal microscopy and angle-resolved spectroscopy were used for study of far-field transmittance and reflectance. The near-fields were investigated by SNOM and confocal Raman microscopy. Simulations were carried out to obtain the near-fields and optical resonances.

DS 16.4 Mon 18:00 PHY C213

Light Localization Effects in Commensurate Gratings — •Aude Barbara[1,2], Jerôme Le Perchec[3], Stéphane Collin[4], Camille Maxime[1,2], and Pascal Quémerais[1,5] — [1]Institut Néel, CNRS-UJF, Grenoble, France — [2]IAPP, TU Dresden, Germany — [3]CEA, Grenoble, France — [4]LPN, Marcoussis, France — [5]MPI-PKS, Dresden, Germany

We present a study in which infrared light localization phenomena are induced in commensurate gratings made of deep sub-wavelength metallic grooves. We combined the effects of light trapping within active sites (the deep cavities) with the properties of self-similar arrangements (commensurate gratings). We show that as the degree of commensuration tends to an irrational number new light localization states are produced. Interestingly, these have properties close to that reported for hot spots on disordered surfaces. In particular they present a very high sensitivity to the variation of the exciting field (wavelength and incident angle). We also experimentally demonstrated the existence of these new resonances and measured their dispersion diagrams. We observed selective light localization within the cavities, transition from localized to delocalized modes and modifications of the mode coupling with the incident light leading to the generation of black modes. The theoretical analyze is in full agreement with the experiments.

A. Barbara et al. *Opt. Exp.* **16**, 19127 (2008)
A. Barbara et al. *Opt. Exp.* **18**, 14913 (2010)

DS 16.5 Mon 18:15 PHY C213

Parallel nanostructuring of fused silica exploiting local near fields — •Sören Maag, Rodica Morarescu, Frank Träger, and Frank Hubenthal — Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

In modern nanotechnology, there is an ongoing interest to decrease the dimensions of surface structures below the diffraction limit. Furthermore, parallel structuring of surfaces with light induced processes is of particular interest. Along these lines we are using nanosphere lithography to create highly ordered triangular gold nanoparticle arrays and exploit their localized optical near field to overcome locally the ablation threshold of fused silicia. Therefore, the nanoparticle arrays were irradiated with a single ultrashort laser pulse (35 fs), at a central wavelength of 790 nm. Depending on the polarization and the fluence of the laser light holes, grooves, or channels, with dimensions well below the diffraction limit have been created. For example, for a polarization along the bisector of the triangular nanoparticles, nanogrooves with a depth of 14 nm, a width at its waist of 45 nm, and a length of 290 nm have been generated, if fluences near the ablation threshold were applied. In contrast, tiny spherical nanoholes with diameters of only 23 nm can be achieved, for fluences significantly below the ablation threshold. The obtained structures can be explained by the enhanced electromagnetic near fields, which overcome locally the ablation threshold of fused silica in the vicinity of the irradiated nanoparticles.

DS 16.6 Mon 18:30 PHY C213

Mapping infrared antenna resonances of particle arrays fabricated by nanosphere lithography — •Jens Richter[1], Andrea Hartung[1], Jón Mattis Hoffmann[1], Xinghui Yin[2], and Thomas Taubner[1,2] — [1]1st Institute of Physics, RWTH-Aachen University, Sommerfeldstrasse 14, 52074 Aachen, Germany — [2]Fraunhofer Institute for Laser Technology, Steinbachstr. 15, 52074 Aachen, Germany

Infrared vibrational spectroscopy is sensitive to characteristic molecule absorption bands, yielding a "fingerprint" spectrum of the molecules involved. The sensitivity of infrared spectroscopy has been increased by several orders of magnitude with optical antennas [1-3]. Arrays of hexagonal sorted triangular metallic infrared antennas created by Nanosphere lithography (NSL) have already been shown to exhibit IR resonances [4].

Our goal is the systematic variation of the NSL fabrication parameters in order to tune the antenna resonance over the whole mid-IR spectrum. We fabricate antenna arrays on different IR-transparent substrates and vary the particles lateral size and height. Using a Fourier-Transform-Infrared-Microscope (FTIR) we determine the plasmon resonance position of each sample. Applications of those structures to surface enhanced IR-Spectroscopy (SEIRA) will be discussed.

[1] R. Adato et al.; PNAS, 106, 19227 (2009)
[2] F. Neubrech et al.; PRL 101, 157403 (2008)
[3] R. Bukasov et al.; Analyt. Chem. 81, 4531 (2009)
[4] C. Haynes et al.; J. Phys. Chem. B, 105, 5599 (2001)

DS 16.7 Mon 18:45 PHY C213

Plasmonic oligomers: the role of individual particles on collective behavior — •Mario Hentschel[1,2], Na Liu[3], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, D-70569 Stuttgart, Germany — [2]Max-Planck-Institute for Solid State Research, Heisenbergstr. 1, D-70569 Stuttgart, Germany — [3]Department of Chemistry, University of California, Berkeley, and Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

We theoretically and experimentally study the transition from isolated to collective modes in plasmonic oligomers which consist of a six-particle outer ring around a single center particle. The inter-particle gap distance plays a key role for the formation of collective modes. The plasmon hybridization method is applied to analyze the optical properties of plasmonic oligomers. The interference between a subradiant and a superradiant mode leads to a pronounced Fano resonance [1]. Furthermore we demonstrate the possibility to switch on and off the Fano resonance by the presence or absence of the central nanoparticle without breaking the system symmetry [2]. We also study the optical response upon modifications such as the introduction of defects by shifting the inner particle from the center position and the variation of the number of individual discs. The ability to observe and tune the collective resonances in metallic nanostructures will allow for the creation of a rich new set of artificial plasmonic molecules with a wide range of controlled optical properties. [1] B. Lukyanchuk et al., Nature Mat. 9, 707 (2010) [2] M. Hentschel et al., Nano Lett. 10, 2721 (2010)

DS 16.8 Mon 19:00 PHY C213

Fabrication of nanocone arrays for high sensitivity biosensing — •Monika Fleischer, Christian Schäfer, Andreas Horrer, Katharina Broch, Dominik Gollmer, Frank Schreiber, and Dieter P. Kern — Institut für Angewandte Physik, Eberhard Karls Universität Tübingen, Auf der Morgenstelle 10, D- 72076 Tübingen

Plasmonic nanostructures, when resonantly interacting with an electromagnetic field, act as optical antennas focusing light to nanoscale volumes. Extremely high near-field enhancement is observed in the direct vicinity of the nanostructure surface, in particular at edges, corners, or tips. A process was developed for the fabrication of metallic nanocones with tip radii on the order of 10 nm. The cones are demonstrated to be efficiently excited by electric field components polarized parallel to the cone axis [1,2]. A narrow spot of high electric field strength is created near each cone apex due to the occurrence of localized surface plasmon resonances. Both serial and parallel methods for the fabrication of regular arrays of nanocones made from e.g. gold, silver, and copper are presented. Dense arrays of metal cones constitute a highly favorable system for high sensitivity sensing of biological or other organic molecules. For molecules located near a cone apex, strong Raman intensity enhancement is observed, similar to the effect of tip-enhanced Raman spectroscopy. This is demonstrated by the example of pentacene molecules [3] on gold cones.

[1] M. Fleischer et al., Nanotechnology 21, 065301 (2010)
[2] M. Fleischer et al., Appl. Phys. Lett. 93, 111114 (2008)
[3] A. Hinderhofer et al., J. Chem. Phys. 127, 194705 (2007)

DS 17: Invited – Grunze

Time: Tuesday 10:15–11:00 Location: GER 37

Invited Talk DS 17.1 Tue 10:15 GER 37

Chemical Nanolithography — •Michael Grunze and Michael Zharnikov — Applied Physical Chemistry, Universität Heidelberg, Im Neuenheimer Feld 253, 69120 Heidelberg, Germany

In this talk the advances in the fabrication of chemical and morphological nano-patterns and gradients by electron beam chemical lithography (EBCL) - or "Chemical Nanolithography" - with monomolecular films as primary resists are discussed. We will show that "Chemical Nanolithography" is an easy and convenient method to create multiphase organic, polymeric or biological surface nanostructures and gradients using stencil masks or electron beam writing, combined with subsequent chemical surface modifications. EBCL can be performed with both aromatic and aliphatic resists. Whereas aromatic monolayers are more robust, aliphatic films are more radiation sensitive and hence require a smaller irradiation dose for patterning. Specific examples given in this talk refer to irradiation-promoting exchange reaction (IPER) lithography, electron beam activation lithography (EBAL), and direct writing chemical lithography (DWCL). In addition, we will demonstrate that chemical patterns that can subsequently be developed into 3D polymer brush architectures can also be made by carbon templating from the gas phase without a pre-adsorbed organic monolayer.

DS 18: Progress in Micro- and Nanopatterning: Techniques and Applications I (Focused Session, jointly with O – Organisers: Graaf, Hartmann)

Time: Tuesday 11:00–13:00 Location: GER 37

Topical Talk DS 18.1 Tue 11:00 GER 37
Microcontact chemistry: surface reactions in nanoscale confinement — •Bart Jan Ravoo — Organic Chemistry Institute, Westfälische Wilhelms-Universität Münster, Correnssstraße 40, 48149 Münster, Germany

Microcontact printing is an established method for the preparation of physical, chemical and biological patterns on solid surfaces. Typically, microcontact printing involves a microstructured elastomer stamp that delivers a molecular ink in the contact area between stamp and substrate. Recently, it has been shown that microcontact printing can also induce chemical reactions when an ink is printed on a substrate, even when the reaction partners are normally unreactive. Rapid and spatially controlled surface reactions induced by microcontact printing enable the molecular modification and patterning of a wide range of inorganic and organic substrates. This lecture will highlight our newest findings concerning the scope and kinetics of surface chemistry by microcontact printing as well as its application in bionanotechnology.

Literature: Ravoo, B.J. J. Mater. Chem. 2009, 18, 8902-8906. Wendeln, C. et al. Langmuir 2010, 26, 15966-15971 Kaufmann, T. et al. Adv. Mater. 2010, DOI: 10.1002/adma.201003564

Topical Talk DS 18.2 Tue 11:30 GER 37
Electrochemical Microstructuring — Xinzhou Ma[1,2], Vadym Halka[1,2], and •Rolf Schuster[1,2] — [1]Physical Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Center for Functional Nanostructures, Karlsruhe, Germany

Small metallic structures of nanometer dimensions are mostly fabricated by lithographic methods, eventually followed by metal deposition under UHV conditions. Recently also electrochemical methods became very promising for microfabrication, because the number of steps involved in the fabrication process may be significantly reduced. However, often the application of conventional electrochemical methods is hampered by long range charging of the double layer and the weak spatial confinement of electrochemical reactions.

In this contribution we review recent methods by which the constraints of conventional electrochemical methods can be circumvented and which allow to structure surfaces on the micrometer to nanometer scale. These approaches are for example based on putting geometrical constraints, using small tools in combination with controlled nucleation or mechanical detachment of metal clusters from the tool or by locally charging the electrochemical double layer upon application of short potential pulses. Also first results on electron beam induced metal deposition from a thin electrolyte film will be presented.

Topical Talk DS 18.3 Tue 12:00 GER 37
Electrochemical Oxidation and Anodization Lithography on Self-Assembled Monolayers — •Stephanie Hoeppener — Laboratory of Organic and Macromolecular Chemistry, Friedrich-Schiller-University Jena, Germany

The use of Scanning Probe Based lithography techniques dates back shortly after the introduction of SXM techniques. In particular bias mediated chemical oxidation processes can be used to induce changes in the substrate's properties, i.e., the conductivity, topography, etc.

Implementing the bias mediated electrochemical oxidation onto self-assembled monolayers was introduced as an alternative that permits the fabrication of surfaces bearing addressable chemically active functional groups. The research activities in this field will be highlighted.

In particular the fabrication of chemically heterogeneous nanostructures introduces the possibility for a site-selective fictionalization of nanostructures – a challenge which is difficult to establish by common photo- and electron lithographic structuring approaches. Besides of fundamental investigations of the electrochemical oxidation process, illustrative examples of the oxidation pattern modification will be presented with respect to nanofabrication approaches.

Topical Talk DS 18.4 Tue 12:30 GER 37
Surface Structuring by Single Pulse Laser Interference: Principles and Applications — •Johannes Boneberg — University of Konstanz

A nanosecond laser pulse is split into several beams. These beams are then overlapped on the sample surface. The resulting interference pattern induces surface modifications. The physical mechanism which lead to surface modification are discussed for thin films and bulk materials. Periods achieved are below 200nm, while the structure sizes could be much smaller. Besides the direct application for the generation of nanostructures, the method can be used as well to generate laterally modified chemical surface structures. These can be utilized in different applications, like the lateral patterning by a sol-gel process.

DS 19: Invited – Chichkov

Time: Tuesday 14:00–14:45 Location: GER 37

Invited Talk DS 19.1 Tue 14:00 GER 37
Laser micro- and nanoprocessing — •Boris Chichkov — Laser Zentrum Hannover e.V., Hollerithallee 8, D-30419 Hannover

Recent progress in the development of laser based micro- and nanoprocessing technologies will be reviewed. Applications in photonics and biomedicine will be discussed.

DS 20: Application of Thin Films

Time: Tuesday 10:15–12:15 Location: GER 38

DS 20.1 Tue 10:15 GER 38
Thin isolators consisting of aluminum oxide and self-assembled monolayers for tunnel diodes — •Andreas Hochmeister[1], Mario Bareiss[1], Ute Zschieschang[2], Hagen Klauk[2], Bernhard Fabel[1], Giuseppe Scarpa[1], and Paolo Lugli[1] — [1]Institute for Nanoelectronics, TU München — [2]Max Planck Institute for Solid State Research, Stuttgart

We present a fabrication method and results of the electrical characterization of metal-oxide-metal (MOM) tunnel diodes. Two different materials (aluminum and gold) were used as metals to produce an asymmetric diode, which can act as a rectifier, e.g. for infrared antenna applications. First an aluminum line was evaporated on a SiO_2/Si substrate through a shadow mask. The dielectric (aluminum oxide) was produced by oxidation using a RIE treatment; the diode was completed by a second evaporation step of gold lines perpendicular to the aluminum line. Gold pads were used for having a better contact during electrical characterization. We could show that by adding a layer of phosphonic acid self-assembled monolayer (SAM) on the isolating aluminum oxide film before the gold evaporation, the effective thickness of the insulator could be tailored. The thickness of the aluminum oxide is approximately 3nm, which could be controlled to 4-6 nm by the additional layer of SAM. Electrical characterization was performed by dc I-V measurements. At high electric fields Fowler-Nordheim tunneling and dielectric breakdown was observed.

DS 20.2 Tue 10:30 GER 38

The influence of the crystallinity of TiO_2 on the resistive switching behavior of memristor devices

— •Hannes Mähne[1], Stefan Slesazeck[1], Stefan Jakschik[1], and Thomas Mikolajick[1,2] — [1]NaMLab gGmbH, Dresden, Germany — [2]Institut für Halbleiter und Mikrosystemtechnik, TU Dresden, Germany

Since 1970, Chua postulates the existing of a memristor and HP found the first device in 2008, a lot of research has been done. Several research groups using successfully titanium oxide without detailed understanding of the switching mechanism. The following work fill a gap of information and create a link between the crystalline structure of TiO_2 and its switching parameters. In this work used structure consists of Si substrate with thermally grown SiO_2 and deposited Ti as adhesion layer before Pt was sputtered as an inert bottom electrode. After deposition of TiO_2, by RF sputtering from a TiO_2 target with additional 2 sccm O_2, the material is in an amorphous phase. To get different phases the samples are annealed in a RTP oven at 500°C and 700°C in Ar atmosphere and with O_2. The top electrode material was evaporated aluminum. To create a temperature stable bottom electrode, several bottom layer stacks are tested and results in a thick Pt layer on a preoxidized Ti adhesion layer. Otherwise the bottom electrode becomes damaged. A reason for this behavior is that thin Pt becomes crystalline and holes are created. Next to this, temperatures above 700°C causes cracks in the TiO_2 films. The change in crystallinity results in a change from a oxygen migration like switching in amorphous to a filament like switching behavior in the crystalline samples.

DS 20.3 Tue 10:45 GER 38

Coexistence of filamentary and homogeneous resistive switching in Fe-doped $SrTiO_3$ thin film memristive devices

— Ruth Münstermann[1], •Regina Dittmann[1], Tobias Menke[1], Ingo Krug[1], Daesung Park[2], Joachim Mayer[2], and Rainer Waser[1,3] — [1]Peter Grünberg Institut, Research Centre Jülich — [2]Central Faculty for Electron Microscopy, RWTH Aachen — [3]Institut fuer Werkstoffe der Elektrotechnik 2, RWTH Aachen

Resistive switching phenomena which are observed in many transition metal oxides are under consideration for future non-volatile memories (so called memristive devices). We used conductive-tip AFM combined with a delamination technique to remove the top electrode of Fe-doped $SrTiO_3$ memristive devices to gain insights into the active switching interface. We observed that resistive switching in Fe-doped $SrTiO_3$ thin films can be either confined to a single strong filament or distributed over larger areas beneath the electrode, in the ideal case the whole junction area. Both types of switching coexist in one and the same sample and exhibit the opposite switching polarity. Combining our electrical date with PEEM and HRTEM analysis, we discuss the nature of the observed switching phenomena.

DS 20.4 Tue 11:00 GER 38

AlN-based microstructures for biocompatible piezo-generation

— •Nicola Heidrich[1,2], Fabian Knöbber[1,2], Vadim Lebedev[1], Ram Ekwal Sah[1], Oliver Ambacher[1,2], and Volker Cimalla[1] — [1]Fraunhofer-Institute for Applied Solid State Physics, Freiburg, Germany — [2]Department of Microsystems Engineering, University of Freiburg, Germany

The aim of this work is to fabricate a biocompatible micro-generator using aluminium nitride (AlN) as piezoelectric material to supply implantable sensors sufficiently with energy, rendering batteries and external power supplies unnecessary. Membranes made from AlN- thin films and silicon nitride (SiN), with diameters of 0.8 to 3 mm were investigated with respect to their material properties, resonant behaviour and power-output in different environments, using internal piezoelectrical and external mechanical excitation of the membranes. The out-of-plane displacement of the surfaces was measured by a laser Doppler vibrometer (LDV) with a precision below 1 pm. It goes to show that tensile stressed membranes almost only generate power at their resonant frequencies well above 50 kHz, while compressive stressed (corrugated) membranes are capable of responding effectively to excitation in the low frequency range, being an appropriate solution for energy harvesting from random body movement. Compared to a single corrugated membrane the peak generated power is increased by almost three orders of magnitude with a 3x4 array of serial and parallel connected membranes.

DS 20.5 Tue 11:15 GER 38

Nanoscaled photoelectron ionisation detector based on lanthanum hexaboride

— •Cordula M. Zimmer[1], Jürgen Schubert[2], Ulrich Kunze[1], and Theodor Doll[3] — [1]Werkstoffe u. Nanoelektronik, Ruhr-Universität Bochum, Germany — [2]Institute of Bio- and Nanosystems (IBN-1), Forschungszentrum Jülich, Germany — [3]Institut für Physik, Johannes-Gutenberg Universität Mainz, Germany

In this work the development of a nanoscaled photo ionisation detector is presented, whose functionality is based on the photoelectric effect of lanthanum hexaboride (LaB_6) thin films. Photoemitted electrons will be brought up to energies of 7 to 18 eV within a nano-electrode arrangement, which does not exceed the mean free path of molecules at 10^5 Pa (70 to 110 nm). This enables the ionising and sensing of specific gases such as hydrocarbons, solvents, organic and inorganic substances under ambient conditions without the risk of molecule fragmentation. The yield of photoelectron current emitted under ultraviolet (UV) irradiation was optimised by tuning the work function of the LaB_6 films. The proper choice of the substrate material and/or the deposition of additional interlayers is important to establish a favourable crystal orientation and stoichiometry of the LaB_6 film which lowers its work function.

DS 20.6 Tue 11:30 GER 38

Characterization of ITO films on fluorescent borate glasses

— •Franziska Steudel[1], Nico Teuscher[2], Susanne Richter[1], Andreas Heilmann[2], Christan Hagendorf[1], Paul-Tiberiu Miclea[1,3], and Stefan Schweizer[1,4] — [1]Fraunhofer Center for Silicon Photovoltaics, Walter-Hülse-Str. 1, 06120 Halle (Saale) — [2]Fraunhofer Institute for Mechanics of Materials, Walter-Hülse-Str. 1, 06120 Halle (Saale) — [3]Institute of Physics, Martin Luther University of Halle-Wittenberg, Heinrich-Damerow-Str. 4, 06120 Halle (Saale) — [4]Centre for Innovation Competence SiLi-nano®, Martin Luther University of Halle-Wittenberg, Karl-Freiherr-von-Fritsch-Str. 3, 06120 Halle (Saale)

For photovoltaic applications, the cover glass is one of the key products in solar modules. For high efficiency modules, it would be advantageous to use the glass not only as a cover but also as a down-converter. Samarium-doped borate glasses, for instance, convert the incident violet and blue part of the solar spectrum to visible red light which is more efficiently absorbed by the solar cell. The chemical composition of borate glasses consists of boron oxide as a network former and metal oxides as network modifiers. In this work, borate glasses with different network modifiers were prepared and used as substrates for the deposition of a conductive indium tin oxide (ITO) film. The deposition is done by magnetron sputtering at room temperature. To understand the electrical and optical properties of the deposited ITO films the diffusion of the glass components into the films is studied by time of flight secondary ion mass spectrometry (ToF-SIMS).

DS 20.7 Tue 11:45 GER 38

A-periodic multilayer development for attosecond pulses in the 300-500 eV photon energy range

— Alexander Guggenmos[1,2], Michael Hofstetter[1,2], Roman Rauhut[1], and •Ulf Kleineberg[1,2] — [1]Fakultät für Physik, Ludwig-Maximilians-Universität München, Garching, Germany — [2]Max-Planck-Institut für Quantenoptik, Garching, Germany

The development of ultrafast X-ray pulses in the sub-femtosecond time regime is a cutting edge technology for studying electron dynamics in atoms, molecules or solid surfaces / nanostructures by means of pump/probe electron spectroscopy. XUV elements as multilayer mirrors and thin metal filters are used to filter and shape attosecond bursts from high harmonic radiation. One near future goal is to extend the current technology to higher photon energies, reaching the water window range around 300 - 500 eV, where the in-vitro investigation of bio-materials on ultra-short time scales becomes possible. Following the ideas of nowadays experimental setups, both the spectral and the temporal resolution can be determined and guided by means of periodic and a-periodic multilayer mirrors, allowing for spectral and temporal soft X-ray pulse shaping. We will present first investigations of periodic and a-periodic multilayer XUV optics in that energy range of 300-400 eV and discuss their applications for filtering single attosecond pulses from High Harmonic radiation. Simulations and optimizations of various binary and ternary multilayer material systems as well as first experimental results achieved by Ion Beam Deposition and insitu-ellispometry of the deposited nanolayers are demonstrated.

DS 20.8 Tue 12:00 GER 38

Ultra fast electrochromic switching of nanoporous tungsten-tantalum oxide films — •Robin Kirchgeorg, Steffen Berger, and Patrik Schmuki — Institute for Surface Science and Corrosion (LKO), Department Material Science and Engineering, Friedrich-Alexander-Universität Erlangen-Nürnberg, Martensstraße 7, 91052 Erlangen, Germany

Self-organized anodic oxide nanostructures have attracted remarkable scientific interest within the last decades. Due to their unique properties, the applicability of these materials were explored in numerous applications, such as in electrochromic devices. The benchmark for electrochromic materials nowadays is WO_3. However, these anodically fabricated WO_3 electrodes still lack cycling stability and performance. Recent results on anodic oxides grown on TiW, TiMo and TiNb alloys indicate a significant enhancement of the stability by the formation of oxide composites, but with the fundamental electrochromic properties being considerably poorer than for pure WO_3. Self-organized nanoporous oxide layers on a W-Ta alloy grown by anodization in a flouride containing electrolyte, show drastically enhanced electrochromic properties combined with high cycling stability. These self-organized, nanostructured, mixed oxide layers show an ultra-fast electrochromic switching behaviour. Up to more than 10 times higher switching frequencies are reached along with a significantly enhanced lifetime and cyclability. The presentation will provide a comparison of anodically selforganized nanostructures of WO_3 and a W-Ta alloy, regarding their electrochromic properties and cycling stability.

DS 21: High-k and Low-k Dielectrics (jointly with DF)

Time: Tuesday 13:45–15:15 Location: GER 38

DS 21.1 Tue 13:45 GER 38

Nondestructive Hard X-ray Photoelectron Spetroscopy Study of Resistive Switching TiN/Ti/HfO_2/TiN RRAM Cells — •Małgorzata Sowińska[1], Sebastian Thiess[2], Christian Walczyk[1], Damian Walczyk[1], Christian Wenger[1], Mindaugas Lukosius[1], Wolfgang Drube[2], and Thomas Schroeder[1] — [1]IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — [2]P09 beamline at Petra III (DESY), Notkestrasse 85, 22607 Hamburg, Germany

Resistive switching metal-insulator-metal (MIM) diodes present a promising approach for back-end-of-line (BEOL) integration of embedded nonvolatile memory (NVM) cells in Si integrated circuits. Research in our group focused on TiN/Ti/HfO_2/TiN devices and one-resistor (1R) as well as one-transistor, one-resistor (1T1R) architectures were successfully processed under Si CMOS BEOL conditions. Switching characteristics in sweep as well as pulse mode were electrically investigated to study NVM characteristics (retention, endurance etc.). To unveil the microscopic origin of the switching mechanism, the Ti/HfO_2 interface was studied by nondestructive Hard X-ray Photoelectron Spectroscopy (HAXPES) studies at the recently constructed P09 beamline at Petra III (Hamburg). Results on RRAM cells in as-deposited, ON and OFF, as well as hard breakdown state will be presented.

DS 21.2 Tue 14:00 GER 38

Improvement of dielectric properties of $Sr_xZr_{(1-x)}O_y$ grown by Molecular Beam Deposition and Sputtering — •Matthias Grube[1], Dominik Martin[1], Walter M. Weber[1], Thomas Mikolajick[1,2], Lutz Geelhaar[3], and Henning Riechert[3] — [1]Namlab gGmbH, 01187 Dresden — [2]Lehrstuhl für Nanoelektronische Materialien, TU Dresden, 01062 Dresden — [3]Paul-Drude-Institut für Festkörperelektronik, 10117 Berlin

Following the demand of replacing conventional dielectrics in the semiconductor industry, a material screening for new high-k dielectrics with nanometer-scale thicknesses is required. Among the many investigated potential materials are ZrO_2 as well as laminates and mixtures of ZrO_2 with HfO_2, Ta_2O_5 and Al_2O_3. We concentrated our efforts to the growth and characterisation of ZrO_2 with the admixture of SrO to form $Sr_xZr_{(1-x)}O_y$. We employed the molecular beam deposition technique (MBD) in a co-deposition regime for this purpose. The capability of MBD for high-k material screening was verified by comparison to deposition via sputtering a stoichiometric $SrZrO_3$ target. The investigated test structures were metal-insulator-metal capacitors (MIM) with a TiN bottom electrode on n^{++}-Si substrates. I-V and C-V measurements revealed a k-value of 19 for amorphous $Sr_xZr_{(1-x)}O_y$ grown by either MBD or sputtering. After surpassing a crystallisation temperature of approximately 650°C the k-value increases to 30 while the dielectric changes into a polycrystalline film with a cubic phase. A comparison of MBD and sputtering of ZrO_2 and $Sr_xZr_{(1-x)}O_y$ will be presented in detail.

DS 21.3 Tue 14:15 GER 38

Phase equilibria at Si-HfO_2 and Pt-HfO_2 interfaces from first principles thermodynamics — •Rampi Ramprasad[1] and Hong Zhu[2] — [1]University of Connecticut, Storrs, USA; Fritz-Haber-Institut der MPG, Berlin, Germany — [2]University of Connecticut, Storrs, USA

In this work, two types of interfaces found in the emerging technologically important high-k MOSFETs have been studied. The phase diagrams of Si-HfO_2 and Pt-HfO_2 interfaces as a function of temperature and oxygen pressure have been determined using first principles thermodynamics (FPT), i.e., by combining conventional density functional theory results with thermodynamics [1]. The vibrational and configurational entropic contributions to the free energies of the condensed phases are explicitly included in this treatment. We demonstrate that the predictions of the FPT approach are in quantitative agreement with experiments for the classes of interfaces considered here. In particular, under UHV conditions, we show that FPT methods predict the correct Si-HfO_2 silica-like interface configurations. Likewise, we also show that an interfacial oxygen coverage of 0.5-1.0 monolayer is favored under UHV conditions at the Pt-HfO_2 interface before rapid oxidation of Pt may be expected (for higher oxygen pressures). These results have important implications both for the applicability of FPT methods for the considered classes of interfaces as well as for high-k dielectrics-based electronic devices in which such interfaces are expected.

[1] H. Zhu, C. Tang and R. Ramprasad, Phys. Rev. B, in print (2010).

DS 21.4 Tue 14:30 GER 38

Bottom-up Modeling of the Elastic Properties of Organosilicate Glasses and their Relation to Composition and Network Defects — •Jan M. Knaup[1,2], Han Li[3], Joost J. Vlassak[3], and Efthimios Kaxiras[1,2,3] — [1]Department of Physics, Harvard University, Cambridge MA, USA — [2]EPFL, Lausanne, Suisse — [3]School of Engineering and Applied Sciences, Harvard University, Cambriudge MA, USA

Organosilicate glasses (OSG), also known as SiCOH or carbon-doped oxide are used as low-k inter-metal dielectrics for integrated circuits. The material must fulfill two conflicting requirements: It has to have low density to reduce the dielectric constant and be mechanically stable enough to withstand mechanical stress during subsequent production steps. Experimental advances in improving their mechanical and electrical properties have not yet been theoretically examined at the ab initio level, due to the relatively large model sizes necessary for amorphous materials. We employ the density-functional based tight-binding (DFTB) method to achieve an accurate description of OSG properties at different compositions. We analyze the influence of composition and topological defects on the density and bulk modulus of non-porous OSG. We find that the dependence of density and stiffness on chemical composition is of different nature. This difference is traced to a transition between different mechanisms of elastic deformation in silica glass and in silicon hydrocarbide, which is also the reason for different sensitivity to topological defects in the two materials.

DS 21.5 Tue 14:45 GER 38

Local I-V characteristics of high-k ultra-thin ZrO_2- and $ZrO_2/Al_2O_3/ZrO_2$-films. — •Dominik Martin[1], Matthias Grube[1], Elke Erben[1], Johannes Müller[2], Wenke Weinreich[2], Uwe Schroeder[1], Lutz Geelhaar[3], Walter Weber[1], Thomas Mikolajick[1,4], and Henning Riechert[3] — [1]namlab Gmbh, D-01187 Dresden — [2]Fraunhofer-CNT, D-01099 Dresden — [3]Paul-Drude-Institut für Festkörperelektronik, D-10117 Berlin — [4]Chair of Nanoelectronic Materials, 01062 Dresden, Germany

In order to produce ultra thin ZrO_2-films, with a dielectric constant high enough to satisfy industry demands, it is necessary to reach the tetragonal crystalline phase. This can be achieved either by high temperature deposition or by a post deposition annealing step. Both however induce high leakage currents. Small amounts of Al_2O_3 can be incorporated in ZrO_2 to reduce leakage current. To get more insight into the charge carrier transport mechanisms involved, a thickness series of ultra thin ZrO_2- and $ZrO_2/Al_2O_3/ZrO_2$-films were deposited by ALD and subjected to different rapid thermal annealing processes. These layers were examined by GI-XRD, TEM, I-V-, C-V-Spectroscopy and conductive atomic force microscopy. Thus, leakage currents are reduced to $3.2 \cdot 10^{-8} \frac{A}{cm^2}$ at 1 V while maintaining the high k value (CET=1 nm at 1V for a 10 nm film) . CAFM studies demonstrate how the crystallization effects the charge transport mechanisms on the mesoscopic scale. Local I-V curves acquired on amorphous films and at grain boundaries in nanocrystalline films in yield lower breakdown voltages and higher leakage currents at crystallite grain boundaries.

DS 21.6 Tue 15:00 GER 38

Post-etch cleaning mechanisms at ultra low k surfaces — •Roman Leitsmann[1], Oliver Böhm[1,2], Philipp Plänitz[1], Christian Radehaus[1], Michael Schreiber[2], and Matthias Schaller[3] — [1]GWT-TUD GmbH, Material Calculations, Chemnitz, Germany — [2]Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz — [3]Globalfoundries Dresden Module Two GmbH & Co. KG, Germany

The usage of materials with an ultra low dielectric constant is necessary due to the decreasing feature size of integrated circuits, which results in smaller distances between the conduction layers, and hence to an increasing resistance capacitance delay. However, the application of such ultra low k (ULK) materials is connected to several problems. For example a fluorocarbon film at the ULK-surfaces at the sidewalls of trenches or vias is formed during the etch process. To remove this film a post-etch cleaning procedure have to be applied. In this study we investigate the cleaning efficiency of diluted HF using state of the art density functional theory. In particular different desorption mechanisms of CF-polymer fragments will be discussed in detail.

DS 22: Focussed Session: Inorganic/Organic Semiconductor Hybrid Structures I (jointly with HL and O)

Time: Tuesday 10:15–13:00 Location: POT 151

Invited Talk DS 22.1 Tue 10:15 POT 151

Self-assembled monolayers on zinc oxide — •Craig L. Perkins — National Renewable Energy Labooratory, Golden, CO USA — Renewable and Sustainable Energy Institute

Two of the most promising schemes for attaching organic molecules to metal oxides are based on the chemistry of the thiol and phosphonic acid moieties. We have made a direct comparison of the efficacy of these two molecular anchors on zinc oxide by comparing the chemical and physical properties of n-hexane derivatives of both. The surface properties of polycrystalline ZnO thin films and ZnO(0001)-O crystals modified with 1-hexanethiol and 1-hexanephosphonic acid were examined with a novel quartz crystal microbalance (QCM)-based flow cell reactor, angle-resolved and temperature-dependent photoelectron spectroscopy, and contact angle measurements. A means of using ammonium chloride as a probe of molecule-ZnO interactions is introduced and used to ascertain the relative quality of self-assembled monolayers (SAMs) based on thiols and phosphonic acids. QCM data shows that a phosphonic acid-anchored alkyl chain only six carbons long can provide significant corrosion protection for ZnO against Brønsted acids, reducing the etch rate relative to the bare ZnO surface by a factor of more than nine. The thermal stability of the two linking groups was also explored and we find that previous claims of highly stable alkanethiolate monolayers on ZnO are suspect. Taken as a whole, our results indicate that the phosphonic acid moiety is preferred over thiols for the attachment of short alkyl groups to ZnO.

Invited Talk DS 22.2 Tue 10:45 POT 151

Inorganic/organic semiconductor heteroepitaxy - towards new hybrid systems for optoelectronics and photonics — •Sylke Blumstengel — Institute of Physics, Humboldt University Berlin, Newtonstr. 15, 12489 Berlin

This talk summarizes our recent efforts to fabricate heterostructures based on ZnO and various conjugated organic materials as well as to tailor their electronic and optical properties. Growth by molecular beam epitaxy of both material components ensures well-defined interfaces and highest structural quality. A unique feature of ZnO and its ternaries ZnCdO and ZnMgO is that films and quantum structures with very good crystalline and optical properties can be epitaxially grown at low temperatures (50°C!) compatible with the stability of organic materials. Thus, not only organic-on-inorganic, but also inorganic-on-organic epitaxy can be performed. Relevant growth mechanisms are discussed. Interfacial energy level alignment including band-offset engineering via the geometric structure of the molecular layer is presented. Direct electronic coupling of the fundamental excitations (Frenkel and Wannier-Mott excitons) across the interface occurs with coupling constants on the meV-energy scale. The superior optoelectronic function of sandwich-type hybrids is demonstrated by the achievement of stimulated emission of the enclosed organic layer at markedly reduced pump thresholds due to efficient energy transfer from ZnO.

15 min. break

Invited Talk DS 22.3 Tue 11:30 POT 151

Electrostatic Field Driven Alignment of Organic Oligomers on ZnO Surfaces — •Fabio Della Sala[1], Sylke Blumstengel[2], and Fritz Henneberger[2] — [1]Nanoscience Institute (CNR), Via per Arnesano, 73100 Lecce — [2]Institut fuer Physik, Humboldt-Universitaet zu Berlin, Newtonstrasse 15, 12489 Berlin, Germany

We present a theoretical study on the physisorption process of organic oligomers on the ZnO(10$\bar{1}$0) surface. Using first-principles density-functional theory and non-empirical embedding methods, we find that both in-plane location and orientation of the molecules are completely determined by the coupling of their quadrupole moments to the periodic dipolar electric field present at the semiconductor surface. The adsorption is associated with the formation of a molecular dipole moment perpendicular to the surface, which bears an unexpected linear relation to the molecule-substrate interaction energy. Long oligomers such as sexiphenyl become well-aligned with stabilization energies of several 100 meV along rows of positive electric field, in full agreement with recent experiments. These findings define a new route towards the realization of highly-ordered self-assembled arrays of oligomers/polymers on ZnO(10$\bar{1}$0) and similar surfaces.

Invited Talk DS 22.4 Tue 12:00 POT 151

The incorporation of metal nanostructures at organic/inorganic semiconductor interfaces — •Dietrich RT Zahn, Michael Ludemann, Ovidiu Gordan, Philipp Schäfer, and Georgeta Salvan — Semiconductor Physics, Chemnitz University of Technology, 09107 Chemnitz

Raman spectroscopy is applied in situ and online to study the interface formation of organic semiconductors such as perylene derivatives and phthalocyanines on inorganic semiconductor like gallium arsenide and silicon. Moreover, also the interface formation between metals and organic semiconductors has been extensively investigated. In the latter case the surface enhanced Raman scattering (SERS) effect is observed and it provides useful information regarding e.g. metal reactivity and metal diffusion. More recently well defined metal nanostructures were prepared on oxidised silicon samples using nanosphere lithography. When organic molecules are deposited onto such structured substrates strong enhancement effects are again observed. However, the enhancement effect shows an unusual resonance behaviour at excitation wavelengths well away from the metal cluster plasmon energy. The potential of such structures for application will be illuminated.

DS 22.5 Tue 12:30 POT 151

Fabrication of ZnO/polymer hybride devices using chemical vapor deposition of polymers — •Jan Richters and Tobias Voss — Institut für Festkörperphysik, Universität Bremen, Otto-Hahn-Allee 1, 28359 Bremen

Due to their large surface area and good electrical conductivity, ZnO nanowires are interesting candidates for the fabrication of hybrid inorganic/organic optoelectronic devices. As an example, dye-sensitized solar cells can be prepared using a ZnO nanowire-array as one electrode with a monolayer of dye adsorbed on their surface. An additional hole-conductive material is required to form the connection with the counter electrode, where PEDOT:PSS or similar polymers can be applied. These polymer layers are usually fabricated using liquid-based synthesis-methods such as dip-coating or spin-coating which suffer from a limited penetration depth of the polymer into the pores of the nanowire array.

Here, we present a vapor-transport technique for the fabrication of dye-sensitized solar cells based on ZnO nanowires and the polymers PEDOT and polystyrene. We compare the electrical and optical properties of the devices, describe the microscopic properties of the polymer layers and provide details of the fabrication technique.

DS 22.6 Tue 12:45 POT 151

Electrical investigations of different polymer and substrate materials for dye-sensitized ZnO-NW/polymer hybrid solar cells — •Kay-Michael Günther[1], Julia Waltermann[1], Stefan Kontermann[2], and Wolfgang Schade[1,2] — [1]Clausthal University of Technology, EFZN, EnergieCampus, 38640 Goslar — [2]Fraunhofer Heinrich-Hertz-Institute, EnergieCampus, 38640 Goslar

Dye-sensitized solar cells composed of a n-doped ZnO nanowire (NW) array and a p-doped polymer layer appear to be a promising candidate for low-cost production of environment-friendly solar cells. In this study, we compare the commonly used polymer layers PEDOT:PSS and P3HT. While the former one provides a better conductivity, the latter one shows itself a photoabsorbance below $\lambda =$ 400 nm. In addition, we investigate three different TCO substrates (ITO, FTO and ZnO:Al) using Impedance Spectroscopy (IS), current-voltage-measurements (IV), as well as IV-transients. The results show that in our setup an additional polycrystalline ZnO layer beneath the ZnO NWs is needed to prevent short circuits caused by polymer seeping between the NWs towards the counter electrode. Furthermore, the confinement to a simple ZnO layer enables us to optimize the polymer layer independently from the NWs. Hence, we compare devices with and without NWs and with different processing parameters. We achieve the best results with P3HT and FTO substrates. With ZnO:Al, we observe additional RC-combinations which partly result from a Schottky barrier formed at the ZnO:Al interface leading to a significant higher series resistance. An equivalent circuit is derived and discussed.

DS 23: Focussed Session: Inorganic/Organic Semiconductor Hybrid Structures II (jointly with HL and O)

Time: Tuesday 14:15–15:15 Location: POT 151

Invited Talk DS 23.1 Tue 14:15 POT 151

Interfacial charge-carrier energetics probed by electromodulated absorption spectroscopy: implication for organic-inorganic hybrid photovoltaic devices — •Peter Ho — Dept of Physics, National University of Singapore

The transition from vacuum-level alignment to Fermi-level pinning of the organic semiconductor contact as the work function of the "metallic" electrode crosses a certain threshold value has been well-established by numerous careful ultraviolet photoemission spectroscopy stuides. In this talk, I will discuss the use of electromodulated absorption spectroscopy to probe this transition within the devices directly through the built-in potential measured at the Stark feature, and also the interface polaron density measured in the subgap. Therefore the results are particularly relevant to the operation of light-emitting diodes and photovoltaic cells. We found that the pinning crossover occurs surprisingly at different work-function threshold values. The implications of this result for energy-level alignment and contact optimisation in light-emitting diodes and photovoltaic devices, and in hybrid inorganic-organic semiconductor photovoltaic devices, will also be discussed.

Invited Talk DS 23.2 Tue 14:45 POT 151

Organic layers on Si, SiC, and diamond substrates: structural and electronic properties — •Martin Stutzmann, Ian D. Sharp, Jose Antonio Garrido, and Martin S. Brandt — Walter Schottky Institut, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany

In this contribution, we address the structural and electronic properties of hybrid heterostructures of organic functional layers on silicon, silicon carbide, and diamond substrates. For the covalent grafting of alkenes or phenyls on H- or OH-terminated surfaces, distinct differences in the reactivity of the different substrates and the quality of the resulting self-assembled monolayers are observed. These surfaces can be further functionalized with proteins such as enzymes or photosystems to investigate charge transfer processes between the solid substrate and the bioorganic layer. In addition, we have investigated the electronic properties of thin films of P3HT or pentacene deposited on Si, SiC, and diamond by spin coating or organic MBE. Based on current-voltage characteristics of such heterojunctions in the dark and under illumination we discuss basic questions of band alignment and charge transfer at the different heterointerfaces.

DS 24: Organic Electronics and Photovoltaics CPP-II (jointly with CPP, HL, and O)

Time: Tuesday 10:30–13:00 Location: ZEU 222

Topical Talk DS 24.1 Tue 10:30 ZEU 222

Modelling charge transport in organic semiconductors — •Denis Andrienko — MPI for Polymer Research, Mainz, Germany

The role of material morphology on charge carrier mobility in partially disordered organic semiconductors is discussed for several classes of materials: derivatives of hexabenzocoronenes,[1] perylenediimides,[2] triangularly shaped polyaromatic hydrocarbons,[3] Alq3,[4] polypyrrole and a variety of organic crystals. Simulations are performed using a package developed by Imperial College, London and MPI for Polymer Research, Mainz (www.votca.org[5]). This package combines: quantum chemical methods for the calculation of molecular electronic structures and reorganization energies; molecular dynamics and systematic coarse-graining approaches for simulation of self-assembly and relative positions and orientations of molecules on large scales; kinetic Monte Carlo and master equation for studies of charge transport.

[1]. J. Kirkpatrick, V. Marcon, J. Nelson, K. Kremer, D. Andrienko, *Phys. Rev. Lett.*, 98, 227402, 2007

[2]. V. Marcon, W. Pisula, J. Dahl, D. W. Breiby, J. Kirkpatrick, S. Patwardhan, F. Grozema, D. Andrienko, *J. Am. Chem. Soc.*, 131, 11426, 2009

[3]. X. Feng, V. Marcon, W. Pisula, M. R. Hansen, J. Kirkpatrick, F. Grozema, D. Andrienko, K. Kremer, and K. Müllen, *Nature Materials* 8, 421, 2009

[4]. A. Lukyanov, D. Andrienko, *Phys. Rev. B*, 82, 193202, 2010

[5]. V. Rühle, C. Junghans, A. Lukyanov, K. Kremer, D. Andrienko, *J. Chem. Theor. Comp.* 5, 3211, 2009

DS 24.2 Tue 11:00 ZEU 222

Performance of density functional theory for donor-acceptor systems: a case study for TTF and TCNQ molecules — •Viktor Atalla[1], Mina Yoon[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Oak Ridge National Laboratory, USA

Organic materials are promising candidates for a next generation of electronic devices, since they offer a variety of new intriguing properties. However, from a theoretical point of view these materials are challenging because they are often composed of donor-acceptor systems, for which density-functional theory (DFT) with state-of-the-art exchange-correlation (XC) functionals is often suspected to fail. Here we study the performance of DFT in describing electron affinities, ionization potentials, and charge transfer for clusters of the prototypical electron donor molecule TTF and acceptor molecule TCNQ.

For the indivdual molecules we calculate the dependence of the HOMO and LUMO levels on the fraction of exact exchange and the screening length [1]. We find that conventional semilocal and hybrid XC functionals severely underestimate HOMO-LUMO gaps. For weakly bound TTF-TCNQ dimers all investigated XC functionals consistently give charge transfer from the donor to the acceptor, however the amount of transfered charge is strongly functional dependent - in particular all semilocal functionals have significant aritificial charge transfer in the asymptotic limit.

[1] A. Krukau *et al.*, J. Chem. Phys. **125**, 2006

DS 24.3 Tue 11:15 ZEU 222

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

We present external quantum efficiency (EQE) studies of P3HT:PCBM based bulk heterojunction polymer solar cells with improved intensity resolution in the sub-bandgap (SBG) region, i.e. the energy range below the optical bandgaps of the pristine materials. Varying the P3HT:PCBM blending ratio, we find that in addition to a Gaussian profile an exponential tail is needed for a quantitative description of the SBG EQE spectra. To gain insights into the origin of the single contributions, absorption and emission spectra covering several decades of intensity and SBG EQE signals are discussed in detail.

DS 24.4 Tue 11:30 ZEU 222

Quantitative analysis of optical spectra and solar cell performance of P3HT:PCBM blends — •Sarah T. Turner, Patrick Pingel, Robert Steyrleuthner, and Dieter Neher — Institute of Physics and Astronomy, University of Potsdam, Germany

The properties of solar cells made from a blend of regioregular poly(3-hexylthiophene) (P3HT) with [6,6]-phenyl-C_{61}-butyric acid methyl ester (PCBM) are known to depend largely on the layer morphology. Here, we present the results of optical studies on P3HT:PCBM blends coated from chloroform and dichlorobenzene with subsequent thermal annealing. A recently established analytical model developed by Spano for the absorption of weakly interacting H-aggregates was used to obtain information about the fraction of crystallized chains, the width of the aggregates, and the energetic disorder in the P3HT phase [1]. In terms of an increased aggregate width and a decreased energetic disorder in the P3HT phase, thermal annealing was found to have little effect on the films prepared from dichlorobenzene and an appreciable effect on the films prepared from chloroform. The results from the model were compared with the performance of solar cell devices and single-carrier devices with the same active layer. Most importantly, the initial increase in P3HT aggregate size upon thermal annealing showed a good correlation with an increase in hole mobility. Further increases in solar cell device performance at higher annealing temperatures were correlated with a decrease in P3HT energetic disorder and an increase in PCBM aggregation.

[1] F.C. Spano, J. Chem. Phys. 2005, 122, 234701.

DS 24.5 Tue 11:45 ZEU 222

Influence of Phase Segregation on the Dynamics of Charge Carriers in Organic Solar Cells — •Andreas Baumann[1], Tom J. Savenije[3], Dharmapura H. K. Murthy[3], Martin J. Heeney[4], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Physical Institute, Julius-Maximilians-University of Würzburg, Am Hubland, D-97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), Am Hubland, D-97074 Würzburg — [3]Optoelectronic Materials Section, Department of Chemical Engineering, Delft University of Technology, 2628 BL Delft, The Netherlands — [4]Department of Chemistry, Imperial College London, London, SW7 2AZ, United Kingdom

The morphology of a bulk heterojunction solar cell plays an important role in the dynamics of charge carriers, whereas the donor–acceptor ratio have a great impact on the extent of phase segregation. A fine phase intermixing is believed to be beneficial for an efficient photogeneration. However, the charge transport is strongly related to percolated pathways to the electrodes. We studied the influence of phase segregation on the dynamics in the blend system poly(2,5-bis(3-dodecyl thiophen-2-yl) thieno[2,3-b]thiophene) (pBTCT) mixed with [6,6]-phenyl-C61-butyric acid methyl ester. We used the technique of charge extraction by linearly increasing voltage and transient microwave conductivity to study the macroscopic and microscopic transport properties, respectively. We found an enhanced geminate recombination in the 1:1 ratio blends due to fine phase intermixing, whereas extensive phase segregation in the 1:4 ratio led to an efficient polaron pair dissociation.

DS 24.6 Tue 12:00 ZEU 222

Charge separation at molecular donor-acceptor interfaces: correlation between interface morphology and solar cell performance — •Andreas Opitz, Julia Wagner, Mark Gruber, Ulrich Hörmann, and Wolfgang Brütting — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Combinations of organic electron and hole conductive materials are widely used for ambipolar charge carrier transport and donor/acceptor photovoltaic cells. Thereby the efficiency of these excitonic solar cells is correlated to the morphology of the interface between the donor and the acceptor materials.

In this contribution we show the effect of crystallization behaviour on molecular bulk and planar heterojunction solar cells [1]. Different donor (copper phthalocyanine – CuPc, diindenoperylene – DIP) and acceptor (Fullerene – C_{60}, per-fluorinated copper phthalocyanine – F_{16}CuPc) materials are analysed for their growth morphology in planar and mixed films as well as for their performance in photovoltaic cells. The morphology of the blended layer ranges from molecularly mixed films in the case of the two phthalocyanines to phase-separated films when mixing CuPc or DIP with C_{60}. A corrugated interface is found for bilayered structure of DIP/C_{60} [2]. Additionally a good crystallization behaviour of DIP improves the solar cell performance even for its lower absorption in comparison to CuPc.

[1] A. Opitz et al., IEEE J. Sel. Top. Quant. (2010), early view.

[2] J. Wagner et al. Adv. Func. Mater. (2010), early view.

DS 24.7 Tue 12:15 ZEU 222

Towards Ideal Morphology of Polymer Bulk Heterojunction Solar Cells — •Chetan Raj Singh[1], Michael Sommer[2,3], Marcel Himmerlich[1], André Wicklein[3], Stefan Krischok[1], Mukundan Thelakkat[3], and Harald Hoppe[1] — [1]Institute of Physics, Ilmenau University of Technology, Germany — [2]Department of Chemistry, University of Cambridge, United Kingdom — [3]Applied Functional Polymers, University of Bayreuth, Germany

We present the thorough optimization of block copolymer (BCP) based polymer solar cells utilizing a blend of a self-assembling P3HT-b-PPerAcr BCP and an PPerAcr acceptor homopolymer. As an effect of increasing acceptor content in the block copolymer/homopolymer blend, we observe a continuous rise in the open circuit voltage (Voc) and the short circuit current (Isc) leading to an overall improved photovoltaic performance. The improved performance with increasing acceptor content is attributed to (a) an increase of the acceptor domain size leading to improved charge transport and to (b) a reduced recombination of charge carriers at the cathode interface due to the surface segregation of the acceptor. The surface segregation of the acceptor is identified by atomic force microscopy and X-ray photoelectron spectroscopy. Furthermore we show that by deliberately introducing an acceptor buffer layer at the cathode interface, we are able to control Voc at relatively high values (~ 640 mV), independently of the bulk heterojunction morphology underneath.

DS 24.8 Tue 12:30 ZEU 222

Triplet Excitons and Cations in dicyanovinyl end-capped quaterthiophenes with varying side chain length — •Christian Koerner[1], Hannah Ziehlke[1], Roland Fitzner[2], Egon Reinold[2], Peter Bäuerle[2], Karl Leo[1], and Moritz Riede[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden — [2]Institut für Organische Chemie II und Neue Materialien, Universität Ulm

Dicyanovinyl end-capped oligothiophenes (DCV-nT) are highly suitable for systematical investigations of energy and charge transfer processes in donor-acceptor blends because of the tunability of electronic and morphological properties by varying e.g. length of backbone or side chains. Moreover, it has been shown to work well as absorber in small molecule organic solar cells (OSC) achieving up to 5.2% power conversion efficiency (PCE) for DCV-5T in a bulk heterojunction (BHJ) device[1].

We use photoinduced absorption spectroscopy (PIA) to probe the long-living (μs-ms) excited states (triplet excitons, cations) after photoexcitation of DCV-nT:C_{60} blends. With PIA, their generation and recombination behaviour can be investigated. Here, we report our results obtained on a series of DCV-4Ts with varying side chains from none to methyl side chains which supposedly mainly influences the morphology of the thin film. We complement our studies by exploring the potential of these materials as absorber layer in planar and BHJ solar cells. For example, DCV-4T without side chains gives an open circuit voltage of 1V and PCEs of 1.9% in a BHJ solar cell with C_{60}.

[1] Fitzner et al., Adv. Func. Mat., accepted

DS 24.9 Tue 12:45 ZEU 222

Surface structure of organic heterojunction solar cells — •M. Zerson[1], E.-C. Spitzner[1], C. Riesch[1], A. Sperlich[2], H. Kraus[2], A. Förtig[2], C. Deibel[2], V. Dyakonov[2], R. Lohwasser[3], M. Thelakkat[3], and R. Magerle[1] — [1]Chemische Physik, TU Chemnitz — [2]Experimental Physics VI, Julius-Maximilians-University of Würzburg — [3]Makromolekulare Chemie I, Univ. Bayreuth

In organic heterojunction solar cells based on P3HT and PCBM, the charge transfer within the active layer as well as the charge transport towards the electrodes are determined by the electronic properties of the interfaces and their microstructure. The surface of semicrystalline polypropylene has been shown to be covered by a thin layer of amorphous material. We aim at investigating potential similarities between organic semiconductors for photovoltaics. We report on 3D depth profiling of the surface structure of different types of P3HT and blends of P3HT with PCBM using amplitude modulation atomic force microscopy. From a map of amplitude-phase-distance curves, the tip indentation into the soft (compliant) amorphous surface layer is measured. This spatial information serves as depth coordinate for reconstructing high resolution cross sections and 3D depth profiles of the top 10 nm of the specimen. Furthermore, the shape of the unperturbed (true) surface and the thickness of the amorphous top layer are determined. The latter is found to be between 4 and 10 nm thick, depending on the type of material and the sample preparation conditions (thermal and solvent annealing). We discuss the impact of the thickness of the amorphous top layer on the efficiency of organic solar cells.

DS 25: Organic Electronics and Photovoltaics CPP-III (jointly with CPP, HL, and O)

Time: Tuesday 14:00–15:15 Location: ZEU 222

DS 25.1 Tue 14:00 ZEU 222

Substituted Perylene Diimides as Electron Acceptors in Organic Solar Cells: Suppressing Aggregate Formation to Increase Device Efficiency — •Valentin Kamm, Glauco Battagliarin, Ian A. Howard, Michael Hansen, Hans W. Spiess, Alexey Mavrinskiy, Wojciech Pisula, Chen Li, Klaus Müllen, and Frédéric Laquai — Max-Planck-Institut für Polymerforschung, Mainz, Deutschland

Perylene diimide (PDI) is a promising electron acceptor material for high open circuit voltage bulk heterojunction organic solar cells. However, many PDI molecules have the drawback of strong aggregation leading to intermolecular excited state formation that results in exciton trapping. These traps can effectively limit the diffusion of excitons to the interface where charge separation occurs and thus strongly reduce the charge generation efficiency. In this contribution we study the influence of substitution of PDI molecules with side groups attached to the terminal and to the perylene core positions on the formation of aggregates. In particular transient photoluminescence and absorption spectroscopy are used to probe the impact of aggregation on the dynamics of charge generation and recombination in bulk heterojunction solar cells. Besides, AFM, x-ray and solid state NMR techniques are used to get further insight into the solid state morphology of polymer:PDI blends on different length scales. Finally, we correlate the photophysical properties of the PDI derivatives with the efficiency of bulk heterojunction organic solar cells and present unprecedented efficiencies from polymer:PDI solar cells.

DS 25.2 Tue 14:15 ZEU 222

Near-field spectroscopic mapping of the nanoscale phase separation of low band-gap polymer:fullerene blend film — •xiao wang[1], hamed azimi[2], hans-georg mack[1], mauro morana[2], hans-joachim egelhaaf[3], alfred j. meixner[1], and dai zhang[1] — [1]Institute of Physical and Theoretical Chemistry, Auf der Morgenstelle 18, University of Tübingen, Germany — [2]Konarka Austria F&E GmbH, Linz, Austria — [3]Konarka Technologies GmbH, Nürnberg, Germany

We present the study of the influences of the additive 1,8-octanedithiol (ODT) on the nanometer scale morphology and local photophysics properties of low band-gap polymer blends, PCPDTBT and PCBM. Near-Field spectroscopic mapping provides the possibility to obtain simultaneously morphology and spectroscopic (photoluminescence and Raman) information correlated with high spatial resolution.[1] We observe the phase separations of the PCPDTBT:PCBM blend film induced by ODT by the dramatically increased PL emission from PCPDTBT that was originally largely quenched, by the fluctuations of spectral features at different locations of the sample surface, by the fibril-shaped topographic features evolve to spherical bumps. The correlations between the local photo physics properties and the morphology of the blend film with/without ODT at both the micrometer and nanometer scales were revealed by the confocal and high-resolution near-field spectroscopic mapping technique. 1.Wang, X.; Zhang, D.; Braun, K.; Egelhaaf, H. J.; Brabec, C. J.; Meixner, A. J. Adv. Funct. Mater. 2010, 20, (3), 492-499.

DS 25.3 Tue 14:30 ZEU 222

High Crystallinity and Nature of Crystal–Crystal Phase Transformations in Regioregular Poly(3-hexylthiophene) — •Ovidiu F. Pascui[1,3], Ruth Lohwassser[2], Michael Sommer[2], Mukundan Thelakkat[2], Thomas Thurn-Albrecht[1], and Kay Saalwächter[1] — [1]Institut für Physik, Martin-Luther-Univ. Halle-Wittenberg, Halle, Germany — [2]Makromolekulare Chemie I, Universität Bayreuth, Germany — [3]Experimentelle Physik III, TU Dortmund, Germany

Molecular weight and stereoregularity affect the morphology and the crystallinity of conjugated polymers and are thus of pivotal relevance for the mobility of charge carriers in electro-optical device applications. We use ^{13}C solid-state NMR to determine the crystallinity and details on crystal–crystal phase transformations in regioregular head-to-tail poly(3-hexylthiophene) of well-defined molecular weight and demonstrate that the crystallinity was previously severely underestimated. Typical crystallinities are at least around 37% for the lowest molecular weights and as high as about 64% upon increasing MW, corresponding to a corrected maximum value for the reference melting enthalpy of $\Delta H_\mathrm{m} \approx 37$ J/g for use in DSC experiments. Using one- and two-dimensional NMR, we observe that the crystal-crystal phase transition between a 3D- and a 2D-ordered crystalline phase at around 60°C entails a structural disordering process of the alkyl side chains, while not affecting the backbones. The formation of the 3D-ordered phase is kinetically suppressed at higher molecular weights.

see: O. F. Pascui et al., *Macromolecules* **43**, 9401 (2010).

DS 25.4 Tue 14:45 ZEU 222

Self-Assembled Ultralong Organic Semiconducting Nano/Microwires — Julia Lambrecht, •Tobat P. I. Saragi, and Josef Salbeck — Macromolecular Chemistry and Molecular Materials (mmCmm), Department of Mathematics and Science and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Strasse 40, D 34132 Kassel, Germany

We report on the simple process in fabrication of spiro-substituted perylene diimide nano/microwires (NMWs) by using self-assembly approach, namely drying under solvent atmosphere. This method results in a controllable number of NMWs on the substrate, which enables us to fabricate single NMW electronic device. Furthermore, we are able to control the growth direction of NMWs by using a structured substrate. An aspect ratio as high as ~9200 can be obtained in our experiment and the longest wire is determined to be 5.5 mm. The resistivity of the single NMW is characterized and the value is in the range of 100 Ohm m and 10000 ohm m.

DS 25.5 Tue 15:00 ZEU 222

Plasmonic enhancement of light absorption in organic semiconductors using silver nanowire arrays — •Matthias Handloser[1], Ricky Dunbar[2], Philipp Altpeter[2], Lukas Schmidt-Mende[2], and Achim Hartschuh[1] — [1]Department Chemie and CeNS, Ludwig-Maximilians-Universität, München, Germany — [2]Department Physik and CeNS, Ludwig-Maximilians-Universität, München, Germany

Plasmonics can be used to improve light absorption in photovoltaic devices, permitting a considerable reduction in the physical thickness of absorber layers, and yielding new options for solar-cell design [1]. We investigated arrays of aligned silver nanowires embedded in different organic polymers via confocal microscopy in combination with Time Correlated Single Photon Counting (TCSPC) and Pump-Probe techniques. The wires had a length of 10 um, a height of 20 nm, and variable widths and spacings. Thin films of different organic semiconductors were then deposited onto these arrays. Plasmon modes were excited through one and two photon absorption between 500 to 900 nm and photoluminescence maps and transients of the arrays were recorded. We observed a clear correlation between photoluminescence intensity, lifetime and nanowire spacing. We analyzed our data to distinguish between absorption and radiative rate enhancement and energy transfer to the metal followed by quenching. [1] H.A.Atwater, A.Polman, Nature Materials 9, 205 (2010)

DS 26: Plasmonics and Nanophotonics O-III (jointly with HL and O)

Time: Tuesday 11:15–13:00 Location: WIL A317

DS 26.1 Tue 11:15 WIL A317

Tip-enhanced Spectroscopic Mapping — •Dai Zhang, Xiao Wang, and Alfred J. Meixner — Inst. Phys. Theo. Chem.

When a sharp Au tip approaching very closely to the sample surface, the tip-sample system behaves as an optical antenna. It confines and enhances the excitation field to a small sub-diffraction volume in the gap between the tip-apex and the surface and retrieving emitted or scattered photons to the far field for detection.

In my talk, the influence of several parameters, such as the gap distance, the material properties of the tip and the substrate as well as the size of the tip, on the performance of the gap-mode near-field optical microscopy will be systematically discussed. Gap-mode near-field spectroscopic mapping technique has been recently developed in our lab. I will demonstrate the Raman and photoluminescence spectroscopic imaging of the chemical distribution in the polymer:fullerene organic solar cell blend film [1]. From the simultaneously recorded morphology and spectroscopic information, the interplay among the blend film morphology, the local donor and acceptor molecular distributions, and the photoluminescence quenching efficiency will be discussed. With the above demonstrations, we propose that the gap-mode near-field optical microscopy is a promising, high-resolution and multi-function characterization technique for material science [1,2].

References [1] X. Wang et al, Advanced Functional Materials 20, 492 (2010). [2] D. Zhang et al, Physical Revew Letters, 104, 056601 (2010).

DS 26.2 Tue 11:30 WIL A317

Near-Field Imaging of Directive Optical Yagi-Uda Nanoantennas — •Jens Dorfmüller[1], Daniel Drégely[1], Moritz Esslinger[2], Worawut Khunsin[2], Ralf Vogelgesang[2], Klaus Kern[2,3], and Harald Giessen[1] — [1]4. Physikalisches Institut und Research Center SCoPE, Pfaffenwaldring 57, Universität Stuttgart, 70569 Stuttgart, Germany — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, 70569 Stuttgart, Germany — [3]Institut de Physique de la Matière Condensée, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Apertureless Scanning Near-field Optical Microscopy (aSNOM) in a cross-polarization scheme allows us to map the E-fields of plasmonic nano-structures in real-space with a resolution far beyond the diffraction limit [1,2]. Maps of near-field amplitude and phase allow us to determine the excitation mode. Analyzing the amplitude at elements of optical nano-antennas allows us to measure the receptivity in dependence of antenna geometry as well as illumination conditions.

Here, we investigate the reception directionality of optical Yagi-Uda antennas. Depending on the illumination direction, the electromagnetic energy is either concentrated at the feed element or distributed over several antenna elements. Comparison with simulations shows a very good agreement.

[1] J. Dorfmüller, R. Vogelgesang, R. T. Weitz, C. Rockstuhl, C. Etrich, T. Pertsch, F. Lederer, K. Kern, *Nano Lett.* **9**, 2372 (2009).

[2] J. Dorfmüller, R. Vogelgesang, W. Khunsin, C. Rockstuhl, C. Etrich, K. Kern, *Nano Lett.* **10**, 3596 (2010).

DS 26.3 Tue 11:45 WIL A317

Surface-Plasmon-Polariton interation with gratings — •Andreas Englisch, Stefan Griesing, Uwe Schmitt, and Uwe Hartmann — Institute of Experimental Physics, Saarland University, Postfach 151150, D-66041,

Surface-Plasmon-Polaritons (SPP) couple with light through suitable periodical structures. In the case of SPP-excitation a typical decrease of the intensity in the diffracted orders can be observed. Two different kinds of gratings are investigated: periodically corrugated metal surfaces on the one hand and structured dielectric layers on flat metal surfaces on the other hand. The intensities of the diffracted orders as well as the near-field intensities are measured in dependence of the grating profile. The near-field is characterized with respect to the amplitude and the phase by the use of a phase-sensitive scanning near-field optical microscope (SNOM. Numerical modeling based on finite element simulations in Fourier space as well as in real space were performed and compared with the measurements.

DS 26.4 Tue 12:00 WIL A317

Nonlocal, grating-coupled scattering-type near-field scanning optical microscopy of individual gold nano-particles — •Diyar Sadiq[1], Javid Shirdel[1], Jae Sung Lee[2], Namkyoo Park[2], and Christoph Lienau[1] — [1]Institut für Physik, Carl von Ossietzky Universität, 26111 Oldenburg, Germany — [2]Photonic Systems Laboratory, School of EECS, Seoul

Scattering-type near-field scanning optical microscopy (s-NSOM) is now routinely used for (sub-) 10-nm-resolution optical imaging of surfaces. The performance is, however, often limited by a rather substantial signal background resulting from a direct optical illumination of the scattering antenna. Various ideas for a nonlocal optical excitation have therefore been proposed, e.g., by grating-coupling of surface plasmon polaritons (SPP) onto adiabatic metallic tapers and three-dimensional focusing of SPP wavepackets towards the tip apex [1]. Recently, first line-scan images recorded by using such probes demonstrated 20 nm resolution and coupling of about 15% of the SPP intensity onto the tip apex [2]. Here, we use such a grating-coupled SPP microscope for the first time for s-NSOM imaging of single metallic nano-particles. We demonstrate sub-20-nm-resolution imaging of localized SPP fields and observe that more than 40% of the grating-coupled SPP field is localized at the taper apex. The results are supported with numerical simulation based on the finite-difference time-domain (FDTD) method. [1] C. Ropers et al. Nano Letters 7, 2784 (2007). [2] C. C. Neacsu et al, Nano Letters 10, 592 (2010).

DS 26.5 Tue 12:15 WIL A317

Enhanced vibrational near-field spectroscopy of PMMA with infrared antennas — •Jón Mattis Hoffmann, Jens Richter, and Thomas Taubner — I. Institute of Physics (IA), RWTH Aachen University, Sommerfeldstraße 14, 52074 Aachen, Germany

Infrared spectroscopy allows for the investigation of chemical properties of a sample material by directly probing molecular vibrations. Combined with scattering-type near-field optical microscopy (s-SNOM), which relies on the scattering of light at a sharp metallic tip, it is possible to obtain such spectroscopic information in images with strongly subwavelength resolution [1]. For the probing of weakly absorbing samples, such as molecular vibrations in thin polymer layers [2], increased sensitivity of infrared near-field spectroscopy is needed. It has been shown that signals in near-field vibrational spectroscopy of thin films can be enhanced by reflecting substrates [3]. For even higher enhancement factors we investigate the possibility of using resonant substrates.

Here we employ triangular nanostructures fabricated by nanosphere lithography that exhibit strong resonances in the infrared region as substrate. We want to measure the resonant enhanced near-field spectra of a thin PMMA film on top of these infrared antennas.

[1] F. Keilmann et al. in Nano-Optics and Near-Field Optical Microscopy ed. by A. Zayats and D. Richards, 235 (ArtechHouse, 2009).

[2] T. Taubner et al., Applied Physics Letters 85, 5064 (2004).

[3] J. Aizpurua et al., Optics Express 16, 1529 (2008).

DS 26.6 Tue 12:30 WIL A317

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

We present scattering-type scanning near-field optical micro spectroscopy (s SNOM) investigations successfully operated in the THz range with a wavelength independent spatial resolution of 90 nm. Our microscopy set-up bases on a true noncontact atomic force microscope (nc-AFM) combined with the free-electron laser (FEL) source at the Helmholtz-Zentrum Dresden-Rossendorf. This laser provides tunability from 30 to 250 μm. We were able to record, for the first time ever, s-SNOM signatures with a FEL at wavelengths ranging from 30 μm to 180 μm (10 to 1.67 THz). In addition to the near-field dependent optical signals we also demonstrate the imaging and spectroscopy capabilities of our THz-s-SNOM. Image scans were performed on a specially designed test structure consisting of a topography-free composite of a polymer/gold sample. On these samples a topography independent strong optical material contrast could be demonstrated at 150 μm wavelength. Furthermore we achieve a resolution of better than 90 nm on a Fischer-Pattern test structure, corresponding to an optical improvement of better than 1500 times the wavelength.

DS 26.7 Tue 12:45 WIL A317

Background-Free Imaging with an Apertureless Scanning Nearfield Optical Microscope — •Moritz Esslinger[1], Jens Dorfmüller[1,2], Ralf Vogelgesang[1], Worawut Khunsin[1], and Klaus Kern[1,3] — [1]Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany — [2]presently at 4. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany — [3]de Physique de la Matière Condensée, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

We present advances in experimental techniques of apertureless near-field optical microscopy (aSNOM). This technique achieves high spatial resolution by utilizing the field enhancement at the apex of sharp tips. Many conventional setups utilize p-polarized light in the illumination as well as in the detection path. The detected light of such a setup not only contains the optical near field signal, but is affected also by coupling effects between tip and sample.

By using p-polarized light for illumination and detecting the s-polarized component of the backscattered light we are able to measure the z-component of the electric field on the sample essentially without coupling effects. Here we outline how the proper choice of tip position, together with optimizing polarizer and analyzer angles of our cross-polarization scheme ensures plasmonic eigenmode mapping with a background of exactly zero. By comparison with simulation data not including the tip we show that the measurement has little to no influence on the eigenmodes.

DS 27: Invited – D'Agosta

Time: Wednesday 10:15–11:00 Location: GER 37

Invited Talk DS 27.1 Wed 10:15 GER 37

Stochastic approach to electronic and spin thermal transport — •Roberto D'Agosta — Nano-bio spectroscopy group, UPV/EHU, E-20018 San Sebastian, Spain — Ikerbasque, Basque Foundation for Science, E-48011 Bilbao, Spain

The theory of open quantum systems aimed at describing the interaction of a thermal bath with a quantum mechanical system is a field of intense research activity.

In this talk, I will present some recent developments in this area used to investigate the thermal transport both in electronic and spin systems. Especially at the nanoscale, the *standard* approaches based on the Fourier law or the Landauer formalism have been put under serious scrutiny and it has been shown that they can be in contrast with both analytical and numerical results.

After a brief introduction to the field, I will discuss the differences between the two main approaches, the stochastic Schroedinger equation (SSE) and the reduced density matrix formalisms, and show how the SSE can be used to describe the dynamics of a spin chain or an electron system coupled to an external thermal bath. I will discuss how the coupling with the environment might induce correlation between the states of the system and how we can explore the dynamical approach to thermal steady states.

DS 28: Spins in Organic Materials I (Focused Session, jointly with MA – Organisers: Salvan, Hess, Timm)

Time: Wednesday 11:00–13:00 Location: GER 37

Topical Talk DS 28.1 Wed 11:00 GER 37

Selective spin-blockade in interacting molecular interferometers — •Milena Grifoni, Andrea Donarini, and Georg Begemann — Institut für Theoretische Physik, Universität Regensburg, Regensburg, Germany

We consider molecular junctions in the single-electron tunneling regime which, due to a high degree of spatial symmetry, have a degenerate many-body spectrum. As a consequence, interference phenomena which cause a current blocking can occur at specific values of the bias and gate voltage. We present here necessary and sufficient conditions for interference blockade also in the presence of spin-polarized leads. As an example we analyze a benzene single-electron transistor. For a setup with parallel polarized leads, we show how to exploit the current blocking to selectively prepare the system in a defined spin state without application of any external magnetic field.

References:

A. Donarini, G. Begemann and M. Grifoni, Nano Lett. 9, 2897 (2009)

A. Donarini, G. Begemann and M. Grifoni, Phys. Rev. B 82, 125451 (2010)

Topical Talk DS 28.2 Wed 11:30 GER 37

Charge and Spin Transport through Single-Atom and Single-Molecule Junctions — •Jörg Kröger — Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany

The tip of a scanning tunnelling microscope is used to controllably contact single atoms and molecules adsorbed to surfaces. Owing to atomically precise imaging, the conductance dependence of a single-C_{60} junction on the C_{60} orientation has been unambiguously demonstrated. Time-resolved measurements of these junctions show two-level variations of the conductance and indicate an enhanced coupling of electrons to molecular vibrations. Orders-of-magnitude modifications of single-molecule contact conductances have been achieved by dehydrogenating tin-phthalocyanine molecules on Ag(111). Concomitant calculations visualize the current flow through the molecule and highlight the importance of chemical bonds to the electrodes. Spin valve effects have been observed at the ultimate size for magnetic single-atom contacts, which exhibit spin-dependent conductance in the ballistic electron transport regime.

Topical Talk DS 28.3 Wed 12:00 GER 37

The strange life of a molecular spin observed under a microscope — •Germar Hoffmann — University of Hamburg, Germany — Academia Sinica, Taiwan

The 90ies saw the emerging of a new and fascinating class of magnetic materials based on molecules [1]. Although, the spin density is low, spin information can be efficiently stored in and transmitted by spatially and energetically well defined molecular orbitals. These orbitals can be experimentally precisely addressed. The internal and external spin interaction through molecular orbitals can be engineered by the molecular design. This opens also new concepts for spintronic devices through the combination of the molecular spin with additional functionality - on a length scale not accessible by classical systems. Though, the further development lacks of precise experimental access to understand the behavior of the individual molecular spin in a given environment and to guide toward an improved design of molecular spin-systems.

Here, I will present and discuss recent results on molecular magnetism. By means of spin-polarized scanning tunneling microscopy, scanning tunneling spectroscopy, and local manipulation, single magnetic molecules are locally and energetically investigated in different environments. Thereby, molecular systems cover commercially available [2], specially synthesized, and on-surface synthesized systems.

[1] R. Sessoli et al., JACS 115, 1804 (1993); M. Tamura et al., Chem. Phys. Lett. 186, 401 (1991). [2] J. Brede et al., Phys. Rev. Lett. 105, 047204 (2010); N. Atodiresei et al., Phys. Rev. Lett. 105, 066601 (2010).

DS 28.4 Wed 12:30 GER 37

Design of the Local Spin-Polarization at Hybrid Organic-Ferromagnetic Interfaces — •Nicolae Atodiresei[1], Predrag Lazić[2], Vasile Caciuc[1], and Stefan Blügel[1] — [1]Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425-Jülich, Germany — [2]Massachusetts Institute of Technology, Cambridge, 02139-Massachusetts, USA

Combining molecular electronics with spintronics represents one of the most exciting avenues in building future nanoelectronic devices. In this context, a clear understanding of the physics at magnetic electrode-molecule interfaces is highly desirable and, in particular, first principles simulations are used to elucidate and design the functionality of specific molecules in a given organic-metal surface environment. We will present a conceptual study to understand the manipulation of the local spin-polarization present at the interface for several single organic molecules adsorbed on a ferromagnetic surface. The generality of the concept predicted by the theoretical calculations on model systems is further strengthened by the spin-polarized scanning tunneling microscopy (SP-STM)experiments. In this study it is demonstrated that, by an appropriate selection of the adsorbed molecules, the electrons of different spin [i.e. up and down] can selectively be injected from the same ferromagnetic surface by locally controlling the spin-polarization. [1] N. Atodiresei *et al.* Phys. Rev. Lett. 102, 136809 (2009); [2] J. Brede *et al.* Phys. Rev. Lett. 105, 047204 (2010); [3] N. Atodiresei *et al.* Phys. Rev. Lett. 105, 066601 (2010).

DS 28.5 Wed 12:45 GER 37

Structural and magnetic properties of trinuclear-Cu(II)-complexes — •Torsten Hahn[1], Tobias Rueffer[2], and Vladislav Kataev[3] — [1]Institute for Theoretical Physics, TU Bergakademie Freiberg, Germany — [2]Department of Chemistry, Chemnitz University of Technology, Germany — [3]Leibniz Institute for Solid State and Materials Research Dresden, Germany

The magnetic super-exchange interactions in Cu(II) bis(oxamato) and bis(oxamidato) complexes [1] are shown to be highly sensitive to structural modifications coordinating close to the central copper. This work presents a detailed theoretical investigation of the influence of such modifications of the molecular structure on the magnetic coupling by means of DFT using the broken symmetry approach. The relation between structural parameters, the local spin density and the corresponding magnetic exchange parameters is discussed and compared to experimental results from EPR studies and magnetic measurements. Special attention was paid to the relationship between the spin population of the monomeric building blocks and the trends of the exchange interaction in case of the corresponding trinuclear complexes. Furthermore, the use of a simplified transport model based on the Non-Equilibrium-Green-Functions formalism delivers first insights into transport properties of these complexes for possible spintronic applications.

Funding by the DFG via the research unit 1154 "Towards Molecular Spintronics" is gratefully acknowledged.

[1] B. Braeuer, et. al., Inorg. Chem. 47, 6633 (2008)

DS 29: Gaede Prize Talk – Philip Hofmann

Time: Wednesday 14:00–14:45 Location: TRE Phy

Prize Talk DS 29.1 Wed 14:00 TRE Phy

Spin-split metallic surface states on semimetals and topological insulators — •Philip Hofmann — Department of Physics and Astronomy, Interdisciplinary Nanoscience Center Aarhus University, 8000 Århus C, Denmark

The surfaces of Bi, Sb and the so-called topological insulators (TIs) all share the property that their electronic structure is metallic, in sharp contrast to the bulk which is either semimetallic (Bi, Sb) or semiconducting (TI). The main reason for the existence of the metallic surface states is not bond-breaking but the loss of inversion symmetry at the surface, combined with a strong spin-orbit interaction. The surface states are almost completely non-degenerate with respect to the electron's spin and this has interesting consequences for their electron dynamics. Indeed, the surface states on TIs are predicted to exhibit a number of novel and exotic physical phenomena and have potential applications in spintronics and quantum computing. In this talk I will review some basic properties of spin-split surface states, relate the findings on semimetal surfaces to topological considerations and discuss the similarities and differences of surface states on semimetals and topological insulators.

DS 30: Invited – Johnston-Halperin

Time: Wednesday 15:00–15:45 Location: GER 37

Invited Talk DS 30.1 Wed 15:00 GER 37

Electrical spin injection in a hybrid organic/inorganic spin-polarized light emitting diode (spin-LED) — •Ezekiel Johnston-Halperin — Department of Physics, The Ohio State University, USA

The development of organic-based magnets with room temperature magnetic ordering and semiconducting functionality promises a route to all-organic spintronic devices and hybrid organic/inorganic structures capable of exploiting both the multifunctionality of organic systems as well as the established spintronic functionality of inorganic materials. Here we report the successful extraction of spin polarized current from a thin film of the organic-based room-temperature ferrimagnetic semiconductor V[TCNE]x (x~2; TCNE: tetracyanoethylene) and its subsequent injection into a GaAs/AlGaAs light-emitting diode

(LED). The orientation of this spin current is determined by polarization analysis of the electroluminescence from the LED and is found to be parallel to the magnetization of the V[TCNE] layer, in agreement with theoretical predictions. Detailed analysis of the optical selection rules in the LED, coupled with control measurements of magnetic circular dichroism in the V[TCNE] layer, reveals the magnitude of the electron spin polarization to be largely insensitive to both electrical bias and temperature. This successful demonstration of spin injection in a hybrid organic/inorganic structure opens the door to a new class of active, hybrid spintronic devices with the potential for multifunctional behavior defined by the optical, electronic and chemical sensitivity of the organic layer.

DS 31: Spins in Organic Materials II (Focused Session, jointly with MA – Organisers: Salvan, Hess, Timm)

Time: Wednesday 15:45–16:45 Location: GER 37

Topical Talk DS 31.1 Wed 15:45 GER 37

Organic spintronics and the great potential of ferromagnetic metal-organic interfaces — •Martin Aeschlimann — Department of Physics, University of Kaiserslautern

The study of the spin properties of organic semiconductors (OSC) is recently receiving great attention. One of the most promising routes to employ them for spintronics applications is to exploit the high spin injection achievable across ferromagnetic metal-organic interfaces [1]. Combined with the extreme flexibility and tunability of OSC, it is expected that such hybrid interfaces will constitute a fundamental building block for advanced spintronics devices, where spin-injection is controlled by fine-tuning of the interface physical and chemical properties. An example has been recently presented in [2], where doping of the OSC copper phthalocyanine (CuPc) has been successfully used to tune the spin functionality of a cobalt-CuPc interface. In particular, the presence of a spin-polarized hybrid interface state, acting as a spin-filter at the interface, has been used to enhance the efficiency of spin injection to values above 100%. Besides the cobalt-CuPc interface, we have studied the iron-CuPc, cobalt-Tris(8-hydroxyquinolinato)aluminium (Alq3) and iron-Alq3 interfaces. The studies have been conducted by means of spin polarized scanning tunnelling microscopy and spectroscopy, spin-resolved ultraviolet photoemission spectroscopy and spin- and time-resolved two-photon photoemission.

[1] M. Cinchetti et al., Nature Materials 8, 115-119 (2009)

[2] M. Cinchetti et al., Phys. Rev. Lett. 104, 217602 (2010)

DS 31.2 Wed 16:15 GER 37

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

In this work monolayers and multilayers of cobalt(II)phthalocyanine (CoPc) were analysed with respect to their chemical and electronical properties. The organic material was deposited under ultra high vacuum conditions on single crystalline Au(100) (5×20 reconstruction) and Ag(111) surfaces that were cleaned by Ar$^+$ bombardment and annealing cycles. The molecular ordering has been studied by low energy electron diffraction (LEED) and the morphology of thick films by scanning probe microscopy (AFM) that indicates a polycristalline growth.

The results of combined X-ray and ultraviolet photoemission spectroscopy (XPS, UPS) indicate clear differences in the valence band and Co2p core level spectra for mono- and multilayer due to charge transfer to the monolayer cobalt ion and a possible influence of image charge screening effects enhanced by the metal substrates. An additional interface state in the vicinity of the Fermi level was observed in the monolayer spectra.

DS 31.3 Wed 16:30 GER 37

Cobalt-Meq$_3$ (Me=Al, In, Ga) interface formation studied by spin- and time-resolved photoemission spectroscopy — •Nicolas Grossmann, Sabine Steil, Martin Laux, Andreas Ruffing, Indranil Sarkar, Mirko Cinchetti, and Martin Aeschlimann — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany

We have studied the formation of the interface between an epitaxially grown Co(001) thin film and the organic semiconductors tris(8-hydroxyquinoline)aluminium(III) (Alq$_3$), tris(8-hydroxyquinoline)gallium(III)(Gaq$_3$) and tris(8-hydroxyquinoline) indium(III)(Inq$_3$). The organic semiconductors were progressively grown on the cobalt substrate up to a coverage of 5 monolayers. The grown interfaces have been characterized by means of spin-resolved ultraviolet photoemission spectroscopy and spin- and time-resolved two-photon photoemission spectroscopy. For every growth step we have monitored the changes in the work function, the energetic position of the occupied and unoccupied molecular orbitals and interface states, and the changes in the cobalt spin polarization induced by interface formation. In addition, we have measured the spin-resolved lifetime of unoccupied hybrid interface states. The results will be discussed with focus on the relevance of spin-polarized hybrid interface states on the sign of the magnetoresistance observed in organic spin valves based on Alq$_3$ [1].

[1] V. A. Dediu, et al., Nature Mater. 8, 707 (2009);

DS 32: Spins in Organic Materials III (Focused Session, jointly with MA – Organisers: Salvan, Hess, Timm)

Time: Wednesday 17:00–18:30 Location: GER 37

DS 32.1 Wed 17:00 GER 37

Highly controlled deposition, environment, and surfaces in paramagnetic organic radicals — •Sabine-Antonia Savu, Indro Biswas, Mathias Glaser, Maria Benedetta Casu, and Thomas Chassé — IPTC, University of Tübingen, Tübingen, Germany

Organic radicals are a promising class of molecules which combine magnetic properties with the considerable advantages of organic molecules for example chemical and mechanical flexibility. For electronic applications, a comprehensive knowledge of the electronic, structural and morphological properties of organic magnets is indispensable. Nitpyrene is a pyrene-based nitronyl radical which belongs to a new class of organic magnets with high stability and promising magnetic properties. In this work we present a multi-technique investigation of nitpyrene thin films in order to get information on the electronic structure, growth modes, and thin film processes of this molecule. We show the results of investigations on nitpyrene thin films using X-ray based techniques, together with atomic force microscopy (AFM). Nitpyrene was deposited under ultra high vacuum conditions onto the well-characterized single crystal Au(111) surface using strictly controlled evaporation conditions. By analyzing the attenuation of the substrate core level signal, we find indications for a Stranski-Krastanov growth mode (layer plus islands). This information is also supported by AFM measurements. Furthermore, we find evidence for Ostwald ripening processes. ESR measurements confirmed the persistence of the radical nature in the thin films.

DS 32.2 Wed 17:15 GER 37

The influence of molecular orientation on triplet excitons in various oligo- and polythiophenes — •Hannes Kraus[1], Andreas Sperlich[1], Anja Keckeisen[1], Carsten Deibel[1], Vladimir Dyakonov[1,2], Hannah Ziehlke[3], Moritz Riede[3], Karl Leo[3], Roland Fitzner[4], Egon Reinhold[4], and Peter Bäuerle[4] —

[1]Experimental Physics VI, Julius Maximilian University of Würzburg, D-97074 Würzburg — [2]ZAE Bayern, D-97074 Würzburg — [3]Institut für Angewandte Photophysik, TU Dresden, D-01062 Dresden — [4]Institute of Organic Chemistry II and Advanced Materials, Ulm University, D-89081 Ulm

One of the intriguing issues in oPV materials is the role of triplet excitons on photogeneration of charge carriers. Evaporated oligothiophene films and solution-processed polythiophenes have been used in high-efficiency organic solar cells. Thus the electronic properties of both material classes are of great interest. Utilizing angle resolved optically detected magnetic resonance (ODMR), we investigated the triplet excitons of thin films of the quinquethiophene DCV5T (evaporated), the polythiophene P3HT and the block copolymer PCPDTBT (both spin-cast). We found a strong dependence of the triplet signatures on the crystalline ordering, especially for oligothiophenes, and attempt to connect this dependence to the intrinsic ordering of the corresponding molecular system. In combination with structural analysis, angle resolved ODMR allows to gain new insights into the physics of triplet excited states.

DS 32.3 Wed 17:30 GER 37

Light induced spin-interacting charge-transfer states in polymer:C60-fullerene blends — •Andreas Sperlich[1], Tom J. Savenije[1,3], Magdalena Zawadzki[1], Hannes Kraus[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — [2]ZAE Bayern, D-97074 Würzburg — [3]Department of Chemical Engineering, Delft University of Technology, NL-2628 BL Delft, The Netherlands

Charge-transfer states (CTS) are widely considered to be an intermediate species between the primary photo-excited singlet exciton and the formation of separate electrons and holes in organic semiconductors and their blends. We demonstrate that these CTS, being interacting e-h pairs, can be studied using electron spin resonance (ESR).

At temperatures below 100K a spin-polarized pattern (E-A-E-A) of microwave emission (E) and absorption (A) can be detected. Several microseconds after the excitation pulse this polarization pattern transforms to a purely absorptive spectrum with two peaks (A-A). This spectrum is identical to the one obtained by cw ESR, which has previously been assigned to non-interacting positive and negative charges. For lower temperatures (<20K) additional features assigned to spin-interacting persistent e-h pairs were observed.

DS 32.4 Wed 17:45 GER 37

Comparison of the magneto-optical response of different metal-phthalocyanines measured by MOKE — •Michael Fronk, Klaus Seidel, Dietrich R.T. Zahn, and Georgeta Salvan — Chemnitz University of Technology, Chemnitz, Germany

In recent years organic materials experience much attention because of their potential applications in spintronic devices predominantly due to their long spin life-times. This work focusses on the magneto-optical characterisation of paramagnetic phthalocyanines. While a part of this investigation (mainly on VOPc and CuPc) is already published [1] additional magneto-optical Kerr effect (MOKE) spectra of MnPc, FePc, and CoPc will be presented. The films in the typical thickness range between 30 nm and 100 nm were prepared by organic molecular beam deposition in high vacuum. The magneto-optical Voigt constant is obtained using optical model calculations. A fit of the Voigt data using an oscillator model was performed in order to gain more insight in the electronic origin of the features in the Voigt constant and subsequently in the MOKE spectra. For instance, the hybridisation of Co-3d states with the HOMO π-orbital of CoPc leads to additional features in the magneto-optical spectra compared to *e.g.* CuPc. This effect is much more pronounced in the magneto-optical spectra than in the dielectric function components that are commonly assessed by spectroscopic ellipsometry.

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

DS 32.5 Wed 18:00 GER 37

Hybrid organic/inorganic heterojunctions based on rolled-up nanomembranes — •Carlos Cesar Bof Bufon[1], Juan Diego Ariaz Espinosa[1], Maria Esperanza Navarro Fuentes[1], Dominic J. Thurmer[1], and Oliver G. Schmidt[1,2] — [1]Institute for Integrative Nanosciences, IFW-Dresden, Dresden, Germnay — [2]Material Systems for Nanoelectronics, Chemnitz University of Technology, Chemnitz, Germany

We present a novel method, based on self-released strained nanomembranes, for contacting molecules by using metals and/or semiconductors as electrodes to form hybrid heterojunctions. 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 molecular layer was previously deposited. By this means, we are able to fabricate not only the standards metal-molecule-metal and metal-molecule-semiconductor heterojunctions but also the unique semiconductor-molecule-semiconductor heterojunctions. In this last case, the type of doping and its concentration can be independently for each electrode in order to tune the device electronic properties. The strained nanomembrane based electrodes provide a soft and robust contact on top of the molecular layer. Consequently, no damage to the molecules and no short circuits via possible pinholes have been observed. 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.

DS 32.6 Wed 18:15 GER 37

Degradation effect on the magnetoresistance in organic light emitting diodes — •Andreas Buchschuster, Tobias Schmidt, and Wolfgang Brütting — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

The effect of a magnetic field on the resistance and the luminance of organic light emitting diodes (OLEDs) is commonly observed but not yet fully understood. One of the recent findings was that the magnetic field effect on the resistance (OMR) as well as the effect on the luminance (OML) can be enhanced drastically by electrical stressing of the device.

To investigate both phenomena we studied OLEDs based on small molecules with tris(8-hydroxyquinoline)aluminium (Alq$_3$) as emitting material. Measurements were performed on two different types of hetero-layer devices which only differed in their hole injection layer (HIL) whereat one of the devices exhibited a significantly longer lifetime. Magnetic field effects on the current and the luminance have been detected up to 100 mT while the stressing time was 500 h at the most. We found values up to 5.6 % for the OMR and about 9 % for the OML as well as a correlation of both effects with the degradation of the device. As a result we could show that the transport properties of the hole injection layer has a strong influence on the magnetic field effects.

DS 33: Progress in Micro- and Nanopatterning: Techniques and Applications II (Focused Session, jointly with O – Organisers: Graaf, Hartmann)

Time: Wednesday 11:00–13:00 Location: GER 38

DS 33.1 Wed 11:00 GER 38

Tuning the electrical conductivity of Pt-containing granular metals by postgrowth electron irradiation — •Fabrizio Porrati, Roland Sachser, Christian H. Schwalb, and Michael Huth — Physikalisches Institut, Goethe-Universität, D-60438 Frankfurt am Main, Germany

We have fabricated Pt-containing granular metals by focused electron beam induceddeposition from the $(CH_3)_3CH_3C_5H_4Pt$ precursor gas. The granular metals are made of platinum nanocrystallites embedded in a carbonaceous matrix. We have exposed the as-grown nanocomposites to low energy electron beam irradiation and we have measured the electrical conductivity as a function of the irradiation dose. Postgrowth electron beam irradiation transforms the matrix microstructure and thus the strength of the tunnel coupling between the Pt nanocrystallites. For as-grown samples (weak tunnel coupling regime) we find that the temperature dependence of the electrical conductivity follows the stretched exponential behavior characteristic of the correlated variable-range hopping transport regime. For briefly irradiated samples (strong tunnel coupling regime) the electrical conductivity is tuned across the metal-insulator transition. For long-time irradiated samples the electrical conductivity behaves like that of a metal. In order to further analyze changes of the microstructure as a function of the electron irradiation dose we have carried out atomic force microscopy (AFM) and micro-Raman measurements. These measurements reveal that by increasing the irradiation dose the matrix changes following a graphitization trajectory between amorphous carbon and nanocrystalline graphite.

DS 33.2 Wed 11:15 GER 38

Ordered triple color patterns based on two dye molecules — •Wang Wenchong, Fuchs Harald, and Chi Lifeng — Physikalisches Institut and Center for Nanotechnology (CeNTech), Universität Münster, 48149 Münster, Germany

Functional, small molecular weight organic molecules have received great scientific and technological interest due to their promising potential applications in molecular electronics and optoelectronics. Since last two decades, exciting progress has been witnessed in both materials and film preparation that applied for organic field effect transistors (OFETs),light emission diodes (OLEDs), solar cells,Memories, Sensors, and so on. However, device processing techniques yielding high performances, high levels of integration and uniformity over large area are still underdevelopment. Template directed growth of molecules has been demonstrated as a promising technique for patterning,functionalizing materials at predefined areas and improving device performance.[1-3] Here, based on liquid behavior and solid solvation of molecuoes on patterned surface, the technique can further be applied to fabricate high resolution, ordered triple color patterns with only two molecules.

[1] W. C. Wang, L. F. Chi, et al, Phys. Rev. Lett.2007, 98, 225504.

[2] W. C. Wang, L. F. Chi, et al, Adv. Mat. 2009, 21, 4721.

[3] W. C. Wang, L. F. Chi, et al, Adv. Mat. 2010, 22, 2764.

DS 33.3 Wed 11:30 GER 38

Artificial Hierarchical Gecko-mimicking Structures — •Michael Röhrig, Alexander Kolew, Fabian Pfannes, Matthias Worgull, and Hendrik Hölscher — Institute for Microstructure Technology (IMT), Karlsruhe Institute of Technology (KIT), Germany

Geckos have an impressive attachment system that makes them able to climb on nearly every surface. Like various other mechanisms developed by nature, the gecko effect is strongly connected to the structuring of surfaces. The toes of the Tokay Gecko for example are divided into several lamellae which are covered with millions of setae, delicate hairs which are about $100\,\mu m$ in height and $4\,\mu m$ in diameter. The setae branch into hundreds of tiny endings, the so called spatulae. Thus the gecko is capable of achieving intimate contact with smooth and rough surfaces which leads to a strong adhesion due to intermolecular forces, in particular van der Waals forces.

Mimicking these micro- and nanostructures leads to artificial dry attachment systems. *Hot embossing* is a well-suited molding technique to fabricate such biomimetic structures. In this talk a new variation of hot embossing, the so called *hot pulling* will be presented. Hot pulling allows the fabrication of fibrillar, gecko-mimicking surfaces. Beyond that, the method of measuring the adhesion of structures via AFM force distance curves by using spherical tips will be depicted.

DS 33.4 Wed 11:45 GER 38

Self-arranged anodic nanostructured thin films on titanium — •Robin Kirchgeorg, Steffen Berger, and Patrik Schmuki — Institute for Surface Science and Corrosion (LKO), Department Material Science and Engineering, Fridrich-Alexander-Universität Erlangen-Nürnberg, Martensstraße 7, 91052 Erlangen, Germany

Self-organized anodic oxide nanostructures, in particular highly ordered titania nanotubes offer several interesting functional properties that have been explored in a wide field of applications, such as wettability tuning of surfaces, bio medicine, electrochromic devices, and solar energy conversion. The nanotubular oxides can be tailored, for example with respect to layer thickness, tube diameter, and other morphological, electrical or chemical properties. For many applications these patterned surfaces are at prime importance. The self-organization and growth mechanism of TiO_2 nanotubes during anodization were investigated on photolithographically masked titanium thin films. The influence of potential, time and anodization conditions on the growth mechanism of TiO_2 nanotubes are evaluated. The presentation will provide an overview on the mechanisms of growth and self-ordering of TiO_2 nanotubes.

DS 33.5 Wed 12:00 GER 38

Flexible, free-standing and electrically active TiO_2 nanotubular membranes via lithographic approaches — •Sergiu P. Albu, Steffen Berger, Himendra Jha, and Patrik Schmuki — Department of Materials Science, WW4-LKO, University of Erlangen-Nuremberg, Martensstrasse 7, D-91058 Erlangen, Germany

In the presentation we show the fabrication of a new generation of TiO_2 nanotube membranes. The anodic oxide nanotube growth can be performed through a patterned Ti foil into an underlying Al metal layer [1]. After the selective dissolution of the Al/alumina layer, a very well defined both side open suspended TiO_2 nanotube layer can be obtained. Using lithographic patterning of the anodization area allows to achieve large scale, flexible and well electrically connected nanotubular flow-through membranes with fast electrical switching features over the entire membrane. The removal of the top-initiation layer is based on carrying out anodization through a slowly soluble photoresist coating [2]. These approaches facilitate a better quality and new features of the TiO_2 nanotubular structures.

[1] S. P. Albu, A. Ghicov, S. Berger, H. Jha, P. Schmuki, Electrochem. Commun. 2010, 12, 1352.

[2] S. P. Albu, P. Schmuki, Phys. Status Solidi RRL 2010, 4, 151.

DS 33.6 Wed 12:15 GER 38

ALD Growth of Highly Ordered ZnO Nanotube Arrays with Tunable Structures and Their Device Applications — •Hui Sun, Kin-Mun Wong, Stefan Bartels, Gerhard Wilde, and Yong Lei — Institute of Materials Physics and Center for Nanotechnology, University of Münster, Münster 48149, Germany

Because of the highly ordered feature, anodic alumina membranes have been widely used as nano-templates for growing one-dimensional (1D) nanostructures of various materials. The structural parameters of the template-prepared 1D nanostructures are adjustable including the size, spacing, and aspect ratio of the nanostructures. Recently, we successfully fabricated large-scale ordered arrays of ZnO nanotubes using a synthesizing route combining the template technique and atomic layer deposition (ALD) process. The advantages of the template technique together with the natures of the ALD process (e.g., precisely controllable atomic-scale growing process) results in attractive features of the obtained ZnO nanotube arrays, including tunable tube diameter, wall thickness, length and array density. These nanostructures are of extremely high and variable surface-to-volume ratio, which means that the change of surface status would affect the state of the material significantly. We believe that those constructions will largely enhance the utility of surface electronics devices, such as chemical sensors, biosensors etc., and the structure meets the requirement for conductometric semiconductor gas sensors of high sensitivity. Potential applications, such as photonic detector of super high resolution and band edge mode surface emitting laser are discussed.

DS 33.7 Wed 12:30 GER 38

Surface Patterning using Nano-Templates For Realizing Highly Ordered Nanostructure Arrays with Controllable Properties — •Huaping Zhao, Shikuan Yang, Fabian Grote, Feng Xu, and Yong Lei — Institute of Materials Physics and Center for Nanotechnology, University of Muenster, Muenster 48149, Germany

Here we present the research progress of template-based surface nanopatterning techniques [1-5] in our group. Two kinds of templates were used in the surface patterning process: ultra-thin alumina membranes and monolayer polystyrene spheres. Using the templates, surface patterns of different materials with diverse shapes were synthesized. The structural parameters of the template-prepared surface patterns largely depend on those of the templates. The feature size of the building blocks of the patterns can be adjusted from the quantum size to nanoscale and microscale range [1]. The cost-effective and time-saving fabrication processes of template-based surface patterning approaches are highly desirable for industrial applications in fabricating different nano-devices, giving rise to broad applications of template-prepared surface nanostructures.

References:

1.Lei Y, Yang SH, Wu MH, et al., Chem. Soc. Rev., in press, 2010 (DOI:10.1039/ B924854B).

2. Wu MH, Wen LY, Lei Y, et al., Small, 6 (5), 695, 2010.

3. Lei Y, Cai WP, Wilde G, Prog. Mater. Sci., 52, 465, 2007.

DS 33.8 Wed 12:45 GER 38

Dynamics of step bunches on vicinal surfaces: Sublimation, electromigration and transparent steps — •Marian Ivanov[1], Vladislav Popkov[2], and Joachim Krug[1] — [1]Institut für Theoretische Physik, Universität zu Köln, Köln — [2]Dipartimento di Fisica Teorica, Università degli Studi di Salerno, Salerno, Italy

Using morphological instabilities one can produce templates for nanoscale technology. One example of such an instability is step bunching, which splits a regular vicinal surface into regions of low and high density of monoatomic steps. We consider a one-dimensional step train evolving in the presence of sublimation, step-step interactions, fast kinetics and an Ehrlich-Schwoebel effect. We show that the interplay of sublimation and step-step interactions removes the conservation law for the crystal volume in the co-moving frame, which has been assumed in previous work [1,2]. As a consequence large step bunches are found to break up into smaller bunches of a characteristic size, and the monotonic coarsening dynamics of the volume-conserving model is replaced by a complex quasiperiodic pattern [3]. This interesting behavior is preserved by adding the corresponding terms due to the effect of electromigration. In the case of fast diffusion we consider a recently introduced model for transparent steps [4] and present simulation results for the evolution of the bunch geometry.

[1] V. Popkov, J. Krug, Europhys. Lett. 72, 1025 (2005) [2] V. Popkov, J. Krug, Phys. Rev. B 73, 235430 (2006) [3] M. Ivanov, V. Popkov, J. Krug, Phys. Rev. E 82, 011606 (2010) [4] B. Ranguelov, S. Stoyanov, Surf. Sci. 603, 2907 (2009)

DS 34: Progress in Micro- and Nanopatterning: Techniques and Applications III (Focused Session, jointly with O – Organisers: Graaf, Hartmann)

Time: Wednesday 15:00–17:00 Location: GER 38

DS 34.1 Wed 15:00 GER 38

Femtosecond laser induced recrystallization and ablation of hydrogenated amorphous silicon films — •Babak Soleymanzadeh[1], Christian Strüber[1], Helmut Stiebig[1,2], and Walter Pfeiffer[1] — [1]Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany — [2]Malibu GmbH & Co. KG, Böttcher Str. 7, 33609 Bielefeld, Germany

Ultrashort laser pulses offer new and fascinating possibilities in the field of laser material processing. Here we investigate the femtosecond laser induced recrystallization and ablation of hydrogenated amorphous silicon films (300 nm thickness) grown on glass substrates by large area (>1 m^2) plasma-enhanced chemical-vapor deposition. At laser fluences of <40 mJcm^{-2} (800 nm, <100 fs pulse duration) recrystallization of the amorphous silicon layer is observed in spatially resolved Raman micro-spectroscopy. The fluence dependence of this recrystallization indicates that a nonlinear excitation mechanism is responsible. At slightly higher fluences the amorphous silicon thin-film is ablated. Scanning electron microscopy and energy-dispersive X-ray spectroscopy (EDX) is applied to investigate the ablation process for various laser fluences. The prospect of using femtosecond laser induced material processing in silicon thin-film photovoltaics is discussed.

DS 34.2 Wed 15:15 GER 38

Photothermal Laser Micro- and Nanoprocessing of Mesoporous Gold — •Lina Schade[1], Mareike Mathieu[1,2], Monika Biener[2], Juergen Biener[2], and Nils Hartmann[1] — [1]Fakultät für Chemie, NETZ, CeNIDE, Universität Duisburg-Essen, Universitätsstr. 5, 45141 Essen, Germany — [2]LLNL, Livermore, CA 94550, USA

In recent years, mesoporous gold has gained significant attention as a novel material in actuation, sensing and catalysis. The particular properties of this material result from its spongelike open-cell morphology with pore sizes of about 25 nm. Techniques which allow one to engineer mesoporous gold on a micro- and nanoscale, of course, are of high interest in view of fundamental studies and technical applications. Common annealing procedures, for example, provide a means to adjust the pore size in the range of 50 - 600 nm and investigate size dependent properties, such as the enhancement effect in surface enhanced Raman spectroscopy (SERS) [1]. Here we report on a photothermal laser technique for micro- and nanoprocessing of mesoporous gold [2]. A focused beam of a cw-laser with a wavelength of 532 nm and a 1/e spot size of 1.4 microns is used to locally anneal the substrate surface and fine tune the pore structure. This allows one to fabricate porous gradients on micrometer length scales. In addition, thiol-based self-assembled monolayers provide unique opportunities to functionalize these porous structures [2]. Prospects in SERS measurements and other applications are discussed.

[1] S.O Kucheyev, et al., Appl. Phys. Lett. 89 (2006) 053102.

[2] M. Mathieu, N. Hartmann, NJP, in press.

DS 34.3 Wed 15:30 GER 38

Photothermal laser patterning of buried polymer interfaces — •Anja Schröter, Steffen Franzka, and Nils Hartmann — Fakultät für Chemie, CeNIDE and NETZ, Universität Duisburg-Essen, Universitätsstr. 5, 45141 Essen, Germany

Covalent attachment of polymer films provides a versatile means to taylor chemical and physical surface properties. Alternative to the approach of growing a polymer on a surface [1], here we report on a facile and flexible photothermal procedure for local grafting of thin polymer films to solid surfaces. Surface-oxidized silicon samples are coated with alkylsiloxane monolayers. After wet-chemical treatment in order to form azide-terminated monolayers a thin polymer film is spin-coated on top of the monolayer. Local irradiation with a focused beam of a diode-pumped solid-state laser at a wavelength of 532 nm thermally activates the azide groups at the buried polymer interface and leads to local covalent attachment of the polymer. Subsequently, polymer material, which is not coupled to the surface, is removed via sonication. The influence of incident laser power and irradiation time is investigated. At a 1/e focal spot diameter of 2.1 microns dots with diameters close to 1 micron can be fabricated. This procedure allows for rapid large-scale patterned attachment of a wide spectrum of polymers.

[1] M. Mathieu, A. Friebe, S. Franzka, M. Ulbricht, N. Hartmann, Langmuir 25 (2009) 12393.

DS 34.4 Wed 15:45 GER 38

Photothermally induced chemical patterning of organic monolayers on oxide-free silicon substrates — •Martin Przyklenk[1], Benjamin Klingebiel[1], Luc Scheres[2], Han Zuilhof[2], and Nils Hartmann[1] — [1]Fakultät für Chemie, CeNIDE, NETZ, Universität Duisburg-Essen, Universitätsstr. 5, 45141 Essen — [2]Laboratory of Organic Chemistry, Wageningen University, Dreijenplein 8, 6703 HB Wageningen, The Netherlands

Patterned self-assembeld organic monolayers (SAMs) are widely used as templates to build up complex functional surface structures. A simple routine for nanopattering of organic monolayers down to 100 nm and below relies on photothermal processes [1,2]. In photothermal processing a focused laser beam is used to locally heat the substrate and initiate thermal decomposition of the monolayer. Here we use a simple photothermal procedure for direct chemical functionalization of organic monolayers [1]. Oxide-free silicon samples are coated with alkyl and alkenyl monolayers [2]. Through irradiation with a focused beam of an argon ion laser at a wavelength of 514 nm in gaseous bromine local bromination of the monolayer takes place. Mechanistic aspects and prospects of photothermal routines in micro- and nanofabrication of multifunctional organic monolayers are discussed.

[1] B. Klingebiel, A. Schröter, S. Franzka, N. Hartmann, ChemPhysChem 10 (2009) 2000.

[2] L. Scheres, B. Klingebiel, J. ter Maat, M. Giesbers, H. de Jong, N. Hartmann, H. Zuilhof, Small 6 (2010) 1918.

DS 34.5 Wed 16:00 GER 38

Pattern transfer on large samples using a sub-aperture reactive ion beam — •André Miessler, Agnes Mill, Jürgen W. Gerlach, 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 CF_4 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 as well as an accumulation of carbon (up to 40 atomic percent) in the beam periphery, respectively. The substitution of CF_4 by NF_3 as reactive gas reveals a lot of benefits: more stable ion beam conditions in combination with a reduction of the beam size down to a diameter of 5 mm and a reduced amount of the Ni, Fe and Cr contaminations. However, a layer formation of silicon nitride handicaps the chemical contribution of the etching process. These negative side effects influence the transfer of trench structures on quartz by changing the selectivity due to altered chemical reaction of the modified resist layer. Concerning this we investigate the pattern transfer on large fused silica plates using NF_3-sub-aperture RIBE.

DS 34.6 Wed 16:15 GER 38

Swift Heavy Ion Beam Shaping Of Sub-Micron Structures — •R. Ferhati[1], N. Guilliard[1], T. Weishaar[1], S. Amirthapandian[1], M. Fritschke[2], L. Bischoff[2], and W. Bolse[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart — [2]Forschungszentrum Dresden

Already in 1983 it was discovered, that swift heavy ion (SHI) irradiation of metallic glasses results in anisotropic deformation (shrinking along the beam direction expansion in perpendicular directions) [1]. We have employed this "hammering effect" to reshape sub-micrometer structures by SHI bombardment under proper variation of the beam incidence angle. Utilizing the focused ion beam (FIB) technique, a rectangular grid with varying lateral distances of 100 to 5000 nm was cut into a 100 nm thick NiO- resp. ZnO-film from their surfaces down to the oxidized Si-substrate, in order to produce small oxide "ashlars". The samples were then irradiated under grazing incidence and continuous azimuthal target rotation with 1.4 GeV U- (NiO) and 0.95 GeV Au-ions (ZnO), respectively, in our new in-situ SEM at the UNILAC accelerator of GSI [2]. After certain fluence steps, the irradiation was stopped and one and the same spot was analyzed by means of SEM in order to investigate the evolution of the irradiated objects. Depending on their initial size complex structures (egg-, cone-, pillar-, forceps-, tooth-like) were formed, which can only be understood if besides the hammering effect deformation due to surface tension and yield stress are taken into account. [1] S. Klaumünzer, G. Schumacher, Phys. Rev. Lett. 51 (1983), [2] S. Amirthapandian, et al., Rev.Sci.Instr. 81, (2010)

DS 34.7 Wed 16:30 GER 38

Surfactant driven self-organized surface patterns by ion beam erosion — •Hans Hofsäss and Kun Zhang — II. Physikalisches Institut, Universität Göttingen, 37077 Göttingen, Germany

Self-organized pattern formation on surfaces by ion beam erosion and driven by metal surfactant atoms is discussed. Si substrates were irradiated with 5 keV Xe ions at normal incidence and ion fluences up to $5x10^{17}$ Xe^+/cm^2 under continuous deposition of surfactant atoms. In the absence of surfactants uniform flat surfaces are obtained. With surfactants pronounced patterns like dots, combinations of dots and ripples as well as ripples with about 100 nm wavelength are generated. 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 between about 10^{15} and $5x10^{15}$ atoms/cm^2. With increasing ion fluence the pattern contrast increases but the pattern type remains unchanged. The 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. Directed deposition of metal surfactant causes preferential deposition and shadowing and determines the final pattern orientation and morphology. First results on the dynamic behaviour of the ripples are presented.

DS 34.8 Wed 16:45 GER 38

Dynamics of surfactant induced ripple patterns on Si generated by ion beam erosion — •Kun Zhang, Hans Hofsäss, Hans-Gregor Gehrke, and Oliver Göpfert — II.Physikalisches Institut, Universität Göttingen, 37077 Göttingen, Germany

Some metallic surfactants induce pronounced dot and ripple patterns on Si substrates during normal and near normal ion incidence sputter erosion. In the absence of metal co-deposition uniform flat surfaces are obtained. It is known that surface ripples generated by ion beam erosion at glancing ion incidence propagate across the surface. In this work we investigate the propagation of ripple patterns triggered by surfactant atoms and a possible correlation between ripple propagation and directed deposition of surfactant atoms. Si substrates were irradiated with 5 keV Xe ions at normal ion incidence under continuous deposition of Fe or Mo surfactant atoms. With surfactants pronounced patterns like dots, combinations of dots and ripples as well as ripples with about 100 nm wavelength and up to 12 nm in height are generated. The dynamics of patterns, in particular the propagation of ripples across the surface with increasing ion fluence was investigated using sequential ion irradiation and scanning electron microscopy analysis. Specific regions on the irradiated samples were identified using thin marker grooves prepared by focused ion beam milling. Using pattern recognition methods we are able to determine the fluence dependent shift of the ripple patterns with respect to the marker grooves. We find dynamic patterns with a propagation velocity of about 0.7 nm per 10^{15} ions/cm^2. A qualitative model for the ripple propagation is presented.

DS 35: Plasmonics and Nanophotonics (jointly with HL and O)

Time: Wednesday 17:15–19:15 Location: GER 38

DS 35.1 Wed 17:15 GER 38

Simulation of second harmonic generation from split ring resonators with the Discontinuous Galerkin Time Domain method — •Yevgen Grynko, Torsten Meier, and Jens Förstner — Universität Paderborn, Warburger Str. 100, 33098 Paderborn

We report our results of the application of the Discontinuous Galerkin Time Domain (DGTD) method [1] for the simulation of the linear and non-linear response of plasmonic nanostructures. We use DGTD as it has a number of attractive features including adaptive grid refinement and nonlinear stability. In this work, we consider an array of U-shaped split ring resonators. Metallic dispersion is described with a current density equation based on the representation of electron dynamics in terms of electron plasma. It includes linear Drude terms and nonlinear terms for the Lorentz force and convective acceleration of the electron flow. The nonlinear part of the equation causes the doubling of the transmitted frequency leading to the the SH peak in the spectrum. Switching between the terms shows that the "convective" term plays the main role in the observed phenomena. The strength of the the SH peak is comparable to the values reported previously in the experiments [2] and FDTD simulations [3].

[1] J. S. Hesthaven, T. Warburton, 2002, J. Comp. Phys., 181, 186-221. [2] M. W. Klein, et al., 2007, Opt. Express, 15, 5238. [3] Y. Zeng, et al., 2009, Phys. Rev. B 79, 235109-1 - 235109-9.

DS 35.2 Wed 17:30 GER 38

Analysis of optimization techniques for coherent optical control in nanostructures — •Tobias Fankhänel, Torsten Meier, and Jens Förstner — University of Paderborn, Department of Physics and CeOPP, Warburger Str. 100, D-33098 Paderborn, Germany

We compare the efficiency of optimization approaches for shaping coherent optical control in nanostructures. The optical response of various structures is calculated using the Finite-Difference Time-Domain (FDTD, [1]) method. Standard optimization algorithms (L-BFGS gradient method [2], genetic algorithm [3]) are used to maximize target function like the flux transmission or spatio-temporal response; the algorithms' convergence time and computational effort is analyzed.

[1] A. Taflove, S. C. Hagness. Computational electrodynamics: the finite-difference time-domain method, third edition (Artech House Inc., Norwood 2005)

[2] J. Nocedal. Updating Quasi-Newton Matrices with Limited Storage (1980), Mathematics of Computation 35, pp. 773-782.

[3] GALib, http://lancet.mit.edu/ga/

DS 35.3 Wed 17:45 GER 38

Two state lasing from a quantum dot laser — •Diana Khabipova, Kathy Lüdge, Niels Majer, and Eckehard Schöll — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We investigate the emission properties of a quantum dot (QD) laser with two confined electron and two hole levels, respectively. Our microscopically based rate equation model for quantum dot lasers [1] is extended by including the first excited state of the QDs as a second lasing state besides the ground state. The model treats separately the dynamics of QD electrons and holes, photon densities of the ground and excited state lasing, respectively, and the electron and hole densities in the 2D wetting layer as carrier reservoir. The carrier-carrier scattering rates include the direct capture from the wetting layer into the ground and excited state as well as relaxation processes from excited to ground state. The influence of the energy differences between the excited state, ground state, and wetting layer on the turn-on dynamics is investigated. We analyse also the effect of the excited state upon the relaxation oscillations, their turn-on delay and damping rate. Furthermore we study the excited state dynamics under thermal heating conditions and for different device dimensions.

[1] K. Lüdge, R. Aust, G. Fiol, M. Stubenrauch, D. Arsenijevic, D. Bimberg, and E. Schöll, IEEE J.Quantum Electron. 46, 12, 1755 (2010).

DS 35.4 Wed 18:00 GER 38

Analytical approach to modulation properties of quantum dot lasers — •Kathy Lüdge[1], Evgeny Viktorov[2], Thomas Erneux[2], and Eckehard Schöll[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Universite Libre de Bruxelles, Optique Nonlineaire Theorique, Campus Plaine, C.P. 231, 1050 Bruxelles, Belgium

We analyze a microscopically based rate equation model for quantum dot lasers. The model separately treats the dynamics of electrons and holes, and the carrier-carrier scattering rates depend nonlinearly on the wetting layer carrier densities [1]. Our objective is to determine analytical expressions for the relaxation oscillation frequency and damping rate. To this end, we consider the Class B limit of the five rate equations and apply asymptotic techniques. We consider two cases corresponding to either equivalent or drastically different decay rates for the electrons and holes. We show how they contribute to increase the relaxation oscillation damping rate compared to the damping rate of the conventional laser and that there exist optimal conditions on the control parameters in order to observe maximum damping.

[1] K. Lüdge, E. Schöll, IEEE J.Quantum Electron. 45, 1396 (2009).

DS 35.5 Wed 18:15 GER 38

Periodic Nanostructures: Spatial dispersion mimics chirality — •Bruno Gompf[1], Julia Braun[1], Thomas Weiss[1], Harald Giessen[1], Martin Dressel[1], and Uwe Hübner[2] — [1]Physikalisches Institut and Research Center SCOPE, Universität Stuttgart — [2]Institut für Photonische Technologien, Jena

The underlying idea of metamaterials is that it should be possible to construct artificial materials with completely new effective dielectric properties from nanometer-sized photonic atoms. One of these new fascinating properties is, for example, the recently achieved optical activity in photonic metamaterials. In our work we demonstrate that even a simple isotropic metal-dielectric nanostructure, i.e., a subwavelength hole array on a square lattice in a semitransparent Au film, rotates the polarization state at oblique incidence, but this behaviour cannot be explained by effective optical parameters. The structure was characterized by Mueller matrix spectroscopic ellipsometry at various angles of incidence and azimuthal orientations in the energy range of 0.73 to 4.6 eV. For the additional theoretical simulations, we employed a Fourier modal approach. To visualize the theoretical and experimental results, we plot the matrix elements in polar coordinates. Already from a brief look at the off-diagonal elements, it becomes obvious that the hole array mixes different incoming polarization states upon reflection in a complex way, which can not be explained by purely dielectric optical constants. It can be shown that for our square array even a bi-anisotropic model must fail. Rather spatial dispersion has to be taken into account.

DS 35.6 Wed 18:30 GER 38

New transparent conductive metal based on polymer composite — •mehdi keshavarz hedayati[1], mohammad jamali[1], thomas strunkus[2], vladimir zaporochentko[2], franz faupel[2], and mady elbahri[1,3] — [1]Nanochemistry and Nanoengineering, Institute for Materials Science, Faculty of engineering, Christian-Albrechts-University of Kiel — [2]Multicomponent Materials, Institute for Materials Science, Faculty of engineering, Christian-Albrechts-University of Kiel — [3]Helmholtz-Zentrum Geesthacht GmbH, Institute of Polymer Research, Nanochemistry and Nanoengineering

Currently great efforts are made to develop new kind of transparent conductors (TCs) to replace ITO. In this regard different materials and composites have been proposed and studied including conductive polymers, carbon nanotubes (CNTs), metal grids, and random networks of metallic nanowires. But so far none of them could be used as a replacing material, since either they are either fragile and brittle or their electrical conductivity is below the typical ITO. Thin metallic films due to their high electrical conductivity could be one of the best replacing materials for ITO, however their poor transparency makes their application as TCs limited. Here we design and fabricate a new polymeric composite coating which enhances the transparency of the thin metal film up to 100% relative to the initial value while having a high electrical conductivity of typical metals. Therefore our proposed device has a great potential to be used as new transparent conductor.

DS 35.7 Wed 18:45 GER 38

A self-assembly route to mesoporous Bragg reflectors — •Stefan Guldin[1], Matthias Kolle[1], Morgan Stefik[3], Richard Langford[1], Dominik Eder[2], Ulrich Wiesner[3], and Ullrich Steiner[1] — [1]Physics Department, Cavendish Laboratory, University of Cambridge, UK — [2]Materials Science Department, University of Cambridge, UK — [3]Materials Science Department, Cornell University, Ithaca, NY, USA

Mesoporous distributed Bragg reflectors (MDBRs) consist of a periodic lattice of alternating high and low refractive index, while exhibiting porosity on the sub-optical length scale. MDBRs have great potential as sensing materials in biology and chemistry, as adsorption and desorption of gas phase molecules lead to reversible changes in the refractive index of the stack. Optoelectronics is another promising field of applications. MDBRs can be used as light harvesting element in excitonic solar cells. When infiltrated with light emitting polymers, MDBRs have exhibited distributed feedback lasing.

We present a new route for the fabrication of MDBRs which relies on the self-assembling properties of the block copolymer PI-*b*-PEO in combination with sol-gel chemistry to finely tune porosity and pore size in the resulting inorganic material. Stacking-up multiple layers of alternating refractive index results in a fast and reliable assembly of a continuous network with well defined interfaces. The outcome are MDBRs of high quality optical properties even when built from a single material, in our case TiO_2.

DS 35.8 Wed 19:00 GER 38

Launching Surface Plasmons by Carbon Nanotube Photoluminescence — •Nicolai Hartmann[1], Johann Berthelot[2], Alexandre Bouhelier[2], and Achim Hartschuh[1] — [1]Department Chemie and CeNS, Ludwig-Maximilians-Universität München, Germany — [2]Département Nanosciences, Laboratoire Interdisciplinaire Carnot Bourgogne, Université de Bourgogne, Dijon, France

We report on the excitation of propagating surface plasmons in metal films and waveguides via photoluminescence emission from semiconducting single-walled carbon nanotubes. Upon excitation in the visible regime a single carbon nanotube acts as a directive near-infrared point dipole source for surface plasmons propagating along the direction of the nanotube axis. To investigate this behaviour we used leakage radiation microscopy [1,2]. The excitation of propagating surface plasmons manifests itself by a narrow emission of leakage radiation in Fourier space appearing at angles according to the surface plasmon resonance. In real space we observe the exponential decay of the intensity along the propagation direction of the plasmon. Propagation lengths between 11 and 13 μm could be extracted and supported by calculations, depending on the thickness of the dielectric spacer layer separating carbon nanotubes and metal film. Combining surface plasmon coupling with electroluminescence from carbon nanotubes [3] opens up the possibility to create an electrically driven plasmon source.

[1] B. Hecht, et.al., Phys. rev. Lett. 77, 1889 (1996) [2] M. Böhmler, et.al., Opt. Express 18, 16443 (2010) [3] P. Avouris, et.al., Nat. Photonics 2, 341 (2008)

DS 36: Plasmonics and Nanophotonics HL-I (jointly with HL and O)

Time: Wednesday 10:15–12:15 Location: POT 251

DS 36.1 Wed 10:15 POT 251

Optical Gain in Rolled-up Semiconductor/Metal Metamaterials — Stephan Schwaiger, Markus Broell, Ricardo Costa, Matthias Klingbeil, Aune Koitmae, Wolfgang Hansen, Detlef Heitmann, and •Stefan Mendach — Institute for Applied Physics, University of Hamburg, Jungiusstrasse 11, 20355 Hamburg, Germany

Stimulated emission from optically active gain material is one of the most promising ways to solve the problem of losses in metamaterials [1, 2]. Here, we present gain measurements on rolled-up semiconductor/metal hybrid metamaterials [3] containing InGaAs quantum wells. We find a characteristic increase and decrease of the transmission through the metamaterial when optically pumping the quantum well. We observe positive gain of up to 15% at the high energy tails of the photoluminescence peaks of the quantum well and negative gain of similar magnitude at the low energy tails. This behaviour can be well reproduced with transfer matrix calculations which model each peak in the quantum well photoluminescence by a Lorentz oscillator.

[1] Y. Sivan, S. Xiao, U. K. Chettiar, A.V. Kildishev, and V. M. Shalaev, Opt. Exp. 26, 24060 (2009). [2] S. Xiao, V. P. Drachev, A.V. Kildishev, X. Ni, U. K. Chettiar, H.-K. Yuan, and V.M. Shalaev, Nature 466, 735 (2010). [3] S. Schwaiger, M. Bröll, A. Krohn, A. Stemmann, C. Heyn, Y. Stark, D. Stickler, D. Heitmann, and S. Mendach, Physical Review Letters 102, 163903 (2009)

DS 36.2 Wed 10:30 POT 251

Calculation of Transmission through rolled-up three dimensional Metamaterials — •Andreas Rottler, Stephan Schwaiger, Aune Koitmäe, Matthias Klingbeil, Markus Bröll, Detlef Heitmann, and Stefan Mendach — Institute of Applied Physics, University of Hamburg, Germany

Metamaterials are artificial structures where permittivity and permeability can be designed on demand and may exhibit values which are not observed in nature. In this talk, we present finite-difference time-domain simulation results on a metamaterial which consists of curved alternating layers of metal/semiconductor films. Such structures can be prepared from self-rolling strained metal/semiconductor layers and exhibit an anisotropic permittivity with tunable plasma frequency allowing for hyperlensing in the visible [1]. We performed simulations where we varied the parameters of the structure in order to optimize the transmission through the curved metamaterial.

We gratefully acknowledge support by the DFG via the Graduiertenkolleg 1286.

[1] S. Schwaiger et al., Phys. Rev. Lett. 102, 163903 (2009)

DS 36.3 Wed 10:45 POT 251

Auxiliary basis functions for the Wannier function based 2D TE photonic crystal circuit design — •Patrick Mack, Christian Wolff, and Kurt Busch — Institut für Theoretische Festkörperphysik (TFP) and DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany

Photonic crystals are periodic dielectric heterostructures exhibiting a band structure for light. Adjusting fabricational parameters offers the possibility to open complete, photonic band gaps prohibiting light propagation regardless of direction. Purposely designed defect structures introduce localized light modes in these forbidden frequency ranges, creating resonator modes, waveguides and functional elements for photonic devices, whose design optimization has to be carried out numerically.

The Wannier function (WF) approach yields a tight-binding like numerical method which expands these localized states in a set of localized basis functions and proved to be particularly efficient for E-polarized (TM) light in the combination with an S-matrix approach. In the H-polarized (TE) case, however, slow convergence limited the applicability of this Ansatz. We propose to use additional auxiliary basis functions, that improve convergence and are capable of modeling 2D TE large scale photonic circuitry (typically air holes in silicon) involving non-etched holes and tunable linear anisotropic media, such as liquid crystals and magneto-optic materials.

DS 36.4 Wed 11:00 POT 251

Coupling model for the derivation of optical resonances in stacked nanogratings — •Thomas Weiss[1,2], Nikolay A. Gippius[2,3], Sergei G. Tikhodeev[3], Gérard Granet[2], Liwei Fu[1], Richard Taubert[1], and Harald Giessen[1] — [1]4th Physics Institute and Research Center Scope, University of Stuttgart, Stuttgart, Germany — [2]LASEMA, University Blaise Pascal, Aubière, France — [3]A. M. Prokhorov General Physics Institute, Russian Academy of Sciences, Moscow, Russia

Nanogratings have become one of the most important structures in modern nanooptics over the last few years. They can be used in different fields such as photonic crystals and metamaterials. However, the experimental fabrication as well as the corresponding numerical calculation is usually very time-consuming. Hence, simple models are required for a qualitative derivation of the optical behavior of such structures. Here, we present a method to approximate the optical resonances of stacked nanogratings using the Fourier modal method and optical scattering matrix theory. The resulting equations form a low-dimensional linear eigenvalue problem that can easily be solved for varying grating distances, including near field effects as well as multiple scattering in the far field regime with strong coupling to Fabry-Perot resonances. The method is not only accurate and fast; it provides also additional physical insight, as the individual components of the coupling mechanism can be studied independently. Furthermore, the model involves no fitting parameters. All quantities can be derived ab initio by the scattering matrix formalism.

DS 36.5 Wed 11:15 POT 251

3D photonic crystal integrated in a mircomorph thin film silicon tandem cell — •Johannes Üpping[1], Thomas Beckers[2], Reinhard Carius[2], Uwe Rau[2], Stephan Fahr[3], Carsten Rockstuhl[3], Falk Lederer[3], Matthias Kroll[4], Thomas Pertsch[4], Lorenz Steidl[5], Rudolf Zentel[5], and Ralf B. Wehrspohn[1] — [1]Institute of Physics, mikroMD, University of Halle Wittenberg — [2]Institute of Energy Research, IEF-5 Photovoltaics, Forschungszentrum Jülich GmbH — [3]Institute of Condensed Matter Theory and Sold State Optics, Friedrich-Schiller-Universität Jena — [4]Institute of Applied Physics, Friedrich-Schiller-Universität Jena — [5]Institute of Organic Chemistry, Johannes Gutenberg-Universität Mainz

A 3D photonic intermediate reflector for textured micromorph silicon tandem solar cells has been investigated. In thin-film silicon tandem solar cells consisting of amorphous and microcrystalline silicon with two junctions of a-Si/μc-Si, efficiency enhancements can be achieved by increasing the current density in the a-Si top cell. It is one goal to provide an optimized current matching at high current densities. For an ideal photon-management between top and bottom cell, a spectrally selective intermediate reflective layer (IRL) is necessary. We we present the first fully integrated 3D photonic thin-film IRL device incorporated in a state-of-the-art textured tandem solar cell. The design, the preparation and numerical calculations of a 3D self organized inverted opal photonic crystal structure in a textured micromorph tandem solar cell are presented.

DS 36.6 Wed 11:30 POT 251

Angle-resolved fluorescence spectroscopy in photonic crystals — •Rebecca Wagner, Lars Heerklotz, and Frank Cichos — Molecular Nanophotonics, University of Leipzig, Germany

Photonic Crystals (PCs) are materials with periodically varying dielectric constant. Multiple scattering of light on this spatially modulated refractive index leads to the formation of a photonic band structure including photonic band gaps. The optical density of states is redistributed as compared to a homogeneous material and is described by the fractional local density of states (FLDoS). This leads to a modified propagation of light in the material.

The spectral and angular position of the band gaps can, for example, be probed by reflection spectroscopy. Since reflections can occur on different lattice plane families, the detection angle has to be varied for every angle of incidence, making this method very time consuming. Further, an average of the reflectivity over differently oriented crystal domains is taken.

We develop a method to overcome these problems using fluorescence spectroscopy of single internal emitters. By applying a special technique we are able to measure angle resolved fluorescence spectra for many emission angles at the same time. Comparison of these spectra to spectra of emitters outside the PC gives the FLDoS, which also contains information about the symmetry of the emitter's local environment. By varying emitters and lattice constants of the PC, different regions of the band structure can be probed.

DS 36.7 Wed 11:45 POT 251

The Concepts of Self-assembled 3D Photonic Crystals for High Temperature IR reflective coatings — •Hooi Sing Lee[1], Alexander Petrov[1], Manfred Eich[1], Roman Kubrin[2], Gerold Scheider[2], Julien Bachmann[3], and Kornelius Nielsch[3] — [1]Institut für Optische und Elektronische Materialien, TUHH, Hamburg, Deutschaland — [2]Institut für keramische Hochleistungswerkstoffe , TUHH, Hamburg, Deutschaland — [3]nstitut für Angewandte Physik, Uni Hamburg, Hamburg, Deutschaland

The study is undertaken to develope a self-assembled 3D microporous structure which is based solely on low thermal conductivity ceramic materials and is capable of reflecting IR radiation at any incident angle over a wide spectral range.The practical applications which will benefite most from this study are ceramic thermal barrier coatings (TBC) and selective filters for thermophotovoltaics (TPV). Finite Integration Technique (FIT) simulations have shown that yttria stabilized zirconia (YSZ) inverse opal with the pore size of $>$ 500nm possesses stopgap in the IR regime and can be tailored to reflect target range of wavelength by changing the lattice constants. The width of the stopgap can be effectively enlarged by stacking several inverse opal with different pore sizes in the subsequent layers and it was shown in simulation and experiment. It was estimated that 9 stacks of such structures can achieved 91% of total hemispherical reflectance in the wavelegth range of 1-6 *m, where the major blackbody radiant power at 1500 K tends to be concentrated. The optical properties of direct opal and inverse opal were measured and compared with the simulations.

DS 36.8 Wed 12:00 POT 251

Bio-inspired multifunctional photonic systems — •Mathias Kolle[1], Peter Vukusic[2], and Joanna Aizenberg[1] — [1]School of Engineering and Applied Sciences, Harvard University, 9 Oxford St, Cambridge, MA-02138, US — [2]School of Physics, Stocker Road, Exeter, EX4 4QL

Biomimetic and bio-inspired attempts to produce novel photonic structures have attracted increasing research interest in recent years. Nature offers an enormous amount of multifunctional micro- and nanostructures that provide outstanding, distinctive, dynamic and tailored coloration and high reflectivity. Various intriguing photonic structures have been identified on the wing scales of beetles, butterflies, the feathers of birds or in marine animals. Nature offers a huge reservoir of blueprints for novel artificial optical materials and photonic structures. We present the development of bio-inspired, dynamic, micro-optical elements that are comparable to some of natures efficient optical systems. Artificially controlled self-assembly combined with established nanofabrication techniques can be used for the development of new optically-adaptive devices. Novel optical elements have to address the aspect of tunability and multifunctionality to be versatile for a wide range of applications. Furthermore, we propose a technique to create fully organic adaptive optical systems based on elastic multilayer micro-rolls.

DS 37: Plasmonics and Nanophotonics O-IV (jointly with HL and O)

Time: Wednesday 11:15–13:00 Location: WIL A317

DS 37.1 Wed 11:15 WIL A317

Steering and Negative Refraction of Surface Plasmon Beams — •Benedikt Stein, Jean-Yves Laluet, Eloïse Devaux, Cyriaque Genet, and Thomas W. Ebbesen — ISIS, Université de Strasbourg & CNRS, 8 allée Gaspard Monge, 67000 Strasbourg, France

Surface plasmon polaritons have raised renewed interest over the past decade for their potential in optical devices and circuits [1]. Inspired by the design principles of photonic bandgap materials [2,3], we have studied the propagation of surface plasmon beams through singly and doubly periodic metallic gratings. Large beam steering effects are experimentally revealed by probing the isofrequency surfaces related to propagating Bloch waves inside the gratings. In particular, negative refraction is demonstrated close to the Bragg condition. We also analyze how the local structure of the isofrequency surface can amplify the sensitivity of surface plasmon based refractive-index sensors [4].

[1] Barnes, W. L.; Dereux, A.; Ebbesen, T. W. *Nature* 2003, 424, 824
[2] Zengerle, R. *Journal of Modern Optics* 1987, 34, 1589
[3] Russell, P.S.J. *Phys. Rev. A.* 1986, 33, 3232
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DS 37.2 Wed 11:30 WIL A317

Far-field optical characterization of ultrafast plasmon propagation in nanostructures — •Christian Rewitz[1], Thomas Keitzl[1], Philip Tuchscherer[1], Jer-Shing Huang[2], Peter Geisler[3], Bert Hecht[3], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg — [2]Department of Chemistry, National Tsing Hua University, Hsinchu 30013, Taiwan — [3]Nano-Optics and Biophotonics Group, Department of Experimental Physics 5, University of Würzburg, Am Hubland, 97074 Würzburg

Our goal is to characterize and control the propagation of ultrafast excitations in optical nanocircuits. For this purpose, the technique of spectral interferometry (SI) is combined with a microscope setup. This allows for a full characterization (amplitude and phase) of an ultrafast pulse emitted at the output of a nanocircuit. The input and output of the nanostructure can be addressed with a diffraction-limited resolution. As a first experiment, we investigate the propagation of plasmons in silver wires with nanometer radial and micrometer longitudinal dimensions. Once the excitation pulse is focused on one end of a wire, part of the energy is converted into a propagating plasmon mode. Upon propagation the plasmon is modified by dispersion and attenuation that is specific to the nanostructure. After the plasmon is converted into a radiative far-field mode at the other end of the wire the field is collected by the microscope objective and can be fully characterized via SI. Thus, specific plasmonic properties of the nanostructure can be determined. One of them is the propagation speed of the plasmon.

DS 37.3 Wed 11:45 WIL A317

Ultrafast optical nonlinearities in hybrid metal-semiconductor nanostructures — •Parinda Vasa[1], Robert Pomraenke[1], Giovanni Cirmi[2], Elenora De Re[2], Wei Wang[1], Stephan Schwieger[3], David Leipold[3], Erich Runge[3], Giulio Cerullo[2], and Christoph Lienau[1] — [1]Institut für Physik, Carl von Ossietzky Universität Oldenburg, Germany — [2]IFN-CNR, Dipartimento di Fisica, Politecnico di Milano, Milano, Italy — [3]Institut für Physik and Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, Germany

Understanding and manipulating the interactions between quantum emitters and surface plasmon polaritons (SPPs) is the key to designing and implementing novel nano-optical devices. We report the measurements of ultrafast optical nonlinearity resulting from the strong interaction between SPPs on a gold grating and excitons in either a semiconductor QW or a J-aggregated cyanine dye. The hybrid structures are characterized by linear reflectivity measurements and exhibit enhanced SPP-exciton coupling. The nonlinearity is investigated by low-temperature, angle-resolved, ultrafast pump-probe spectroscopy under different excitation schemes. Strong optical excitation drastically alters the hybrid nanostructure response by transiently changing the exciton density. A significant shift in the polariton resonance wavelength and changes in the response time are observed. The results are explained within a semi-classical density matrix formalism. Such a strong ultrafast nonlinear interaction between SPPs and excitons will be of key importance in adding active functionality to plasmonic devices.

DS 37.4 Wed 12:00 WIL A317

Characteristics of the Electron Emission from Metal Nanotips due to Ultrashort Laser Pulses — •Steve Lenk and Erich Runge — Institut für Physik und Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, 98693 Ilmenau, Germany

We investigate the electron emission process from sharp gold nanotips illuminated by ultrashort femtosecond laser pulses theoretically. The emission processes under discussion for few-femtosecond laser pulses are multiphoton emission [1] and optical field emission [2]. We calculate the probability current from a numerical solution in two spatial dimensions of an initial-value problem [3] via an exponential split-operator method and a real-space product-formula algorithm [4]. The time-dependent electromagnetic potentials used for the study of the electron emission are derived from a finite-difference time-domain method calculation. We observe spatial emission spot changes dependent on the bias voltage as well as different time characteristics due to different laser pulse powers. The electric field and the photoelectron current are compared to experimental results.

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[3] S. Glutsch, *Excitons in Low−Dimensional Semiconductors*, Springer Heidelberg (2004).
[4] H. De Raedt, Comp. Phys. Rep. **7**, 1 (1987).

DS 37.5 Wed 12:15 WIL A317

Theory of ultrashort plasmon pulse generation by mode-locked surface plasmon polariton lasers — •Kwang-Hyon Kim, Anton Husakou, and Joachim Herrmann — Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy, Max-Born-Str. 2a, 12489 Berlin

Amplification of surface plasmon polaritons (SPP) by embedding a dielectric with a gain medium is of great importance for a variety of applications including surface spectroscopy, imaging and information processing. By adding a feedback and a fast modulator, mode-locked lasing of SPPs becomes possible. In this contribution, we extend a semiclassical theory of surface plasmon polariton lasers to the case of mode-locked SPP lasers. In the considered scheme feedback is provided by a Bragg reflector of SPPs, and the SPP laser is composed of a metal film deposited on a polymer host as well as a saturable absorber layer and a gain layer. We investigate mode-locking characteristics, such as pulse duration and peak intensity, in dependence on the layer thickness of the metal film and the absorber layer, the pump intensity, and densities of gain and absorber molecules. We consider the dyes R6G as gain and DQOCI as saturable absorber and predict the possibility of SPP pulse generation with maximum peak intensity of more than 500 GW/cm^2 and shortest pulse duration of 280 fs.

DS 37.6 Wed 12:30 WIL A317

Spatiotemporal nanofocusing in random nanostructures achieved by time-reversal, adaptive optimization, and optimal open-loop control of ultrashort laser pulses — •Dominik Differt[1], Javier Garcia de Abajo[2], Christian Strüber[1], Dmitri Voronine[1,3], and Walter Pfeiffer[1] — [1]Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany — [2]Instituto de Optica, CSIC, Serrano 121, 28006 Madrid, Spain — [3]Department of Physics, Texas A&M University, 4242 TAMU, College Station, USA

Because of the reciprocity of electromagnetic wave propagation the time-reversal of a wave emitted from a nanoemitter embedded in a random scattering environment should refocus in space and time at the emitter site. If only partial waves, e.g. one particular planar wave component, of the outgoing wave are time-reversed this nanolocalization of the back-propagated wave is not perfect. Here we investigate the degree of spatiotemporal nanolocalization of time-reversed partial planar waves. The chosen nanostructure consists of two nanoemitter particles embedded in a random assembly of metallic nanospheres acting as scattering environment. A multiple elastic scattering of multipole expansion (MESME) code is used for solving Maxwell's equations in frequency domain. The degree of nanolocalization varies significantly and depends critically on which partial planar wave is time-reversed. In addition, direct adaptive optimization or optimal open-loop control of the spatiotemporal nanofocusing of planar waves at the emitter position exhibits a much higher degree of nanolocalization.

DS 37.7 Wed 12:45 WIL A317

Investigating Ag Nanostructures by TOF-PEEM using High Harmonic Radiation — •Soo Hoon Chew[1], Frederik Süssmann[2], Christian K. Späth[1], Alexander Guggenmos[2], Yingying Yang[2], Jürgen Schmidt[1], Adrian Wirth[2], Sergey Zherebtsov[2], Michael Hofstetter[2], Matthias F. Kling[2], Mark I. Stockman[3], Ferenc Krausz[2], and Ulf Kleineberg[1] — [1]Department of Physics, Ludwig Maximilian University of Munich, Garching, Germany — [2]Max Planck Institute of Quantum Optics, Garching, Germany — [3]Georgia State University, Altanta, USA

We demonstrate first experimental results on imaging plasmonic nanostructures by Time-of Flight-Photoelectron Emission Microscope (TOF-PEEM) in combination with Extreme Ultraviolet (XUV) attosecond pulses from a High Harmonic Generation source. The 1 kHz coherent attosecond XUV radiation is produced by ionizing neon atoms with waveform-controlled near-infrared (0.6 mJ, 5 fs) laser pulses and spectrally filtered at 93 eV by means of a multilayer mirror. We have characterized various polycrystalline Cu microstructures and Ag nanostructures using these ultrashort XUV pulses by TOF-PEEM with a spatial resolution approaching 100 nm. The electron energy spectrum have been investigated at different sample positions and energy filtering has been applied to improve image resolution. The experiments demonstrate first steps towards the temporal characterization of nanoscaled localized surface plasmon fields in a femtosecond optical-pump/attosecond XUV-probe experiments.

DS 38: Plasmonics and Nanophotonics O-V (jointly with HL and O)

Time: Wednesday 15:00–17:00 Location: WIL A317

DS 38.1 Wed 15:00 WIL A317

Optical Nanoantennas for Ultrafast Spectroscopy of Single Nanoparticles — •Thorsten Schumacher[1,2], Daniela Ullrich[1,2], Kai Kratzer[1,2], Mario Hentschel[1,2], Harald Giessen[2], and Markus Lippitz[1,2] — [1]Max Planck Institute for Solid State Research, Stuttgart — [2]4th Physics Institute, University of Stuttgart

Nonlinear spectroscopy investigates the deviations from linear light-matter interaction. The already weak signals are reduced further when single nanoobjects such as quantum dots, molecules, or nanoparticles are investigated. Here, we demonstrate how such an extremely weak nonlinear signal can be enhanced by an optical nanoantenna. For this purpose we use the transient optical response of a mechanically oscillating single gold nanodisc. Our antenna is another gold nanostructure which is placed closely next to the small disc. In this configuration we find a strong plasmonic coupling what can be described by a plasmon hybridization model and numerical simulations. Our calculations show how this plasmonic interaction cause a transfer of the weak nonlinear response of the nanoparticle to the much stronger antenna signal. With ultrafast pump-probe spectroscopy we verify the theoretical predictions and show a measured signal enhancement by a factor of 10, what is in good agreement with our simulations. Finally we can give an outlook for more advanced antenna structures to further increase the enhancement factor.

DS 38.2 Wed 15:15 WIL A317

Connecting antennas, waveguides and couplers in nanoplasmonics — •Arian Kriesch[1,2,3], Jing Wen[1,2], Daniel Ploss[1,2,3], Peter Banzer[1,2], and Ulf Peschel[1,2] — [1]MPI für die Physik des Lichts, Erlangen, Germany — [2]Friedrich-Alexander-Universtität Erlangen-Nürnberg, Erlangen, Germany — [3]Erlangen Graduate School in Advanced Optical Technologies (SAOT)

Subwavelength, plasmonic waveguides open the way to the manipulation of light in photonic circuits at the nanoscale. However, they demand new techniques to efficiently transfer light from the far-field into these highly confined waveguide modes. Recent technological progress has enabled the fabrication of plasmonic metal gap waveguides on dielectric substrates with a width in the range of a few tens of nanometers as well as connected optical nanoantennas by Focussed Ion Beam (FIB) and e-beam lithography. We present experimental measurements of the properties of such waveguides, namely transmission and bend losses, which are compared to Finite Element Method (FEM) calculations.

Our optimized optical antennas (coupling efficiency from the far-field to waveguide ≈ 15%) allow for efficient, selective coupling to single waveguides. Utilizing these antennas together with a setup for high-numerical-aperture focal scanning, we have demonstrated and quantitatively analyzed the coupling between closely adjacent waveguides, thus realizing discrete diffraction and coupling effects in nanoplasmonic waveguide arrays. Efficient optical antennas, low loss bent waveguides and interwaveguide couplers are each a building block in future highly confined plasmonic nanocircuitry.

DS 38.3 Wed 15:30 WIL A317

Spiral Optical Nanoantenna — •Daniel Dregely, Martin Schäferling, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, D-70569 Stuttgart, Germany

Advances in nanofabrication in the past years allowed for adaption of concepts of the radiofrequency and microwave regime to optical wavelengths [1]. Recently, the road has been opened towards more complex antenna geometries suitable for tailoring light emission on the nanoscale [2,3]. Self-complementary structures are commonly used in the high frequency regime to transmit and receive signals over a broad frequency range.

We investigate a self-complementary spiral nanoantenna for the optical wavelength range. The structure has different handedness for opposite incident directions of light. Albeit being planar, its emission cone is normal to the surface. We study experimentally the optical properties in transmission and reflection for circularly polarized light. Numerical simulations confirm our measurements and give insight to the near-field response of our structure.

References:

[1]P. Mühlschlegel et al., Science 308, 1607 (2005)

[2]T. Kosako, Y. Kadoya, and H. F. Hofmann, Nature Photonics 4, 312-315 (2010)

[3]A. G. Curto et al., Science 329, 930-933 (2010)

DS 38.4 Wed 15:45 WIL A317

Plasmonic sensing using multipolar infrared antenna resonances — •Frank Neubrech[1], Daniel Weber[1], Jörg Bochterle[1], Gui Han[2], Tadaaki Nagao[2], and Annemarie Pucci[1] — [1]Kirchhoff-Institute for Physics, Heidelberg University, Germany — [2]National Institute for Materials Science, Tsukuba, Japan

Excited resonantly, antenna-like nanostructures confine the electromagnetic radiation on the nanoscale and therefore enhance the electromagnetic field in their vicinity, which can be exploited for surface enhanced infrared spectroscopy. The only precondition is a good match between the fundamental resonant excitation of the nanoantenna and the vibrational signal of the adsorbate of interest. But not only the near field of the fundamental mode can be used to enhance vibrational signals, but also multipolar modes (l=3, 5, 7) as we will show in this contribution. We performed infrared spectroscopic measurements of nanoantennas supported by a silicon wafer with a natural SiO_2 layer. For parallel polarized light and at a good match of the fundamental resonance mode of the antenna with the SiO_2 phonon, the SiO_2 surface phonon-polariton signal is enhanced. Its line shape reveals a Fano-type interaction with the antenna resonance. Detuning the nanoantenna by increasing its length leads to a decrease of the SiO_2 signal due to the frequency dependence of the antenna resonance. For even longer antennas the SiO_2 signal increases again and reaches a second maximum if the multipolar l=3 excitation of the nanoantenna matches the excitation frequency of the SiO_2 phonon-polariton.

DS 38.5 Wed 16:00 WIL A317

Dispersion engineering in a plasmonic microcavity through mode interaction — •Liwei Fu[1], Heinz Schweizer[1], Thomas Weiss[1,3], Philipp Schau[2], Karsten Frenner[2], Wolfgang Osten[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany — [2]Institut für Technische Optik and Research Center SCoPE, University of Stuttgart, Germany — [3]LASMEA, Université Blaise Pascal, F-63177 Aubière Cedex, France

Microcavities provide the possibility to control and enhance light-matter interaction, which is indispensable for future quantum optical communication [1]. Microcavities with two identical periodically corrugated metallic mirrors supporting surface plasmon polaritons can further confine optical fields into a subwavelength regime. In this report, we demonstrate that mode interactions between surface plasmons and a microcavity mode can be used to tune mode dispersion, which is essential for light matter interaction. We study here numerically how the surface plasmons interact with the cavity modes in both near and far field regimes in a metallic meander cavity via tuning the excitation strength of the surface plasmons [2].

[1] K. J. Vahala, “Optical microcavities,” Nature 424, 839 (2003).

[2] L. Fu, H. Schweizer, T. Weiss, and H. Giessen, “Optical properties of metallic meanders,” J. Opt. Soc. Am. B 26, B111 (2009).

DS 38.6 Wed 16:15 WIL A317

Cavity-enhanced localized plasmonic resonance sensing — •Ralf Ameling, Lutz Langguth, Mario Hentschel, Martin Mesch, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany

We present a method to enhance the sensing properties of a localized plasmon resonance sensor. The concept is based on the combination of localized plasmons in nanostructures and a photonic microcavity. Metal nanorods that are placed at Bragg distance above a metal mirror form a Fabry-Pérot microcavity and constitute a coupled photonic-plasmonic system. The localized plasmon resonances of the nanorods and the phase shifts upon plasmon excitation are extremely sensitive to changes of the refractive index of the material surrounding the nanorods. Compared to the plasmonic nanorods alone, the coupled photonic-plasmonic system allows for a much more sensitive detection of small refractive index changes. We experimentally demonstrate our method with water and glucose solution. Our concept can be applied to many localized plasmonic sensor structures (e.g., colloidal systems such as nanostars) and will considerably increase their sensing properties. Potential applications in the fields of biotechnology, medical diagnostics, or pharmacology including biomolecule detection as well as real-time monitoring of chemical reactions or molecular kinetics might benefit from this concept.

DS 38.7 Wed 16:30 WIL A317

Simulating EELS Spectra using the Discontinuous Galerkin Time Domain Method — •Christian Matyssek[1,2], Jens Niegemann[3], Wolfram Hergert[2], and Kurt Busch[3] — [1]Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany — [2]Institute of Physics, von-Seckendorff-Platz 1, 06120 Halle, Germany — [3]Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology (KIT), D-76128 Karlsruhe, Germany

Electron Energy Loss Spectroscopy (EELS) was recently used to examine single metal nano particles[1] and also systems of particles[2,3]. Frequently, the calculation of these spectra is done in frequency domain, e.g. using the Boundary Element Method[1]. We present the calculation of EEL spectra using the Discontinuous Galerkin Time Domain (DGTD) method, which is well approved in photonics calculations[4]. The numerical results are compared to analytical results that are available for spheres. The influence of substrates on the surface-plasmon excitation is studied. Application of nonlinear material models will be discussed.

[1] Nelayah et al., Nat. Phys. 3, 348 (2007)

[2] Chu et al., Nanotech. 20, 235705 (2009)

[3] Sigle et al., Opt. Lett. 34, 2150 (2009)

[4] Niegemann et al., Phot. and Nanostr. 7, 2 (2009)

DS 38.8 Wed 16:45 WIL A317

Release of the fluorescent dye DAPI via photothermal dissociation of programmable DNA-gold-nanoparticle networks — •Malte Linn[1], Anne Buchkremer[2], Maximilian Reismann[1], Ulrich Simon[2], and Gero von Plessen[1] — [1]Inst. of Physics (IA), RWTH Aachen University, Germany — [2]Institute of Inorganic Chemistry, RWTH Aachen University, Germany

The optical excitation of particle plasmons in gold nanospheres by means of laser light enables a highly localised and contact free heating of the nanoparticles and their immediate surroundings. This effect can be exploited to control temperature-sensitive biochemical reactions. In this work, it is used for the selective release of the DNA-intercalating fluorescent dye 4',6-diamidino-2-phenylindole (DAPI). Here, the release is realized via the photothermal dissociation of networks consisting of DNA-linked gold nanoparticles using focused cw-laser light (532 nm wavelength). Since the DAPI molecules only intercalate into DNA double strands, these molecules are released from the networks due to the photothermal controlled dehybridisation of the DNA into single strands. This process can be spectroscopically observed by measuring the fluorescence intensity, since the fluorescence of DAPI stored in the networks is suppressed by the nearby nanoparticles (fluorescence quenching). By using layer-by-layer networks, consisting of nanoparticles linked by different types of DNA, both a well-defined network structure and a step-by-step release of molecules can be realized. The principle shown here might be the basis for a remote release process of medical agents of future medicines.

DS 39: Organic Electronics and Photovoltaics CPP-IV (jointly with CPP, HL, and O)

Time: Wednesday 14:00–17:00 Location: ZEU 222

Topical Talk DS 39.1 Wed 14:00 ZEU 222

Control of Charge Carrier Dynamics in Disordered Conjugated Polymers — •Dirk Hertel — Physical Chemistry, University of Cologne, Luxemburgerstr. 116, 50939 Cologne, Germany,

We developed a new method to probe charge carrier mobility on ultrafast time scale [1]. It is based on electric field induced second harmonic generation. The method is applied to prototypical amorphous conjugated polymers of the polyphenylene- and polyfluorene-type. Typically the carrier mobility in these organic polymers decreases with time in a power law fashion from about 1 cm^{2}Vs^{-1} at 1 ps to its stationary value of about 10^{-6} cm^{2}Vs^{-1} in hundreds of ns.

The dynamics of the mobility is discussed. It will be shown, that in nanoscale devices the macroscopic mobility is not adequate to describe charge transport. We study the influence of disorder, morphology and temperature on ultrafast transport. At early times the transport is dominated by tunneling [2] and disorder plays already an essential role. Comparison of transient photocurrents with Monte-Carlo simulation reveals that on-chain transport has to be invoked to rationalize our results [3]. The hopping rates for intrachain transport are much larger compared with interchain transport. The results give access to essential transport properties for the development of advanced theoretical models and may help to design improved solar cells.

[1] A. Devižis, et al. *Phys. Rev. Lett.* **103**, (2009) 027404.

[2] A. Devižis, et al. *Phys. Rev. B* **82**, (2010) 155204.

[3] A. Devizis, et al. *Chem. Phys. Lett.* **498**, (2010) 302.

DS 39.2 Wed 14:30 ZEU 222

Light-Emitting Organic Memory — •Peter O. Körner, R. Clayton Shallcross, Vincent Aubert, Eduard Maibach, Philipp Zacharias, and Klaus Meerholz — Department of Chemistry, University of Cologne

We report on light-emitting organic memory (LE-OMEM) devices composed of multiple solution-processed layers. The active layer of our LE-OMEM devices is comprised of crosslinkable dithienylethene photochromes (XDTE) that can be optically switched between two energetically distinct and thermally stable isomers. Exploiting the difference in the HOMO and LUMO levels of these two isomers we use such a layer as an electrical switch within our OLED layer stack. We demonstrate that the ON/OFF ratio in current (OOR$_j$) as well as in electroluminescence (OOR$_L$) of such devices is exponentially dependent on the difference in the largest charge injection barrier between the ON and OFF state of the device. Optimized devices displayed impressive fatigue resistance and afforded values for OOR$_j$ and OOR$_L$ of greater than 10^3. We focus on a variety of crosslinkable DTE molecules of varying structure and functionality with an emphasis on OOR, device stability over multiple read/write/erase cycles (fatigue resistance) and switching rates. Current induced switching allows for electrical writing and reading of grey level information in these XDTE devices. We studied this electrical switching behavior to gain further insight into the distinct switching mechanisms within the XDTE layer. These fundamental studies are a first step towards a completely electrically driven LE-OMEM.

DS 39.3 Wed 14:45 ZEU 222

Determination of the effective radiative quantum efficiency of light-emitting guest-host systems — •Tobias Schmidt[1], Daniel-Steffen Setz[2], Benjamin Lebsanft[1], Thomas Wehlus[1], Jörg Frischeisen[1], Benjamin Krummacher[2], Michael Flämmich[3], Norbert Danz[3], and Wolfgang Brütting[1] — [1]Experimentalphysik IV, Universität Augsburg — [2]OSRAM Opto Semiconductors, Regensburg — [3]Fraunhofer-Institut für angewandte Optik und Feinmechanik (IOF), Jena

The efficiency of organic light-emitting diodes (OLEDs) is still limited as only a small part of the applied electrical power is converted into light and finally extracted from the device to air. Especially the radiative quantum efficiency (RQE) of the used guest-host system is often declared to be unity in phosphorescent emitter/matrix combinations. Due to interference effects, the radiative lifetime of the emitter and thus the effective RQE of the light-emitting guest-host system is influenced by coupling to different modes of the cavity formed by the metallic mirror and the partially reflecting ITO/glass interface. The effective RQE can be determined by measuring the external quantum efficiency of the electrically driven OLED or the photoluminescence lifetime of the emitter inside the OLED at different emitter positions in the cavity. We have investigated the RQE of the commonly used emitter Ir(ppy)$_3$ in neat films with PMMA and CBP as matrices, yielding values of about 70 %, and compare it to OLEDs, where significantly lower values of only 40 % are obtained.

DS 39.4 Wed 15:00 ZEU 222

Exciton quenching in light emitting organic field-effect transistors studied by localized Spectroscopy — •Wouter Koopman, Stefano Toffanin, and Michele Muccini — ISMN-CNR, Via P. Gobetti 101, 40129 Bologna, Italy

The recent development of organic light-emitting transistors (OLETs) promises a new generation of light-emitting organic devices surpassing the efficiency of organic LEDs. The transistor structure prevents non-radiative processes connected to charge-carrier injection as for the ideal OLET the full recombination takes place inside the channel.

In this work we present an investigation of the influence of field-induced quenching on the luminescence intensity in OLETs based on *N,N' ditridecyl-perylene-3,4,9,10-tetracarboxylic diimide* (PTCDI-C13H27) as a model compound. We have used localized photoluminescence and lifetime spectroscopy to study the quenching processes at the electrodes and in the channel region in working devices. Our measurements show a reduction of luminescence intensity up to 20% by applying a forward gate voltage, with a gate field in the order of $1{\times}10^8 Vm^{-1}$. Upon application of a reverse bias a counter-intuitive enhancement of the PL spectrum was found. Excluding polaron-injection by a dielectric barrier, we can identify field induced effects to be responsible for the observed effects.

These results clarify the role of external electric field induced exciton-quenching on the luminescence efficiency of OLETs and establish a bases for the understanding of the limiting processes in more complex devices.

DS 39.5 Wed 15:15 ZEU 222

Triplet Excimer Emission in a Series of CBP-Derivatives — •Sebastian Hoffmann[1], Pamela Schrögel[2], Rodrigo Albuquerque[1], Michael Rothmann[2], Peter Strohriegl[2], and Anna Köhler[1] — [1]Department of Physics, University of Bayreuth, 95440 Bayreuth — [2]Macromolecular Chemistry I, Department of Chemistry, University of Bayreuth, Bayreuth 95440, Germany

Carbazole-based materials such as 4,4*-bis(N-carbazolyl)-2,2*-biphenyl (CBP) and its derivatives are frequently used as matrix materials for phosphorescent emitters in organic light emitting diodes. An essential requirement for such matrix materials is a high energy of their first triplet excited state. Here we present a detailed spectroscopic investigation supported by DFT calculations on two series of CBP derivatives, where CH3 and CF3 substituents introduce strong torsion into the molecular structure. The resulting poor coupling between the two halves of the molecules leads to an electronic structure similar to that of N-phenyl-3,6-dimethyl-carbazole, with high triplet state energy of 2.95 eV. However, we also observe a triplet excimer emission centred at about 2.5-2.6 eV in all compounds. We associate this triplet excimer with a sandwich geometry of neighboring carbazole moieties. For compounds with more polar CF3 substituents, the lifetime of the intermolecular triplet excited state extends into the millisecond range for neat films at room temperature. We attribute this to an increased charge-transfer character of the intermolecular excited state for the more polar substituents. [1] S.T. Hoffmann et al, J. Phys.Chem. B, in press.

15 min. break

DS 39.6 Wed 15:45 ZEU 222

The effect of energetic disorder on the spectral diffusion of singlet and triplet states in phenylene-type polymers — •Anna Köhler[1], Sebastian T Hoffmann[1], Heinz Bässler[1], Jan-Moritz Koenen[2], and Ullrich Scherf[2] — [1]Experimental physics II, Universität Bayreuth — [2]Macromolecular Chemistry, Bergische Universität Wuppertal

We have employed quasicontinuous temperature dependent fluorescence and phosphorescence spectroscopy to monitor the spectral diffusion of singlet and triplet excitons in a series of pi-conjugated polymers.(1) The experimental results are complemented by Monte-Carlo simulations. We investigated (i) how spectral diffusion is controlled by the degree of energetic disorder present in the amorphous film and (ii) how this process depends on the range of the electronic coupling by comparing singlet exciton diffusion via long-range Förster transfer against triplet exciton diffusion by short-range Dexter transfer. For singlets, we find that the fluorescence spectra bear out a bathochromic shift upon cooling the sample down to a critical temperature below which the shift saturates. This bathochromic shift is a signature of spectral relaxation. In contrast we observe a hypsochromic shift of the phosphorescence spectra below a characteristic temperature for triplets in systems with at least moderate energetic disorder. We show that Random-walk theory applied to excitation transport within a Gaussian density-of-states distribution is both necessary and sufficient to rationalize the experimental results in a quantitative fashion. (1) S.T. Hoffmann et al. PRB 81, 115103 (2010)

DS 39.7 Wed 16:00 ZEU 222

Surface Doping of Conjugated-polymer/Insulating-polymer Composite Film for Field-effect-transistor — •Guanghao Lu[1,2], Patrick Pingel[2], Ingo Salzmann[1], Norbert Koch[1], and Dieter Neher[2] — [1]Institut für Physik, Humboldt-Universität zu Berlin, Berlin, Germany — [2]Institut für Physik und Astronomie, Universität Potsdam, Potsdam, Germany

In organic field-effect-transistors, optimized devices are usually achieved at inert environment together with passivated dielectric surface, in order to prevent the possible doping by oxygen or polar groups at dielectric surface. However, in this work, we find that the field-effect properties of poly(3-hexylthiophene)/polystyrene (P3HT/PS) composite can be greatly improved upon surface doping. Upon exposure to air and using oxidablely active dielectric surface, we doped the top surface and bottom surface of P3HT/PS film for top-contact and bottom-contact devices, respectively. The field-effect mobility of these films with only 2-5 wt% P3HT can be enhanced by more than 3 orders, reaching 0.05-0.2 cm2V-1s-1. This phenomenon is strongly contrary to the case of pure P3HT film. We proposed that, for pure P3HT, doping inevitably induces negatively charged sites or charge-transfer complexes, which act as new traps or undesired low energy sites. However, for conjugated-polymer incorporated within insulating-polymer matrix, the interaction between hole and surrounding negative sites is weaker because of the spatial occupation of a-PS among P3HT domains, which largely optimizes the positive aspect of doping and meanwhile restrained its negative role.

DS 39.8 Wed 16:15 ZEU 222

Investigation of single grains in nanoscale P3HT OFETs — •Dileep Dhakal, Steve Pittner, Torsten Balster, and Veit Wagner — School of Engineering and Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen

Regio-regular poly(3-hexylthiophene) (P3HT) has a chain length in the range of several nm up to more than 100 nm, depending on the molecular weight. In addition, the lateral correlation length of 50 nm thick spin-coated P3HT-layers was found to be 150 nm [1] corresponding to the range of structural order within the film. Therefore, the reduction of the channel length L in organic field effect transistors towards the sub-100 nm range will open up the possibility for channels formed by single grains or individual P3HT chains. For this investigation transistor templates on oxidized silicon substrates are prepared by 2 approaches i) by electron beam lithography (EBL) and ii) by metal deposition under defined tilt angle at a preexisting contact edge. The resulting channel length between the source and drain electrode is in the range from 1 μm to 100 nm for EBL and reaches even lower channel sizes using the second approach. At L = 1 μm a mobility of 10^{-2} cm^2/Vs is typically extracted from transfer curve measurements. Without optimization of the gold/P3HT-interface we find a decrease of mobility by more than one order of magnitude for 100 nm devices, which is attributed to an increased influence of the contact resistance. The ratio can be clearly improved by optimizing the interface. [1] B. Gburek and V. Wagner, Org. Electronics 11 (2010) 814.

DS 39.9 Wed 16:30 ZEU 222

The impact of polar bonds on electron transport through self-assembled monolayers — •David A. Egger[1], Ferdinand Rissner[1], Egbert Zojer[1], and Georg Heimel[2] — [1]Institute of Solid State Physics, Graz University of Technology, Austria — [2]Institut für Physik, Humboldt-Universität zu Berlin, Germany

Density functional theory based surface- and transport-calculations are performed to elucidate the role of intra-molecular polar bonds built into self-assembled monolayers (SAMs) sandwiched between two metal electrodes. Conjugated (oligo)phenylene-ethynylenethiols (also known as 'Tour wires') on gold are chosen due to their frequent appearance in past experimental and theoretical studies. Here, we substitute carbon by nitrogen atoms in a systematic way to realize two different molecules with zero dipole moment and virtually identical frontier molecular orbital energies. Despite this similarity in the electronic structure of the isolated species, the charge-transport characteristics of the corresponding SAMs are vastly different. We give a sound explanation for our observations based on an intuitive electrostatic rationale and conclude that the actual orientation of polar bonds in monolayers of preferentially oriented molecules crucially impacts characteristic parameters of molecular electronic devices, such as conductance gap or threshold voltage.

DS 39.10 Wed 16:45 ZEU 222

Photoinduced magnetoresistance in organic field-effect transistors — •Thomas Reichert and Tobat P. I. Saragi — Department of Mathematics and Science and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Strasse 40, D 34132 Kassel, Germany

We report on negative magnetoresistance (MR) in low external magnetic fields in organic field-effect transistors. This effect can only be observed if the device is irradiated. MR strongly depends on gate voltage but is independent of drain voltage. Furthermore, the MR increases as the intensity of irradiation increases and the relationship of both parameters is not linear. The dependency of MR on magnetic field is not linear either, but it follows Non-Lorentian function. The triplet exciton-charge reaction model is a possible explanation for negative MR in irradiated organic field-effect transistors.

DS 40: Organic Electronics and Photovoltaics HL-II (jointly with CPP, HL, and O)

Time: Wednesday 10:15–13:30 Location: FOE Anorg

DS 40.1 Wed 10:15 FOE Anorg

Charge transport and electron trapping in a donor/acceptor-type copolymer — •Marcel Schubert[1], Eduard Preis[2], Ullrich Scherf[2], and Dieter Neher[1] — [1]Universität Potsdam, Institut für Physik und Astronomie, 14476 Potsdam — [2]Bergische Universität Wuppertal, Makromolekulare Chemie, 42119 Wuppertal

Low bandgap polymers are the driving force of the ongoing increase in efficiency of organic solar cells (OSC). Most of them are so called donor/acceptor-type copolymers. The polymer PFTBTT was one of the first of this material class, specially design for use in OSC [1]. It has been successfully incorporated as donor material in combination with soluble fullerenes or as acceptor in all-polymer solar cells.

Here, we present a detailed study of the electron transport properties of PFTBTT. By making use of an ultra thin charge generation layer, we were able to (1) selectively address the charge transport of electrons, (2) perform time-of-flight measurements on samples with less than 200 nm thickness and (3) to combine the time-of-flight and Photo-CELIV technique to investigate charge carrier dynamics. Our measurements proof that PFTBTT is an ambipolar material with a high electron bulk mobility. Furthermore, detailed investigations of the charge carrier dynamics with time-delayed extraction fields revealed a power law-type relaxation of the free electron mobility over two orders in time. These results help to quantify relaxation phenomena reported recently for PFTBTT containing all-polymer solar cells [2].

[1] M. Svensson et al., Adv. Mater. 15, 988 (2003).

[2] C. R. McNeill et al., J. Appl. Phys. 106, 024507 (2009).

DS 40.2 Wed 10:30 FOE Anorg

Investigation of Charge Transfer States in MDMO-PPV:PCBM Solar Cells — •Julia Kern[1], Sebastian Schwab[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Faculty of Physics and Astronomy, Julius-Maximilians-University of Würzburg, Am Hubland, D- 97074 Würzburg — [2]Center for Applied Energy Research (ZAE Bayern e. V.), Am Hubland, D-97074 Würzburg

In recent years, so called charge transfer states (CTS), i.e. interfacial states generated at the donor-acceptor heterojunction in organic solar cells, have attracted a considerable amount of attention and their role in the processes of charge carrier dissociation and recombination has been discussed controversially. In this context, we investigated the photo- (PL) and electroluminescence (EL) originating from blends of MDMO-PPV and various fullerene derivatives. Upon blending donor and acceptor, a peak emerges at the lower energetic side of the pure material excitonic transitions which can be attributed to a CTS. Interestingly, a distinct red shift of this CTS emission is observed between the obtained EL and PL spectra. Furthermore, we studied the influence of temperature and voltage variations on the intensity and spectral shape of the CTS emission.

DS 40.3 Wed 10:45 FOE Anorg

Structure-Property-Relations in PPE-PPV based Polymer Solar Cells — •Christian Kästner[1], Burhan Muhsin[1], Adam Getachew[2], Christoph Ulbricht[2], Özlem Usluer[2], Daniel Ayuk Mbi Egbe[2], and Harald Hoppe[1] — [1]Institute of Physics, Ilmenau University of Technology, Ilmenau, Germany — [2]Linz Institute for Organic Solar Cells, Johannes Kepler University Linz, Austria

Abstract: Photophysical and photovoltaic properties of a series of anthracene-containing and ethylene-3,4-dioxythiophene (EDOT)-containing poly(p-phenylene-ethynylene)-alt-poly(p-phenylene-vinylene)s (PPE-PPV) copolymers with general constitutional units (Ph-C-tC-Anthr-C-tC-Ph-CH-dCH-Ph-CH-dCH-) n and (Ph-C-tC-EDOT-C-tC-Ph-CH-dCH-Ph-CH-dCH-) n have been studied. Mixed linear and branched alkoxy side chains were grafted to the backbone in order to tune the π-π-stacking ability of the materials, which significantly affects their photovoltaic response when used as donor components in a bulk heterojunction construct together with PCBM as acceptor.

DS 40.4 Wed 11:00 FOE Anorg

Morphological aspects of the exciton transport in molecular thin films — •A.K. Topczak[1], T. Roller[2], and J. Pflaum[1,3] — [1]Inst. Exp. Phys. VI, Würzburg University, 97074 Würzburg — [2]3rd Phys. Inst., Stuttgart University, 70550 Stuttgart — [3]ZAE Bayern, 97074 Würzburg

The exciton diffusion length is a key criteria to optimized design of organic thin film photonic devices. This optimisation requires fundamental understanding and control of the excitonic transport. It has been proposed that exciton transport should depend on the extension of crystalline domains [1]. Therefore we performed photoluminescence-quenching measurements to compare the exciton diffusion length (EDL) of the three archetypical semiconductors Diindenoperylene (DIP), Sexithiophene (α-6T) and tris-8-hydroxyquinolate-aluminum (Alq$_3$) and to link this quantity to the polycrystalline structure. A correlation between the exciton transport and the crystalline morphology is demonstrated. Long-range ordered thin films of DIP and α-6T show a high EDL. For these films the necessity of taking interference effects into account for a precise modeling became evident. In comparison, amorphous films of Alq$_3$ showed an EDL which is significantly smaller. We will elucidate the microscopic transport mechanisms and their respective energies by means of temperature dependent measurements. From our results, conclusions on the cell design of planar heterojunction thin film cells can be drawn. Financial support by the DFG (project PF385/4) is gratefully acknowledged. [1] D. Kurrle, J. Pflaum, Appl. Phys. Lett.92 (2008) 133306

DS 40.5 Wed 11:15 FOE Anorg

Electronic Trap States in Methanofullerenes and their Influence on Organic Solar Cells — •Julia Schafferhans[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Physical Institute, Julius-Maximilians University of Würzburg, Am Hubland, D-97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern e.V.), Am Hubland, D-97074 Würzburg, Germany

Methanofullerenes are the most commonly used electron acceptors in organic bulk heterojunction solar cells, due to their advantages that they can be easily processed from solution, possess a high electron affinity and form segregated phases in blends with common donor polymers.

Although trap states can have a significant impact on the performance of organic solar cells, as they can act as recombination centers, lower the mobility and disturb the internal field distribution, the traps in methanofullerenes have not been matter of research so far.

We investigated the trap states of three commonly used fullerene derivatives, namely PC$_{61}$BM, PC$_{71}$BM and bisPC$_{61}$BM, by thermally stimulated current measurements. Each of the studied methanofullerenes exhibit a broad trap distribution, whereby the PC$_{71}$BM and bisPC$_{61}$BM reveal significantly deeper traps compared to PC$_{61}$BM. These findings will be discussed with respect to the solar cell performance.

DS 40.6 Wed 11:30 FOE Anorg

Luminescence imaging of polymer solar cells: visualization of progressing degradation — Marco Seeland, •Roland Rösch, and Harald Hoppe — Institute of Physics, Ilmenau University of Technology, Ilmenau, Germany

We apply luminescence imaging as tool for the non-destructive visualization of degradation processes within bulk heterojunction polymer solar cells. The imaging technique is based on luminescence detection with a highly sensitive silicon-ccd camera and is able to visualize the with time advancing degradation patterns of polymer solar cells. The devices investigated have been aged under defined conditions and were characterized periodically with current-voltage-sweeps. This allows determining the time evolution of the photovoltaic parameters and - in combination with the luminescence images - understanding differences in the observed degradation behaviour. The versatile usability of the method is demonstrated in a correlation between local reduction of lateral luminescence and a fast decrease of the short-circuit-current due to the loss of active area. Differences in the degradation of photovoltaic parameters under varied aging conditions are discussed.

15 min. break

DS 40.7 Wed 12:00 FOE Anorg

Quantitative Description of Electroluminescence Images of Polymer Solar Cells — •Marco Seeland, Roland Rösch, and Harald Hoppe — Institute of Physics, Ilmenau University of Technology, Ilmenau, Germany

We present a quantitative description of electroluminescence images obtained on organic solar cells, which is based on a device modeling employing a network of interconnected microdiodes. The equivalent circuit network model takes interface and bulk resistances as well as the sheet resistance of the transparent electrode into account. The application of this model allows direct calculation of the lateral current and voltage distribution as well as determination of internal resistances and the sheet resistance of the higher resistive electrode. Furthermore, we have extended the microdiode-model to also describe and predict current voltage characteristics for devices under illumation. Finally the local nature of this description enables important conclusions concerning the geometry dependent performance of thin film solar cells.

DS 40.8 Wed 12:15 FOE Anorg

Investigation of Field-dependent Charge Carrier Generation and Recombination in Polymer Based Solar Cells by Transient Extraction Currents — •Juliane Kniepert, James Blakesley, and Dieter Neher — University of Potsdam, Germany

There is an ongoing discussion as to whether photoinduced charge transfer in P3HT:PCBM solar cells leads to fully separated electrons and holes, independent of an electric field, or Coulombically bound interfacial charge pairs. While recent studies by R.A. Marsh et al. with transient absorption spectroscopy gave clear evidence for the formation and field-induced dissociation of bound polaron pairs, measurements by I.A. Howard et al. were in favour of hot exciton dissociation. Here, we present the results of bias-dependent Time Delayed Collection Field (TDCF) measurements to access directly the density of free charge carriers in P3HT:PCBM blends coated from dichlorobenzene. Solvent annealing was applied to yield a phase-separated morphology and the corresponding solar cells exhibit high values for the external quantum efficiency and fill factor. Our setup allowed us to follow the generation and recombination of photogenerated charges with a so far unattained time resolution of 40 ns. Our experiments show that the number of collected carriers is independent of the applied bias during pulsed illumination implying that extractable carriers in P3HT:PCBM blends are not generated by the field-assisted separation of bound polaron pairs. In addition, our experiments support the view that bimolecular recombination of free carriers is strongly suppressed in phase-separated P3HT:PBCM blends.

DS 40.9 Wed 12:30 FOE Anorg

Influence of phase separation on the recombination dynamics of trapped charges in disordered organic semiconductors — •Julien Gorenflot[1], Matthias Gunz[1], Andreas Kämpgen[1], Jens Lohrmann[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius-Maximilians University, D-97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), D-97074 Würzburg

Using a combination of steady-state and transient photoinduced absorption, we explore the recombination of polarons in pristine poly(3-hexylthiophene) (P3HT) as well as in its blend with [6,6]-phenyl-C61 butyric acid methyl ester(PCBM). Interestingly those two systems behave very differently with a recombination order of two for pure P3HT which contrasts with the much higher apparent order in the blend. We explain those results in terms of trap induced delay in the blend where energetically trapped polarons can be unavailable for recombination due to phase separation. We determine the activation energy of the bimolecular recombination in pure P3HT. Our results show that the polaron recombination is caused in both neat polymer and blend by intermolecular rather than intramolecular charge transport.

DS 40.10 Wed 12:45 FOE Anorg

Determination of the built-in voltage of BHJ solar cells by temperature dependent photocurrent measurements — •Markus Mingebach[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Physical Institute, Julius-Maximilians-University of Würzburg, Am Hubland, D-97074 Würzburg — [2]Bavarian Center of Applied Energy Research (ZAE Bayern e. V.), Am Hubland, D-97074 Würzburg

Despite all progresses in the performance of organic BHJ solar cells (up to 8% power conversion efficiency) some very important properties such as the voltage dependent photocurrent or the built-in potential are not fully understood yet. We investigate poly(3-hexyl thiophene) (P3HT) : [6,6]-phenyl-C_{61} butyric acid methyl ester (PCBM) solar cells by means of temperature dependent pulsed photocurrent measurements and impedance spectroscopy. We find a point of optimal symmetry (POS) that represents the case of quasi flat bands (QFB) in the bulk of the cell, which is lower than the built-in voltage. [1] This difference is due to band bending at the contacts, which is reduced at lower temperatures. Therefore we can identify the built-in voltage by measuring the POS (confirmed by temperature dependent current voltage measurements). This leads to the conclusion that the potential determined by Mott-Schottky analysis is not the built-in potential.

[1] M. Limpinsel, A. Wagenpfahl, M. Mingebach, C. Deibel and V. Dyakonov, Phys. Rev. B 81, 085203 (2010).

DS 40.11 Wed 13:00 FOE Anorg

Charge Transport and Recombination Dynamics in Oxygen Exposed P3HT:PCBM Bulk Heterojunction Solar Cells — •Alexander Foertig[1], Andreas Baumann[1], Julia Schafferhans[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Physical Institute, Julius-Maximilians-University of Würzburg, Am Hubland, D-97074 Würzburg — [2]Bavarian Centre for Applied Energy Research (ZAE Bayern e.V.), Am Hubland, D-97074 Würzburg, Germany

The effect of synthetic air exposure on the charge transport and recombination dynamics in poly(3-hexyl thiophene)(P3HT):[6,6]-phenyl-C_{61} butyric acid methyl ester (PCBM) bulk heterojunction solar cells was studied using the complementary measurement techniques of (photogenerated) charge carrier extraction by linearly increasing voltage (photo-CELIV) and transient photovoltage (TPV) and transient photocurrent (TPC). An additional extraction peak appeared in the photo-CELIV transient at larger extraction fields, which is assigned to a field dependent release of previously trapped charge carriers. The complementary techniques consistently revealed an increased charge carrier density and reduced recombination with exposure time to oxygen which we attribute to delayed release from oxygen induced traps and therefore reduced recombination.

DS 40.12 Wed 13:15 FOE Anorg

Charge transport measurements by transient techniques and their detailed evaluation — •Jens Lorrmann[1], David Vocke[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Physical Institute, Julius-Maximilian-University of Würzburg — [2]Bavarian Center for Applied Energy Research e.V. (ZAE Bayern e.V.), Würzburg

The charge carrier transport in pristine poly(3-hexyl thiophene-2,5-diyl) (P3HT) of different regioregularities and in blends with [6,6]-phenyl-C_{61} butyric acid methyl ester (PCBM) was investigated by time-of-flight measurements (TOF). We investigate the field and temperature dependence of hole and electron mobilities down to temperatures of 130 K in order to understand the effects of the transport on the solar cell efficiency. The results from the TOF measurements are compared with the outcome of complementary methods like charge extraction by linearly increasing voltage (CELIV) and field effect transistor measurements. We calculate the disorder parameters from the temperature and field dependencies of the charge mobility using a Gaussian disorder transport formalism. Furthermore, we present the detail evaluation of TOF current transients with an improved method by Scott et al. [1], which provides explicit distributions of the transit times and the mobilities instead of discrete values.

[1] J.C. Scott, L.T. Pautmeier and L.B. Schein, *Mean mobilities of charge carriers in disordered media*, Phys. Rev. B 46:8603, 1992

DS 41: Organic Electronics and Photovoltaics HL-III (jointly with CPP, HL, and O)

Time: Wednesday 18:00–19:30 Location: FOE Anorg

DS 41.1 Wed 18:00 FOE Anorg

Band bending and energy-level alignment in organic semiconductors — Ilja Lange[1], James Blakesley[1], Johannes Frisch[2], Norbert Koch[2], and •Dieter Neher[1] — [1]Universität Potsdam — [2]Humboldt Universität Berlin

Energy level alignment at organic semiconductor / electrode interfaces has been the subject of intensive debate in recent years. In particular, the existence of band bending in undoped organic semiconductors is disputed. It has been proposed that strong band bending should be present due to electronic states within the energy gap of a disordered material. It is also known that such states dominate some crucial properties of organic semiconductor devices, such as charge injection and charge transport. Thus the elucidation of the distribution of these tail states provides a key to understanding fundamental processes in such devices and hence to increasing device efficiency. Unfortunately, the densities of the relevant states are often so low that they are difficult to detect directly. We use a Kelvin probe (KP) to study the energy level alignment of four undoped conjugated polymers deposited on various electrodes. Band bending is observed in all polymers when the substrate work function exceeds certain critical values. Through modeling, we show that the band bending is caused by charge transfer into a low-density population of states that extends several hundred meV into the band gap. KP can therefore be used as a tool to study the energetic distribution of such states. The energetic spread of these states is correlated with charge transport properties, suggesting that these states also determine relevant device properties.

DS 41.2 Wed 18:15 FOE Anorg

Optical Processes in OLEDs: Molecular Photonics — •Michael Flämmich, Dirk Michaelis, and Norbert Danz —

Fraunhofer Institute for Applied Optics and Precision Engineering, 07745 Jena, Germany

Following the OLED display market take-off, huge world wide efforts are spent to develop OLEDs towards competitive sources for general lighting applications. In this context, the light outcoupling problem is well known as the key parameter to improve OLED efficiency in order to tackle existing lighting schemes. From the optical point of view, the device performance is driven (i) by the architecture of the OLEDs layered system and (ii) by the internal features of the emissive material. Studies in recent years have shown that the latter attributes (which are the internal electroluminescence spectrum, the profile of the emission zone, the orientation of the transition dipole moments and the internal luminescence quantum efficiency q) can be determined in situ by measurements of the far-field emission pattern generated by active OLEDs (i.e. in electrical operation) and corresponding optical reverse simulations. Starting from basic considerations of the dipole radiation characteristics, we elaborate specifically how the orientation distribution of the dipole transition moments in the layered system can be analyzed in situ, providing insight into the internal photo-physical processes on the molecular scale of the emitter.

DS 41.3 Wed 18:30 FOE Anorg

Stability of Polarization in Organic Ferroelectric Metal-Insulator-Semiconductor (MIS) Structures — •Rene Kalbitz[1], Peter Frübing[1], Reimund Gerhard[1], and Martin Taylor[2] — [1]Department of Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Straße 24-25, 14476, Potsdam, Germany — [2]School of Electronic Engineering, Bangor University, Dean Street, Bangor Gwynedd, LL57 1UT, UK

Ferroelectric field effect transistors (FeFETs) offer the prospect of an organic-based memory device. Since the charge transport in such devices is confined to the interface between the insulator and the semiconductor, the focus of the present study was on the investigation of this region. Capacitance-voltage (C-V) measurements of all-organic MIS devices with poly(vinylideneflouride- trifluoroethylene) (P(VDF-TrFE)) as gate insulator and poly(3-hexylthiophene)(P3HT) as semiconductor were carried out. When the structure was driven into depletion, a positive flat-band voltage shift was observed arising from the change in polarization state of the ferroelectric insulator. When driven into accumulation, the polarization was reversed. It is shown that both polarization states are stable. However, negative charge trapped at the interface during the depletion cycle masks the negative shift in flat-band voltage expected during the sweep to accumulation voltages. Measurements on P(VDF-TrFE)/P3HT based FeFETs yield further evidence for fixed charges at the interface. Output characteristics suggest the injection of negative charges into the interface region when a depletion voltage is applied between source and gate contact.

DS 41.4 Wed 18:45 FOE Anorg

Ambipolar organic field-effect devices using an aliphatic passivation layer — Michael Kraus, Matthias Horlet, Simon Haug, Stefan Richler, Wolfgang Brütting, and •Andreas Opitz — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

In recent years electron and hole transport has been found to be an intrinsic feature for many organic semiconductors. The charge carrier type depends thereby on the injecting electrodes and the presence of interface traps.

In this contribution we demonstrate the application of the insulating long-chain alkane $C_{44}H_{90}$ tetratetracontane (TTC) as passivation layer, which has been shown to be highly suitable for the elimination of electron traps [1]. The analysis of its growth behaviour on silicon dioxide and of the subsequently deposited organic semiconductor will be shown for different molecular semiconductors like copper-phthalocyanine and diindenoperylene. The charge carrier transport in these semiconductor layers was analysed using top contact organic field-effect transistors. Thereby an asymmetry between electron and hole mobilities was found with diindenoperylene showing the better electron transport whereas copper-phthalocyanine has balanced mobilities at room temperature. The growth of the phthalocyanine gives crystalline needles up to 500 nm in length which improves the transport properties.

[1] M. Kraus et al., J. Appl. Phys. 107, 094503 (2010).

DS 41.5 Wed 19:00 FOE Anorg

Electrolyte-gated organic thin-film transistors for sensing applications — •Felix Buth, Deepu Kumar, Martin Stutzmann, and José Antonio Garrido — Walter Schottky Institut, Technische Universität München, Garching, Germany

Organic thin films can potentially be used in low-cost, disposable devices for chemical or bio-sensing. However, operating organic sensor devices in an aqueous environment raises difficulties when it comes to necessary operation voltages or device stability. One approach to reduce the gate voltage is increasing the capacitance of the gate dielectric. Electrolytic gates offer extraordinarily large capacitances, up to several $\mu F/cm^2$ at low frequencies. This high capacitance, which is the result of the formation of an electrical double layer at the electrolyte/semiconductor interface makes low-voltage operation possible, without high production costs. In this contribution, we investigate the behavior of polycrystalline α-sexithiophene (α6T) thin-film transistors with an aqueous electrolyte gate. Electrochemical impedance spectroscopy and CV measurements indicate a nearly perfectly polarizable interface with negligible parasitic Faradaic currents. For gate voltages below 1 V, a conductive channel is induced at the α6T/electrolyte interface via an electrical field effect. The transistor is stable for several hours and sensitive to changes in the pH or the ionic strength of the solution. The pH sensitivity arises from a shift in the threshold voltage of the transistor, and is not due to changes of the carrier mobility. The pH-dependent threshold voltage shift, in the range of 10 mV/pH, is caused by a change in the surface charge of the thin film.

DS 41.6 Wed 19:15 FOE Anorg

the origin of the short channel effect in organic field effect transistor. — •Ali Veysel Tunc[1], Elizabeth von Hauff[1], Ahmet Lütfi Ugur[2], Ali Erdogmus[2], and Jurgen Parisi[1] — [1]University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory (EHF) Carl-von-Ossietzky Str.9-11, 26129 Oldenburg, Germany — [2]Yildiz Technical University, Department of Chemistry, Davutpasa Campus, 34210 Esenler, Istanbul, Turkey

The origin of the short channel effect in polymer-based field effect transistors (FETs) was investigated. Here, we employed three different molecular weight poly [2-methoxy,5-(3',7'-dimethyl-octyloxy)]-p-phenylene vinylene (MDMO-PPV) and in blends with different ratios of 1-(3-methoxycarbonyl) propyl-1-phenyl[6,6]C61 (PCBM). In this work we demonstrate that the short channel effect is not only influenced by the device geometry but there is also a correlation between intrinsic material properties, the hole current, field effect mobility, contact resistance and short channel behavior in PPV based OFETs. Intrinsic properties, mobility or molecular weight, of the semiconductor influence the onset of the short channel effect. We observed that increasing the PCBM content in the blend leads to an increase in the hole current and field effect mobility, a decrease in the contact resistance, as well as a deviation from the saturation behavior of the output characteristics of the FET. This effect is attributed to a change in the polymer chain ordering in the source channel which in turn influences the charge transport properties in the polymer film.

DS 42: Poster I: Progress in Micro- and Nanopatterning: Techniques and Applications (jointly with O); Spins in Organic Materials; Ion Interactions with Nano Scale Materials; Organic Electronics and Photovoltaics; Plasmonics and Nanophotonics (jointly with HL and O); High-k and Low-k Dielectrics (jointly with DF); Organic Thin Films; Nanoengineered Thin Films; Layer Deposition Processes; Layer Properties: Electrical, Optical, and Mechanical Properties; Thin Film Characterisation: Structure Analysis and Composition; Application of Thin Films

Time: Wednesday 15:00–17:30 Location: P1

DS 42.1 Wed 15:00 P1

Self-organized surface patterns on Si by sputter erosion with molybdenum surfactants — Kun Zhang, •Andre Pape, Marc Brötzmann, and Hans Hofsäss — II. Physikalisches Institut, Universität Göttingen,37077 Göttingen, Germany

We report on the self-organized pattern formation on Si surfaces driven by Mo surfactant atoms. Si substrates were irradiated with 5 keV Xe ions at normal and near normal ion incidence and fluences up to 5x10^{17} Xe^{+}/cm^{2} under continuous deposition of Mo surfactant atoms. In the absence of Mo deposition uniform flat surfaces are obtained. With Mo surfactants pronounced patterns like dots, combinations of dots and ripples as well as ripples with about 100 nm wavelength and up to 12 nm in height are generated. The patterns are analyzed with atomic force microscopy, Rutherford backscattering and transmission electron microscopy. We analyze the critical Mo steady-state coverage for onset of dot formation and onset of ripple formation and the evolution of the pattern contrast with increasing ion fluence. Pattern formation is explained by ion induced diffusion and phase separation of an initially flat amorphous Mo$_x$Si layer and subsequent ion beam erosion with composition dependent sputter yield. Directed deposition of Mo causes preferential deposition and shadowing and determines the final pattern orientation and morphology.

DS 42.2 Wed 15:00 P1

Functionalization of oxide and oxide-metallic nanowire arrays — •Anshuma Pathak[1,2], Hongdan Yan[1], Johannes Dühn[1], Mehmet Fatih Cetin[1], Meinhard Schilling[3], Marc Tornow[2], and Peter Lemmens[1] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]IHT, TU-BS, Braunschweig, Germany — [3]EMG, TU-BS, Braunschweig, Germany

We investigate the functionalization of single crystalline, nanocrystalline and nanoporous Al$_2$O$_3$ surfaces as a coupling enabler to different molecular species. Our aim is to establish nanostructured, composite oxide-molecular materials that can be used as model systems for optically induced energy transfer. Nanoporous oxides are prepared using electrochemical oxidation leading to a dense array of pores. The pore walls are functionalized and in a subsequent step filled by Au wires using electrochemical deposition techniques. The characteristic length scales of the arrays are 20-30 nm with respect to diameter and distance of the pores. Specifically, we investigate the impact of different organic monolayer coatings to the pore walls on the growth and morphology of the Au nanowires.

Work supported by IGSM and NTH.

DS 42.3 Wed 15:00 P1

Surfactant assisted ion beam erosion of GaN and AlN surfaces — •Kun Zhang[1], Ulrich Vetter[1], Nils Borth[1], Hans-Gregor Gehrke[1], Ramasamy Jayavel[2], and Hans Hofsäss[1] — [1]II. Physikalisches Institut, Universität Göttingen, 37077 Göttingen, Germany — [2]Centre for Nanoscience and Technology, Anna University Chennai, 600025 India

We investigate the evolution of the surface morphology of AlN and GaN surfaces during ion beam erosion. AlN and GaN films grown on sapphire substrates were irradiated at room temperature with few keV Xe ions at normal ion incidence with ion fluences up to 4*10^{17} cm^{-2}. The surface morphology was analyzed using atomic force microscopy and scanning electron microscopy. For GaN selective sputtering causes segregation of Ga on the surface, resulting in a dense coverage with small spherical Ga droplets. With increasing ion fluence the droplet size increases. The Ga coverage was quantitatively analyzed with SEM and Rutherford backscattering. For AlN, the rms roughness of the surface decreases with increasing ion fluence from initially 8 nm to about 3 nm at 4*x10^{17} cm^{-2}. No ripple or dot patterns were observed. Sputtering of AlN with simultaneous co-deposition of Ga, results in the formation of randomly distributed small Ga droplets and Al$_{0.8}$Ga$_{0.2}$ islands of few nm in size on the AlN surface. The rms roughness of such a surface is only about 1.3 nm. The density of droplets and islands decreases with increasing ion fluence. In the intermediate regions the AlN surface appears rather flat with rms roughness well below 1 nm.

DS 42.4 Wed 15:00 P1

Selective surface modification of silicon oxide by OTS — •Christian Belgardt[1], Thomas Baumgärtel[1], Thomas Blaudeck[2], Harald Graaf[1], Reinhard R. Baumann[2], and Christian von Borczyskowski[1] — [1]Center for Nanostructured Materials and Analytics (nanoMA), Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — [2]Institute for Print and Media Technology (pmTUC), Chemnitz University of Technology, 09107 Chemnitz, Germany

The key material of electronics is silicon oxide. The chemical modification of its surfaces by self-assembled monolayers (SAMs) is a well-known method to control their physico-chemical properties. SAMs are typically formed by chemical reaction of the constituting molecules with the surface. The common process to prepare highly ordered monolayers is a chemical bath of a silane solution e.g. octadecyltrichlorosilane (OTS).

We report on hydrophobic OTS monolayers formed by standard method from chemical bath and by ink-jet printing which is known as a purely additive dynamic method and scalable technology. Our results indicate that a structured hydrophobization of the silicon oxide surface by inkjet printing is possible using OTS diluted in toluene at millimolar concentrations. The SAM formation is seems to be governed by an evaporation-driven self-assembly of the OTS molecules on the surface.

DS 42.5 Wed 15:00 P1

Influence of process and system parameters on the local oxidation of alkyl-terminated silicon — •Thomas Baumgärtel, Harald Graaf, and Christian von Borczyskowski — Center for Nanostructured Materials and Analytics, Institut für Physik, TU Chemnitz, 09107 Chemnitz, Germany

The local anodic oxidation (LAO) of silicon substrates by an atomic force microscope (AFM) is an electrochemical process which is influenced by multiple parameters. These can be divided into two major groups: system parameters and process parameters. Process parameters such as oxidation voltage, duration and ambient humidity can be tuned over a wide range of values during the experiment. System parameters on the other hand depend on equipment and materials themselves and are only difficult to control e.g. AFM tip shape, substrate conductivity and surface hydrophobicity. We investigated the influence of these parameters on the LAO process of silicon which is passivated by a self-assembled alkyl monolayer. Such monolayers are not only characterized by high molecular order and an excellent physical and chemical stability but offer also a neat way to tune the surface properties by variation of the head groups of the alkenes. A detailed understanding of the dependencies of the LAO process is essential for the controlled generation of silicon oxide nanostructures which can be used to build up functional nanostructures by a combined bottom-up (anchoring of functional molecules) and top-down (AFM LAO lithography) approach.

DS 42.6 Wed 15:00 P1

Permanent bending and alignment of ZnO nanowires — •Christian Borschel[1], Susann Spindler[1], Damiana Lerose[2,3], Arne Bochmann[3], Silke H. Christiansen[3,4], Sandor Nietzsche[5], Michael Oertel[1], and Carsten Ronning[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena — [2]MPI für Mikrostrukturphysik, Weinberg 2, 06120 Halle (Saale) — [3]Institut für Photonische Technologien, Albert-Einstein-Strasse 9, 07745 Jena — [4]MPI für die Physik des Lichts, Günther-Scharowsky-Str. 1, 91058 Erlangen — [5]Zentrum für Elektronenmikroskopie, Friedrich-Schiller-Universität Jena, Ziegelmühlenweg 1, 07743 Jena

Ion beams can be used to bend or re-align nanowires permanently, after they have been grown. We have irradiated ZnO nanowires with ions of different species and energy, achieving bending and alignment in various directions. We study the bending of single nanowires as well as the simultaneous alignment of large ensembles of ZnO nanowires in detail. Computer simulations show that the bending is initiated by ion beam induced damage. Dislocations are identified to relax stresses and make the bending and alignment permanent and resistant against annealing procedures.

DS 42.7 Wed 15:00 P1

Investigation of conducting nanostructures on ta-C films made by FIB lithography — •Peter Philipp and Lothar Bischoff — Institute of Ion Beam Physics and Materials Research, Helmholtzzentrum Dresden-Rossendorf, P.O. Box 51 01 19, 01314

Dresden, Germany

Tetrahedral amorphous carbon (ta-C) films with high sp^3 content produced by mass filtered vacuum arc deposition were modified by Ga$^+$ FIB irradiation. Surface swelling occurs as a function of fluence, caused by ion induced conversion of sp^3 to sp^2 hybridized carbon atoms. A model [1] for diamond swelling was applied to ta-C films to estimate the swelling for fluences up to 1 x 10^{16} cm^{-2}. For higher fluences data from TRIDYN simulations were included due to sputtering in a good agreement with the experiments. Van der Pauw structures were produced by means of Ga$^+$ FIB lithography. A decrease of the sheet resistance with increasing fluence due to the evolution of graphitic regions was observed. The lowest value of 290 $\Omega/\square$ was achieved at 1.6 x 10^{17} cm^{-2}. Additionally, conducting graphitic wires were produced (length: 10 μm, width: 300 nm to 5 μm). The wire resistivity was measured within 130 kΩ (5 μm width) and 0.3 GΩ (300 nm width). Ion induced graphitization of ta-C films by FIB offers prospective applications in nano technology to fabricate conductive nanostructures in an insulating thin film. [1] F. Bosia et al. Nucl. Instrum. Meth. B 268 (2010) 2991.

DS 42.8 Wed 15:00 P1

investigation of the depth profile of ion beam induced nanopatterns on Si with simultaneous metal incorporation — •Behnam Khanbabaee[1], Bahia Arezki[1], Andreas Biermanns[1], Marina Cornejo[2], Frank Frost[2], and Ullrich Pietsch[1] — [1]Festkörperphysik, Universität Siegen, Siegen, Germany — [2]Leibniz-Institut für Oberflächenmodifizierung (IOM), Leipzig, Germany

Ion beam sputtering of semiconductor surfaces can modify the surface and produce a diversity of surface topographies such as periodic ripples or dot structures depended on sputtering parameters. Well ordered nanostructured surfaces have widely technological applications. Recent experiments have shown that the incorporation of metallic impurity atoms during the sputtering process plays a crucial role in pattern formation on the surfaces. These findings offer a new degree of freedom to control pattern formation. In this contribution we report on surface patterning due to Kr ion beam erosion on silicon surfaces with simultaneous Fe and Cr incorporation. We used X-ray reflectivity (XRR) to determine the depth profiles of metal ions as function of ion beam divergence angles and the mean incidence angle of the ions with respect to the surface normal. Depth profiles are correlated with degree of pattern formation determined by AFM. We show that the mean penetration depth and concentration of metal ions depends on the divergence angle of Kr beam provided by Kaufman source which supports the assumption that metal ions are created due to parasitic interaction of the Kr beam with the steel plate lining. The evaluated depth profile by XRR is in good agreement with SIMS and RBS results.

DS 42.9 Wed 15:00 P1

Freestanding Si nanowires fabricated by Ga$^+$ FIB implantation and subsequent anisotropic etching — •Roman Böttger[1], Lothar Bischoff[1], Bernd Schmidt[1], and Matthias Krause[1,2] — [1]Helmholtzzentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, POB 510119, 01314 Dresden, Germany — [2]Technische Universität Dresden, Institut für Festkörperphysik, Zellescher Weg 16, 01062 Dresden, Germany

Localized Ga$^+$ ion implantation in silicon-on-insulator substrates (top layer 2 μm) by focused ion beam and subsequent anisotropic and selective wet etching has been used to fabricate freely suspended nanowires with reproducible widths between 20 and 200 nm. The dependence of the resulting nanowire width on the implanted fluence has been investigated and is supported by a numerical model reproducing the experimental data and enabling an a priori estimation of the nanowire width as a function of the implanted fluence. Moreover, the temperature dependence of the nanowires resistivity and the activation energy for electrical current flow were investigated before and after direct current annealing in air and in vacuum ambient. Annealed nanowires showed a decrease of their resistivity up to two orders of magnitude, indicating a partial recrystallization of the nanowires through self-heating and a change in the conduction mechanism. The assumption of recrystallization is supported by scanning electron microscopy and Raman spectroscopy. The comprehension of the pinpointed fabrication of such Si nanostructures establishes a broad range of application in the field of nano-electro-mechanical systems.

DS 42.10 Wed 15:00 P1

Nano Structure Formation on the Surfaces of SrTiO$_2$ and BaF$_2$ Induced by Impact of Slow Highly Charged Ions — •René Heller, Ayman S. El-Said, Richard A. Wilhelm, and Stefan Facsko — Helmholtz-Zentrum Dresden Rossendorf, Bautzner Landstr. 400, 01328 Dresden, Germany

The interaction of slow highly charged ions with solid surfaces with particular interest on the nano structure formation ability was investigated intensively within the last years. The rapid release of the HCI's potential energy as a unique feature of this kind of projectiles can cause local energy densities at the surface which are comparable to those induced by ultra short laser pulses or swift heavy ions.

Thus HCI give strong rise to be a promising tool for nano structure formation on solid surfaces. Since the potential energy release is strongly restricted to the surface proximity the amount of damage created in the bulk can be strongly suppressed.

In recent time the authors spend much effort in the exploration of the microscopic mechanisms of HCI nano structure creation on the surfaces of the alkali halide KBr and the earth alkali halide CaF$_2$, respectively. Motivated by the promising results and the predictions of the developed models we extended our investigation to the surfaces of SrTiO$_2$ as well as of BaF$_2$.

The results of these measurements are presented and discussed in the present contribution.

DS 42.11 Wed 15:00 P1

Electron exchange in a heterocycle-bridged biferrocene mixed-valence compound — •Nicolas Yèche[1], Yulia Krupskaya[2], Alexander Hildebrandt[3], Hans-Henning Klauss[1], Vladislav Kataev[2], and Heinrich Lang[3] — [1]Institut für Festkörperphysik ,TU Dresden — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden — [3]Institut für Chemie, TU Chemnitz

Symmetrical systems comprising two or more metallocene units sometimes present interesting reduction and oxidation behavior: each of the metallocene unit can be separately oxidized/reduced, giving rise to intermediate valence compounds called "mixed valence" compounds. We present electrochemistry, magnetization, ESR and ^{57}Fe mössbauer spectroscopy measurement of a phenylpyridine bridged biferrocene compound in the mixed valence Fe(II)-Fe(III) state comparing it to normal Fe(II)-Fe(II) state. Resonance forms are observed in mössbauer spectroscopy at room temperature which indicates that the rate of the change between the Fe(II)-Fe(III) state and the Fe(III)-Fe(II) state is greater than 10^{-7}s. Further results and comarative analysis will be discussed.

DS 42.12 Wed 15:00 P1

Energy dependent spin scattering at a hybrid metal-organic interface — •Torsten Methfessel[1], Sabine Steil[2], Nicolas Grossmann[2], Kathrin Koffler[2], Martin Aeschlimann[2], Mirko Cinchetti[2], and Hans-Joachim Elmers[1] — [1]University of Mainz, Institute of Physics, D-55128 Mainz,Germany — [2]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany

In order to exploit the great potential of hybrid organic-inorganic interfaces for spintronics applications [1], fundamental knowledge about their spin-dependent properties is essential [2, 3]. We investigated the iron-copper phthalocyanine (CuPc) interface by means of spin polarized scanning tunneling spectroscopy (SP-STS) and spin polarized ultraviolet photoemission spectroscopy (SP-UPS). The combination of both techniques allows to measure the interface spin-dependent electronic properties in the energy region of relevance for spintronics applications. By comparing SP-STS and SP-UPS measurements on the Fe-CuPc interface we can distinguish two regions in the interface electronic structure: (i) In the first one (close to E$_F$) where no spin polarized hybrid interface states (SP-HISs) are present, the interface acts as a scattering barrier, characterized by an energy-independent spin-flip probability. (ii) In the second region, the spin-dependent tunnelling probability is dominated by SP-HISs, whose presence is confirmed by the SP-UPS measurements. [1] C. Barraud et al. Nat Phys 6 (2010) 615; [2] M. Cinchetti et al. PRL 104 (2010) 217602; [3] M. Cinchetti, et al. Nat Mater 8 (2009) 115.

DS 42.13 Wed 15:00 P1

Installation of a new variable temperature STM and measurements on Cobalt-Phthalocyanine — •Martha Scheffler, Torben Hänke, Danny Baumann, Ronny Schlegel, Dirk Bombor, Christian Hess, and Bernd Büchner — IFW Dresden, Institute for Solid State Research

A new scanning tunneling microscope was implemented in an existing chamber system and tested. It can be completely cooled by a liquid helium flow cryostat and can measure at temperatures down to 10K over a long period. Atomically resolved images as well as scanning tunneling spectroscopy with a high energy resolution can be obtained. Surface studies of Cobalt-Phthalocyanine molecules deposited onto HOPG and Au(001) surfaces will presented.

DS 42.14 Wed 15:00 P1

Organic-metal oxide hybrid thin film phototransistors — •Stephan Rossbauer[1], Stuart Thomas[2], Pichaya Pattanasattayavong[2], Peter Müller-Buschbaum[1], and Thomas D. Anthopoulos[2] — [1]TU München, Physik Department, LS Funkt. Mat., James-Franck-Str. 1, 85748 Garching, Germany — [2]Department of Physics and Centre for Plastic Electronics, Blackett Laboratory, Imperial College London, London SW7 2BW, United Kingdom

Metal oxide semiconductors are an interesting family of materials with great potential for a number of technological applications including transparent electronics, photovoltaics, smart windows and optical displays. This work presents the electronic and morphological effects of light-absorbing organic dyes functionalised directly onto the surface of zinc oxide (ZnO) based transistor channels produced by spray pyrolysis. Dynamic photo response is measured and discussed. The photosensitivity is tunable through the application of the gate voltage. The device produced can be used either as sensing device or as optoelectronic switch.

DS 42.15 Wed 15:00 P1

Dependence of Field-Effect Mobility on Semiconductor Layer Thickness in Organic Thin Film Transistors — •Christopher Keil and Schlettwein Derck — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email:schlettwein@uni-giessen.de

Thin films of $F_{16}PcCu$ from the monolayer regime to thicker nm range were prepared under high vacuum conditions. As substrate a SiO_2 insulating layer was chosen. Metal contacts were evaporated as bottom contacts before the organic layer deposition. Organic thin film transistors of the molecular semiconductors were thereby achieved. Electrical conductivity as well as field-effect mobility were studied to investigate the role of the interface between the semiconductor and the gate insulator in bottom-gate field-effect transistors. The influence of organic film thickness as well as contact resistance between metal electrode and semiconductor layer were discussed to calculate the respective field effect mobility.

DS 42.16 Wed 15:00 P1

Thermally stimulated current measurements on P3HT based MIS-Diodes — •Tobias Könyves-Toth, Christian Melzer, and Heinz von Seggern — Electronic Materials Department, Institute of Materials Science Technische Universität Darmstadt, Petersenstraße 23, 64287 Darmstadt, Germany

Organic electronics show promising abilities even though there are still problems concerning lifetime and performance. These problems are often attributed to trap states in the volume of the employed organic semiconductor and to interface-near trap states. We report on interface traps occurring in state of the art poly(3-hexylthiophene) organic field-effect transistors (OFETs) examined by the technique of thermally stimulated currents (TSC). By using metal-insulator-semiconductor devices the sign of the applied voltage selects the accumulated charge carrier type at the interface and thus, hole or electron interface traps can be addressed. The contribution of the dielectric insulator on the TSC signal was unveiled by reference measurements on devices without the semiconducting layer. Utilizing the TSC method we were thus able to identify different trap states at the insulator-semiconductor and the semiconductor-contact interface and we will present the energetic distribution of the occupied density of states as measured by fractional TSC. Further, we will discuss whether trap states are induced by oxygen, as often stated in literature. The discussed results are crucial for the performance of OFETs as they affect the accumulated charge carriers in the transistor channel.

DS 42.17 Wed 15:00 P1

Organic field effect transistors on thin polyurethane films as gate dielectric — •Steffen Heuser, Jan Hartel, Christopher Keil, and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email:schlettwein@uni-giessen.de

Thin insulating polymer layers (1 – 2.5 μm) of a two-component polyurethane resin were deposited by spin-coating as gate dielectric on a Pt gate electrode on poly(ethyleneterephthalate) PET. An interdigitated source and drain electrode array of gold was prepared to complete the setting of the measurement. Such structures with polymeric gate dielectrics are of interest to realize all-organic field effect transistors (OFET). In this study, 20 nm thin films of a perfluorinated phthalocyanine $F_{16}PcCu$ were prepared by physical vapour deposition (PVD) under fine vacuum conditions as an organic n-type semiconductor. The dielectric properties of the polymer insulating layer were determined by impedance spectroscopy. The transistor structures were measured and as characteristic properties the charge carrier mobility in the $F_{16}PcCu$ film, the threshold voltage and the on/off current ratio of the structures will be discussed.

DS 42.18 Wed 15:00 P1

Electrical and morphological characterization of self assembled nanofibers by means of conducting tip AFM — •Jörn-Oliver Vogel and Paolo Samorì — Institut de Science et d'Ingénierie Supramoléculaires, Strasbourg , Frankreich

Electrical and morphological characterization of self assembled nanofibers by means of conducting tip AFM

The simultaneous characterization of the morphology and the electronic properties of isolated nanostructures is important to understand how the spatial restrictions and the nanoscale order affect the electrical properties of nanoscale objects and organic electronic devices.

Here we report the study of the electrical properties of self organized nanofibers of poly(3-hexylthiophene) polymers adsorbed on an insulating substrate from a mixed p-xylene / chloroform solution.

The fibers were produced by means of spin-coating on a silicon oxide surface with pre-patterned gold electrodes. The P3ht fibers have a typical extension of 20 to 50 nm width, several um length, and 1.5 nm to 5 nm height. The IV characteristics of individual fibers are probed by the conductive AFM tip along the fiber contour in order explore the decay of current through this anisotropic nanostructure.

DS 42.19 Wed 15:00 P1

Integration of self-assembled photonic structures in excitonic solar cells — •Stefan Guldin[1], Sven Hüttner[1], Peter Kohn[1], Morgan Stefik[3], Pablo Docampo[2], Henry Snaith[2], Ulrich Wiesner[3], and Ullrich Steiner[1] — [1]Physics Department, Cavendish Laboratory, University of Cambridge, UK — [2]Physics Department, Clarendon Laboratory, University of Oxford, UK — [3]Materials Science Department, Cornell University, Ithaca, NY, USA

One way to successfully enhance light harvesting of excitonic solar cells in otherwise poorly absorbing spectral regions is the integration of optical elements in the device architecture. Recently concepts for the incorporation of one- or three-dimensional photonic crystal structures have been proposed which are geared towards enhancing absorption in specific parts of the optical spectrum while retaining the cell transparency.

In this work we present a novel route for the fabrication of a photonically active, mesoporous TiO_2 architecture from solution. The method relies on on the self assembly properties of the block copolymer PI-*b*-PEO in combination with sol-gel chemistry. When deposited in a layer-by-layer fashion, porosity and pore size of each individual coating can be controlled in detail, which enables the stacking of alternating high and low refractive index layers of TiO_2. The effects of such a highly reflecting one-dimensional photonic crystal on light absorption properties and cell efficiency of dye-sensitised solar cells will be discussed in detail.

DS 42.20 Wed 15:00 P1

Vertical Organic n-Triodes based on Me-PTCDI and fullerenes — •Axel Fischer, René Michel, Philipp Sebastian, Hans Kleemann, Alexander Zakhidov, Björn Lüssem, and Karl Leo — Institut für Angewandte Photophysik, George-Bähr-Straße 1, 01067 Dresden, Germany

Vertical Organic Triodes (VOT) are promising three terminal transistor devices, which, in contrast to organic field effect transistors (OFETs), can be processed in a vertical structure.

The major advantage of the vertical structure is the possibility to stack them with a second electronic device. For example, VOTs can be combined with an organic memory device to form an active matrix crossbar with the VOT as selection transistor. Due to stacking of the two devices, a high integration density can be achieved.

Furthermore, VOTs exhibit short active lengths which can be precisely controlled by the active layer thickness. Thus, these devices can drive high currents and high switching frequencies are in reach. Although considerable effort has been spent into the research of these devices, a detailed understanding of the working principles of these devices is still missing.

In this contribution, we will introduce the device concept of the VOT and discuss different electronic configurations. We will show organic triodes which are able to drive high current densities. Based on our results, we suggest that the working principle of the device is based on a permeable metal grid.

DS 42.21 Wed 15:00 P1

Charge transport simulations in amorphous organic materials — •Falk May and Denis Andrienko — Max-Planck-Institute for Polymer Research, Mainz, Germany

In the last few years organic materials have become a promising alternative to their inorganic counterparts in various applications for example in field effect transistors, photovoltaics and light emitting diodes. The advantage of using organic materials is due to a shear abundance of compounds that can be specially designed to meet different purposes, e.g. flexibility, light weight, or processability. However, many applications demand a high mobility of charge carriers and organic materials are still lacking behind their inorganic counterparts. Understanding the dynamics of charge carriers in organic materials is therefore a key question in the field, that we are currently addressing with the help of computer simulations in order to design new materials with improved mobilities[1]. We use a multi-scale approach starting from the description of (semi)-classical atomic interactions to generate a realistic morphology by molecular dynamics. At a higher length-scale we then describe charge carrier hopping through Marcus rates by including molecular interactions based on a quantum chemical calculation. On the largest length-scale we use kinetic Monte Carlo simulations to finally obtain charge carrier mobilities.

[1] X. Feng, V. Marcon, W. Pisula, M. R. Hansen, J. Kirkpatrick, F. Grozema, D. Andrienko, K. Kremer, K. Mullen, Nature Materials, 421-426, 2009

DS 42.22 Wed 15:00 P1

Donor-block-acceptor systems for photovoltaic applications — •Sven Hüttner[1], Michael Sommer[2], Kerr Johnson[1], Carol Huang[1], and Richard H. Friend[1] — [1]Cavendish Laboratory, University of Cambridge, UK — [2]Melville Laboratory, University of Cambridge, UK

Polymer solar cells rely on a donor and an acceptor material that form an interpenetrating morphology. This ensures charge separation at the interface, but also a proper charge percolation to the electrodes at the same time. Furthermore, the right position of HOMO and LUMO levels of the respective materials are important for an efficient charge separation. We present novel donor-block-acceptor polymers that can be applied in light harvesting devices. We want to control the heterojunction interface by these donor-block-acceptor molecules. These act as a phase compatibilizer to modify the polymer blend phase separation, but also affect the energetic environment of the heterojunction. Besides their structural characterisation, we investigated these materials by time-resolved spectroscopy. The donor-block-acceptor macromolecules contain P3HT as a donor block, and the acceptor block consists of perylene bisimide derivatives or F8TBT.

DS 42.23 Wed 15:00 P1

Characterization of bulk-heterojunction layers by imaging ellipsometry — •Christian Röling[1], Mathias Vaupel[2], Kristian O. Sylvester-Hvid[3], and Peter H. Thiesen[1] — [1]Accurion GmbH, Stresemannstr. 30, 37079 Göttingen — [2]Zeiss GmbH, Göttingen — [3]Riso National Laboratory for Sustainable Energy, DTU, Denmark

Conductive polymers and polymer-fullerene blends are promising materials for OLED and plastic solar cell applications. Blends prepared by two different methods, silk-printing and spin-coating were imaged, characterized and mapped using the spectroscopic imaging ellipsometer nanofilm_ep3se.

The optical characterization of bulk-heteroconjugate layers with imaging ellipsometry offers new information on the thickness distribution and refractive index distribution. Ellipsometric contrast micrographs are useful tools for the layer inspection concerning homogeneity and morphology, especially for the optimization of the coating process.

DS 42.24 Wed 15:00 P1

SXPS characterization of a donor / acceptor hetero junction for organic solar cells: High photovoltage at the merocyanine / fullerene interface — Eric Mankel, •Philip Reckers, Ludmila Konrad, Corinna Hein, Thomas Mayer, and Wolfram Jaegermann — Technische Universität Darmstadt, Materials Science Institute, Surface Science Division, Petersenstraße 32, 64287 Darmstadt, Germany

Novel absorber molecules are investigated for high efficient organic solar cells. Especially merocyanines provide high photovoltages as donor materials in photoactive organic hetero junction cells. The electronic alignment of a merocyanine / fullerene hetero junction is presented. The band diagram was determined by synchrotron induced photoelectron spectroscopy on in situ stepwise deposited fullerene on a merocyanine layer using the TGM7 dipole beamline at Bessy II. The merocyanine / fullerene HOMO offset is determined to be 850meV leading to a high LUMO offset, the driving force for exciton splitting. In situ bias illumination of the interface with 150W/m^2 of a halogen lamp leads to a reversible shift of the C60 emission features of about 800meV, indicating a high photovoltage. The height of the photovoltage depends on the fullerene layer thickness. It starts at 200mV for submonolayer coverage and increases up to approximately 1V for coverages of some ten nanometers.

DS 42.25 Wed 15:00 P1

Photodegradation of P3HT - a systematic study of environmental factors — •Holger Hintz[1], Ulf Dettinger[1], Hans-Joachim Egelhaaf[2], Larry Luer[3], Heiko Peisert[1], Thomas Chassé[1], and Jens Hauch[2] — [1]Eberhard-Karls-University, Institute for Physical and Theoretical Chemistry, Auf der Morgenstelle 8, D-72076 Tübingen, Germany — [2]Konarka Technologies GmbH, Landgrabenstr. 94, D-90443 Nürnberg, Germany — [3]Madrid Institute for Advanced Studies, IMDEA Nanociencia, Mòdulo 13; Avda Fco Tomas y Valiente, 7, 28049 Madrid, Spain

The influence of environmental factors on the degradation process of P3HT film has been investigated quantitatively. The decay kinetics of the polymer absorption during variation of intensity and spectral distribution of the incident light, oxygen concentration, humidity level as well as temperature are monitored using infrared and UV/VIS absorption spectroscopy. Oxygen diffusion into the polymer film has been investigated using fluorescence spectroscopy. The degradation process is light initiated with a strong increase of the effectiveness towards the ultraviolet region of the spectrum. The photo oxidation is not oxygen diffusion limited although an activation energy of 26 kJmol-1 was observed for both degradation and oxygen diffusion. The observed kinetics, especially its dependence on wavelength of the incident light, point to a radical- based degradation process in the solid state rather than a singlet oxygen based mechanism as it is observed in the liquid phase. The presence of humidity strongly affects the degradation process although water itself does not decompose the polymer.

DS 42.26 Wed 15:00 P1

Orientation and interface properties of a promising low bang gap polymer for organic solar cells — •Umut Aygül[1], David Batchelor[2], Ulf Dettinger[1], Heiko Peisert[1], and Thomas Chassé[1] — [1]Universität Tübingen, Institut für Physikalische und Theoretische Chemie, Auf der Morgenstelle 18, 72076 Tübingen — [2]Karlsruher Institut für Technologie, Institut für Synchrotron Strahlung, 76344 Eggenstein-Leopoldshafen

In polymer based bulk heterojunction-type solar cells so-called low band gap materials with alternating electron-deficient and electron-rich subunits are promising donor components in active layers to improve the efficiency of organic solar cells. A potential candidate in this context is Poly[2,6-(4,4-bis-(2-ethylhexyl)-4H-cyclopenta [2,1-b;3,4-b']dithiophene)-alt-4,7(2,1,3 benzothiadiazole) (PCPDTBT). The application of new materials requires a detailed understanding of the orientation and the electronic properties of the system and interface as these have a dramatic effect on device performance and efficiency. We study the electronic properties of interfaces between PCPDTBT and prototypical electrodes as well as between PCPDTBT and PCBM (acceptor) using X-ray photoemission spectroscopy (XPS) and valence band ultraviolet photoemission spectroscopy (UPS). Furthermore the preferred orientation of thin PCPDTBT films on both ITO and Si was studied with X-ray absorption spectroscopy (XAS) by looking at the sulphur K edge.

DS 42.27 Wed 15:00 P1

Charge Transport in Amorphous Oligothiophenes — •Manuel Schrader[1], Björn Baumeier[1], Chris Elschner[2], Moritz Riede[2], Karl Leo[2], and Denis Andrienko[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]TU Dresden, Institute of Applied Photophysics, Mommsenstr. 13, 01062 Dresden, Germany

Organic semiconducting materials are needed for emerging devices such as photovoltaic solar cells. In this work we combine first principle calculations, molecular dynamics and kinetic Monte Carlo simulations to study charge transport in dicyanovinyl oligothiophenes of different lengths. Poole-Frenkel behavior of the charge carrier mobility is rationalized based on electrostatic and conformational disorder.

DS 42.28 Wed 15:00 P1

Hybrid Solar Cells made of Phthalocyanines and Zinc Oxide Nanowires — •Michael Kozlik, Steffen Milz, Sven Möller, Carsten Ronning, and Torsten Fritz — Institute of Solid State Physics, University of Jena, 07743 Jena, Germany

Hybrid Solar Cells are a topic of recent interest [1]. Usually the inorganic material is combined with organic polymers with increased interface area by using nanostructures. Our aim is to use the better photo current performance of small molecules, i.e. phthalocyanines [2], compared to polymers. Phthalocyanines show a high absorbance in the visible range, which is characterized by UV-Vis spectroscopy. The electronic ground state and the energetic level alignment were investigated using UV photoelectron spectroscopy. ZnO nanowires, synthesized by the vapor-liquid-solid route, are used due to the good conductivity and the transparency in the visible range [3]. A nearly perpendicular nanowire growth was achieved using a ZnO seed layer. The surface-to-volume ratio can be varied by changing the growth parameters. The morphology of the samples was investigated with scanning electron microscopy, while the atomic composition was obtained from X-ray analysis. The substrate and front contact were optimized to remain the high conductivity during nanowire growth. We will also present first results of a hybrid solar cell made of the combination of zinc oxide nanowires and phthalocyanines. References [1] S. Günes et al., Inorg. Chim. Acta 361 (2008) 581. [2] N. Papageorgiou et al., Prog. Surf. Sci. 77 (2004) 139. [3] C. Borchers et al., J. Phys. Chem. B. 110 (2006) 1656.

DS 42.29 Wed 15:00 P1

Influence of different solvents on the morphology in P3HT:PCBM bulk heterojunction systems for organic photovoltaics — •Shuai Guo[1], Matthias A. Ruderer[1], Volker Körstgens[1], Robert Meier[1], Hsin-Yin Chiang[1], Jan Perlich[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik Department, LS Funkt. Mat., James-Franck-Str. 1, 85748 Garching, Germany — [2]HASYLAB at DESY, 22603 Hamburg, Germany

Polymer-based photovoltaics have become of major interest in basic research as well as in application. One very promising system consists of poly(3-hexylthiophene) (P3HT) and the fullerene derivate PCBM. We investigate the morphology of bulk heterojunction films based on P3HT:PCBM. Films are cast from different solvents. It is well known that the solvent properties strongly influence the film formation and therefore influence the performance. In this work the surface structure is investigated by optical microscopy and AFM. In combination with scattering techniques such as XRR, GI(U)SAXS and GIWAXS, revealing the inner structure as well as the crystallinity, the whole morphology of the active layer is detected. Consequently, the different morphologies formed from different solvents are determined and compared with the corresponding performance of these systems.

DS 42.30 Wed 15:00 P1

Characterisation of Organic Field-Effect Transistors using Zinc Tetraphenylporphyrin Monomers and Dimers as Active Layers — •Iulia Genoveva Korodi[1], Daniel Lehmann[1], Simona Pop[2], Aoife Ryan[3], Mathias Senge[3], and Dietrich R. T. Zahn[1] — [1]Chemnitz University of Technology, Semiconductor Physics, D-09107 Chemnitz, Germany — [2]ISAS-Institute for Analytical Sciences, Albert-Einstein-Str.9, D-12489 Berlin, Germany — [3]School of Chemistry, SFI Tetrapyrrole Laboratory, Trinity College Dublin, Dublin 2, Irland

In this work bottom contact organic field-effect transistors (OFETs) using Zinc Tetraphenylporphyrin (ZnTPP) monomers and dimers as active layers were prepared and characterised. The ZnTPP dimer molecules are intramolecularly connected via a $C\equiv C$ bridge. The films were prepared by drop coating from a tetrahydrofuran solution on Si substrates with 100 nm SiO_2 on top with pre-structured gold contacts (from Fraunhofer IPMS Dresden). The channel lengths and the channel width defined by the lithography mask are $L = 2.5$ μm, 5 μm, 10 μm and 20 μm and $W = 10$ mm, respectively. The influence of using ZnTPP monomers or dimers on the on/off ratio, threshold voltage and charge carrier mobility is compared and discussed. The effect of the morphology as revealed by the scanning electron microscopy images is discussed as well.

DS 42.31 Wed 15:00 P1

Time resolved microwave conductivity measurements of Bulk Heterojunction solar cells — •Shine Philip[1], Elias Martinez[2], Klaus Müller[1], Marinus Kunst[2], and Dieter Schmeisser[1] — [1]Brandenburg University of Technology, Department of Applied Physics and sensors, K.-Wachsmann-Allee 17, 03046, Cottbus, Germany — [2]Helmholtz- Zentrum Berlin for Materials and Energy, Hahn-Meitner-Platz 1, 14109 Berlin Germany

The time resolved microwave conductivity (TRMC) method was used in order to study the generation and decay kinetics of charge carriers in the Bulk Heterojunction (BHJ) solar cells. The charge carriers were generated with 532nm laser pulses of 10ns FWHM (Full Width at Half Maximum) induced in the cells. The BHJ solar cells used for the measurements had a photoactive layer consisting of a mixture of Poly (3-Hexylthiophene) P3HT and Phenyl-C61-butyric acid methyl ester (PCBM) which was spin coated onto Indium tin oxide (ITO)/glass substrates. In the field of Organic photovoltaic blends, TRMC method is introduced as a new method of direct investigation of the charge carrier lifetime as well as the charge carrier mobility and we were successful in studying the charge carrier lifetime of the reference BHJ solar cells. We also studied the influence of aligned ferroelectric fields on the charge separation in BHJ solar cells. As ferroelectric material, we used the copolymer Poly (vinylidene fluoride - trifluoroethylene) P(VDF-TrFE).

DS 42.32 Wed 15:00 P1

Sol-Gel Templated Zinc oxide Films for Solar Cell Application — •Kuhu Sarkar and Peter Müller-Buschbaum — TU München, Physik Department, LS Funkt. Mat., James-Franck-Str. 1, 85748 Garching, Germany

Hybrid solar cells consisting of both the organic and the inorganic semiconductor parts are a potential source for low cost green electricity. The organic conjugated polymer acts as a hole-conducting material while the inorganic oxide as an electron acceptor. The nanostructured morphology of inorganic material in the hybrid solar cells leads to enhanced device performance by increasing the active surface area for interfacial interactions. Among the various inorganic metal oxides, zinc oxide is a promising material for use in hybrid solar cells on account of its high electron mobility, a direct band gap of 3.37 eV at room temperature, large excitons binding energy, excellent chemical and thermal stability, suitable optical properties and environment-friendly behaviour. A sol gel approach based on an amphiphilic diblock copolymer acting as a structure directing agent is used to obtain a ZnO network structure via spin coating. Primary structural investigation of the films is carried out using SEM and AFM.

DS 42.33 Wed 15:00 P1

Evaluation of Barrier Films for Organic Solar Cells Using an Electrical Calcium-Test — •Hannes Klumbies[1], Sylvio Schubert[1], Lars Müller-Meskamp[1], Olaf R. Hild[2], and Karl Leo[1,2] — [1]Institut für Angewandte Photophysik, Dresdner Innovationszentrum Energieeffizienz, TU Dresden, 01062 Dresden, Germany — [2]Fraunhofer Institute for Photonic Microsystems, 01109 Dresden, Germany

In contrast to common solar cells based on silicon, organic solar cells have the potential to be cheap and flexible. The latter is especially important for mass-production (Roll-to-Roll-processing), mobile applications and low-cost, lightweight installations. However, flexibility poses a challenge for stable encapsulation of the organic solar cell to prevent it from degradation due to oxygen and water vapor. It is common agreement that the transmission rates for these species should be 1E-4 g/m^2*d or lower - four to five orders of magnitude below the rate of a typical polymer foil. Transmission rates that low are not only difficult to achieve but also difficult to measure. Ready-to-use commercial devices based on coulometry only reach a sensitivity of 5E-4 g/m^2*d.

In this work we use an electrical Ca-test as a sensor for water vapor and oxygen. Its sensitivity is in the range of 5E-5 g/m^2*d or better.

Furthermore we show water-vapour-transmission-rates achieved by different barrier layers on polymer-foil, e. g. sputtered oxides, and compare them with the rates achieved by bare polymer- and commercial barrier-foils.

DS 42.34 Wed 15:00 P1

Solution-processable organic light emitting diode on glass fibers for textile applications — •Björn Gruber, Schulze Kerstin, and Janietz Silvia — Fraunhofer Institute for Applied Polymer Research, Geiselbergstr. 69, 14476 Potsdam-Golm, Germany

Electronic devices based on organic materials offers the possibility to be a low-cost production technology on large area in several years. As a special application organic devices could be used in the field of electronic-textiles in future, for example for safety applications or as smart textiles. Therefore the direct integration of the electronic devices on the textile fibers is interesting.

In this work, organic light emitting diodes (OLEDs) have been manufactured and investigated on cylindrical and flexible substrates. Especially the cylindrical geometry of the substrate hinders a homogeneous deposition of organic layers. Here, we present first results using solution processes for the preparation of the organic materials of an organic light emitting diode on glass fibers. The OLEDs were prepared on thin glass fibers using thermally evaporated metals and dip-coated polymeric layers. We focus on the challenging preparation steps of these layers on cylindrical substrates resulting in working devices. Additionally a current density-voltage-characteristic of a light emitting device on a glass fiber is presented and analyzed.

DS 42.35 Wed 15:00 P1

Inkjet printing of organic layers on nano- and microstructured flexible substrates for organic electronic devices — •Marcel Schmidt[1], Peter Lewer[1], Kerstin Schulze[1], Silvia Janietz[1], Felix Stelzl[2], Chegnui Bekeny[2], and Uli Würfel[2] — [1]Fraunhofer Institute for Applied Polymer Research, Geiselbergstr. 69, 14476 Potsdam-Golm, Germany — [2]Fraunhofer Institute for Solar Energy Systems, Heidenhofstr. 2, 79110 Freiburg, Germany

Inkjet printing as deposition method for organic materials in electronic devices promises to be a low-cost production technology in future. The advantage of this technique is the ability to deposit a small amount of material on defined areas on substrates, e.g. for the preparation of organic field effect transistors (OFETs) or organic solar cells (OSCs). As a special application the use of 3D-nanostructured electrodes on flexible substrates as a high voltage source could be already demonstrated [Adv. Mater. 20, 4055]. The deposition of material layers is especially influenced by the capillary forces of the electrode structures and by the formation of inhomogeneous layers. Here, we present our results on the development of an inkjet printing process for semiconductor materials on nano- and microstructured substrates. The capillary forces resulting from the structure of the substrates as well as the solvents of the ink were examined for the development of the printing process. The prepared layers were analysed using atomic force microscopy (AFM) and scanning electron microscopy (SEM). The fabrication of smooth layers within the microstructure will be demonstrated as well as first results of photovoltaic cells on nanostructured substrates.

DS 42.36 Wed 15:00 P1

Photoelectron Spectroscopy Investigation of the C60/Calcium Interface — •Holger Wetzstein[1], Darius Bunandar[2], Julia Schafferhans[3], Carsten Deibel[3], Achim Schöll[1], and Friedrich Reinert[1] — [1]Experimental Physics VII, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — [2]Department of Physics, University of Texas at Austin, Austin, Tx 78712-0264 — [3]Experimental Physics VI, Julius-Maximilians-University of Würzburg, D-97074 Würzburg

Device lifetime is a crucial point for organic solar cells. Therefore it is important to understand the degradation mechanisms as well as their consequence on the performance of these photovoltaic devices. We observed a characteristic S-shape in the I/V-curves of P3HT/PCBM-bulk heterojunction cells with calcium contacts. A tentative origin of this behavior is a reaction of the calcium with oxygen, which leads to alterations in the regime of the anode interface. To shed more light on this issue we investigated the electronic structure of the Ca/C60 interface, which serves as a model for the PCBM/Ca contact. X-ray (XPS) and ultra-violet photoelectron spectroscopy (UPS) measurements were performed on C60 layers adsorbed on epitaxially grown Calcium as well as on Ca deposited on C60. In both cases, the data clearly show the formation of an interface state due to the charge transfer from the Ca into the C60, which is an indication for a chemical reaction. Moreover, we studied the effect of oxygen exposure on the interfacial chemical and electronic structure under conditions comparable to the conditions during device operation.

DS 42.37 Wed 15:00 P1

Determination of molecular electronic excitations using epitaxial thin film growth: Perfluoropentacene on alkali halides — •Tobias Breuer and Gregor Witte — Molekulare Festkörperphysik, Philipps-Universität Marburg, D-35032 Marburg

The study of optical excitations is an important part of understanding electronic properties in organic semiconductors. As it is in many cases hardly possible to prepare sufficiently sized crystals, optical spectroscopy of organic single crystals is a challenging topic. Here we present an alternative approach: to study optical excitations in Perfluoropentacene ($C_{22}F_{14}$) we prepared epitaxial thin films on the (100)-surfaces of alkali halides. The epitaxial growth of PFP films was proved and studied by AFM and XRD measurements. While exhibiting the same crystalline phase a rather different molecular orientation is adopted on both substrates showing an upright orientation on NaF and a recumbent orientation on KCl which in both cases are stabilized by an electrostatic point-in-line relationship between the outermost fluorine atoms and the alkali cations of the substrate surfaces. While previous studies of optical excitations in PFP were hampered by the laterally isotropic (100)-growth of PFP on amorphous SiO_2[1] the different epitaxial growth modes on the alkali halides enabled access to all molecular axes. A combination of UV/Vis measurements and spectrally and polarization resolved microscopy enabled the determination of the polarization dependence of the observed optical excitations. Evidence of intermolecular coupling was found and will be discussed.

[1] A. Hinderhofer et al., J. Chem. Phys. 127, 194705 (2007).

DS 42.38 Wed 15:00 P1

IR-Spectroscopy on organic charge-transfer complexes — Sebastian Beck[1], •Milan Alt[1], Tobias Glaser[1], Akemi Tamanai[1], Diana Nanova[1], Michael Kröger[2], and Annemarie Pucci[1] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg — [2]InnovationLab GmbH, 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 CT-complexes, such as TTF-TCNQ and its derivates. We studied the optical properties of these CT-complexes in the whole infrared range (100 - 12000 cm^{-1}). The suggested linear relationship between the excitation energy of the C-N-stretching vibration of the acceptor TCNQ and the associated charge-transfer was verified. In addition to the vibronic excitations of the molecules also widely broadened absorption bands in the MIR and NIR were observed. These are attributed to electronic excitations and in the range of the HOMO-LUMO gap of the investigated complexes.

DS 42.39 Wed 15:00 P1

IR studies on an emitter/host mixture — •Tobias Glaser[1], Christian Lennartz[2], Christian Schildknecht[2], and Annemarie Pucci[1] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg — [2]BASF SE, Ludwigshafen

In this study, we show how infrared spectroscopy can be used to investigate the mixing of two organic materials. The materials, in this case a phosphorescent emitter that was developed for organic light emitting devices and a suitable host material, were deposited by vapour sublimation under ultra-high vacuum conditions. By comparing the experimental spectra of thin layers of the pure materials to quantum chemical calculations, the calculated vibrational modes could be assigned to the measured absorption bands. Embedding the emitter into the host by simultaneous evaporation of these two materials gives rise to only small changes in the relative intensity of the IR absorption bands due to the change in background polarisability, but significantly effects the photoluminescence.

DS 42.40 Wed 15:00 P1

Structure and morphology of co-evaporated pentacene-perfluoropentacene thin films[1] — •Christian Frank[1], Alexander Hinderhofer[1], Takuya Hosokai[1], Andrea Resta[2], Alexander Gerlach[1], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany — [2]ESRF, BP 220, F-38043 Grenoble, France

The morphology as well as the structure of thin films, consisting of pentacene (PEN) and perfluoropentacene (PFP)[2] binary blends on SiO_2,

were investigated by means of x-ray reflectivity and grazing incidence x-ray diffraction. Furthermore, reciprocal space maps of these blends with different volume fractions show the co-existence of two intermixing phases in addition to pure PEN and PFP crystallites. The question whether these intermixing occurs on a molecular length scale is addressed. The σ-phase, with its long molecular axis nearly perpendicular to the substrate, is thermally stable and nucleates predominantly at high temperatures. The λ-phase (long molecular axis nearly parallel to the substrate) exhibits a growth behavior, which is enhanced by low temperatures. Additionally, both phases can tentatively be identified within the reciprocal space maps.
[1] A. Hinderhofer, C. Frank, T. Hosokai, A. Resta, A. Gerlach, F. Schreiber, **submitted**
[2] A. Hinderhofer, U. Heinemeyer, A. Gerlach, S. Kowarik, R. M. J. Jacobs, Y. Sakamoto, T. Suzuki, F. Schreiber, J. Chem. Phys. **127**, 194705 (2007)

DS 42.41 Wed 15:00 P1

Structural and Vibrational Properties of C_{60} Fullerene Thin Films on Gold Surfaces — •Caroline Henneke, Philip Schulz, Tobias Schäfer, and Matthias Wuttig — I. Physikalisches Institut (IA), RWTH Aachen University, Germany

The fullerene C_{60} is a widely employed acceptor material for organic solar cells. By tailoring the structure of C_{60} thin films and thus tuning their properties the efficiency of C_{60}-based solar cells can be improved. However, it remains a main challenge to determine the correlation between the structure of C_{60} thin films and their optoelectronic properties.
Here, the influence of substrate temperature during deposition in a vacuum thermal evaporation process (VTE) on the structure and vibrational properties of C_{60} thin films on Au surfaces is investigated. Substrate temperatures ranging from 150 K to 700 K were applied in this study. XRD measurements were conducted to identify structural changes in the C_{60} thin films, while the surface morphology was determined by AFM measurements. The vibrational characteristics of the C_{60} thin films were investigated by Fourier-Transform Infrared spectroscopy (FTIR).

DS 42.42 Wed 15:00 P1

Analysis of structure and electronic alignment of PTCDI-C13 thin films on metal surfaces — •Daniel Gebauer, Philip Schulz, Dominik Meyer, Christian Effertz, and Matthias Wuttig — RWTH Aachen, I. Institute of Physics (IA), D-52056 Aachen, Germany

N,N'-Ditridecylperylene-3,4,9,10-tetracarboxylic diimide (PTCDIC13) depicts a potential acceptor material for organic solar cells. To understand the mechanisms of film formation and charge carrier transfer, it is necessary to examine the interface effects between the organic layer and the metal contact.

In this study thin films of PTCDI-C13 with a thickness varying from single monolayers to 20 nm, are evaporated on Au, Ag, Cu, and Al substrates. The energy level alignment between the valence band of each metal and the molecular orbitals of the subsequently deposited organic layer is analyzed by Ultraviolet Photoelectron Spectroscopy (UPS). Structure and surface morphology of the PTCDI-C13 films have been investigated by Atomic Force Microscopy (AFM) and X-Ray Diffractometry (XRD) in order to study the growth behavior of these films.

DS 42.43 Wed 15:00 P1

Tetrazine Thin Film Growth on SAM-coated Gold Surfaces — •Dominik Meyer[1], Philip Schulz[1], Laurent Galmiche[2], Pierre Audebert[2], and Matthias Wuttig[1] — [1]Institute of Physics (IA), RWTH Aachen University of Technology, 52056 Aachen, Germany — [2]P.P.S.M. (CNRS UMS 8531), École Normale Supérieure de Cachan, 61 Avenue du Président Wilson, 94235 Cachan Cedex, France

The modification of noble metal surfaces by organosulfur self-assembled monolayers (SAM) is a widely studied topic in the field of organic optoelectronics. The assembly of such monolayers alters the electronic structure of the metal surface and strongly affects thin film growth of subsequently deposited organic material employed in optoelectronic devices. Here we present the impact of SAMs on the crystal growth of 3,6-bis(3,5-dimethylpyrazol-1-yl)-1,2,4,5-tetrazine (bpytz). Tetrazines are promising candidates as alternative active materials for optoelectronic and sensor applications as they generally provide a high electron affinity. This study compares the growth of bpytz on pure Au(111) surfaces with modified gold surfaces employing decanethiol and didecyl-dithiocarbamates as self-assembling monolayers. X-ray diffraction (XRD) and Infrared (IR) spectroscopy are employed to investigate the different growth scenarios, while density functional theory (DFT) was utilized to analyze the measured IR data.

DS 42.44 Wed 15:00 P1

Infrared Spectroscopic Ellipsometry Measurements of Polytriarylamine (PTAA) Thin Films — Jens Trollmann, Robert Lovrincic, •Akemi Tamanai, and Annemarie Pucci — Im Neuenheimer Feld 227, 69120 Heidelberg, Germany

Organic materials have been adopted for thin film fabrications since organic molecules are less expensive to produce, and high light absorbing capacity can be expected. For improving the electrical performance, investigation of the dielectric properties for the organic thin films is essential, hence Ψ and Δ measurements have been performed by means of spectroscopic ellipsometry (SE) (Woollam IR-VASE) so as to determine highly accurate dielectric constants (real and imaginary part) and thickness of polytriarylamine (PTAA) thin films (produced by Merck) in the infrared (IR) spectral range between 350 and 5500 cm^{-1}. PTAA is an extraordinarily stable p-type semiconductor material which can be handled in air, high field-effect mobility of organic field-effect transistors (OFETs) fabricated together with PTAA and a low k insulator (low k dielectrics) has been reported. It is possible to obtain the bands not only from molecular vibrations, but also from excitations of free carriers with the SE which dominate the dielectric response of semiconductor thin films in the IR region.

DS 42.45 Wed 15:00 P1

Charge carrier mobility in different donor materials for polymer solar cells — •Oleisa Synooka, Chetan Raj Singh, Marco Seeland, Gerhard Gobsch, and Harald Hoppe — Institüt für Physik, TU Ilmenau, Weimarer str.32, 98693 Ilmenau, Germany

Abstract: During recent years, many donor materials of varying band gap have been synthesized for polymer solar cell applications. Here, we compare the charge carrier mobilities of different commercially available p-type materials (e.g. P3HT and- PCDTBT) by the Space Charge Limited Current (SCLC) method. The mobility measurement results from SCLC are compared with Charge Extraction by Linearly Increasing Voltage (CELIV) measurements. Furthermore, several anode materials (e.g. PEDOT:PSS) have been investigated and compared with respect to their charge injection behavior.

DS 42.46 Wed 15:00 P1

In-situ protein adsorption study using spectroscopic IR-ellipsometry — •Philipp Gehlich, Andreas Furchner, Karsten Hinrichs, Norbert Esser, and Dennis Aulich — Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V.; Albert-Einstein-Str. 9; 12489 Berlin; Germany

In-situ IR-ellipsometry was used to determine the differences in absorption spectra of bovine serum albumin (BSA) films on silicon in aqueous solution. A special flow-cell [1,2] which allows to record spectra at varying temperatures was employed. At an incident angle of 50° tan Ψ - spectra were recorded at different times of the adsorption process. Amide-I- and, partially, amide-II-bands of the thin protein film could be identified and a variation was monitored until the adsorption process was completed. References: [1] K. Hinrichs, K. Roodenko and J. Rappich, Electrochem. Commun. 10 (2008), p. 315.; [2] Y. Mikhaylova, L. Ionov, J. Rappich, M. Gensch, N. Esser, S. Minko, K.-J. Eichhorn, M. Stamm and K. Hinrichs, Anal. Chem. 79 (2007), p. 7676.

DS 42.47 Wed 15:00 P1

Structure and optical properties of binary co-evaporated organic thin films: Diindenoperylene and Perfluoropentacene — •Jens Reinhardt, Alexander Hinderhofer, Katharina Broch, Ute Heinemeyer, Alexander Gerlach, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

The structural and optical properties of co-evaporated thin films of diindenoperylene[1] (DIP) and perfluoropentacene[2] (PFP) on SiO_2 and glass-substrates were studied using x-ray reflectivity, grazing incidence x-ray diffraction, differential reflection spectroscopy (DRS), and absorption spectroscopy. The x-ray data reveal the coexistence of at least one molecular mixed DIP:PFP phase distinct from the pure DIP and PFP thin film phases. In addition the absorption and DRS spectra of the mixture cannot be described by a superposition of the single-component spectra which is attributed to different intermolecular coupling. A systematic variation of growth parameters (substrate temperature: 300 - 360 K; thickness: 5 - 40 nm) and their effect on phase mixing/separation will be discussed.

[1] U. Heinemeyer *et al.*, Phys. Rev. B, **78** (2008) 085210
[2] A. Hinderhofer *et al.*, J. Chem. Phys., **127** (2007) 194705

DS 42.48 Wed 15:00 P1

Molecular anchoring on metal surfaces — Albano Cossaro[2], Dean Cvetko[1,3], Luca Floreano[2], •Michele Puppin[1,2,4], Alberto Verdini[2], and Alberto Morgante[1,2] — [1]Department of Physics, University of Trieste, Trieste, Italy — [2]CNR-IOM, Laboratorio TASC, Trieste, Italy — [3]Department of Physics, University of Ljubljana, Ljubljana, Slovenia — [4]Department of Physical Chemistry, Fritz Haber Institut der Max Planck Gesellschaft, Berlin, Germany

The possibility to control the structural properties of interface layers of an organo-metallic system is a major task of nano-devices engineering. In many cases, a Self Assembled Monolayer (SAM) is used for anchoring molecules or proteins to the substrate or, in organic electronics, for modifying the surface of metallic electrodes in contact with the organic active layers. The Au(111) surface can be functionalized with amine (-NH2) groups by growing a SAM of cysteamine in ultra-high vacuum. The modified surface is used to anchor molecules with a carboxylic (-COOH) functional group. The amine binds to the carboxylic group leading to a second layer in which the anchored molecules have a well defined orientation. To describe the formation and the final geometry of the organic structure we used XPS (X-ray Photoelectron Spectroscopy) and NEXAFS (Near Edge X-ray Absorption Fine Structure) spectroscopies.

DS 42.49 Wed 15:00 P1

Thin films of ethyne-linked porphyrin dimers investigated by spectroscopic ellipsometry — •Simona Pop[1], Peter Kate[1], Aoife Ryan[2], Xin Zhang[3], Jörg Rappich[3], Norbert Esser[1], Karsten Hinrichs[1], and Mathias Senge[2] — [1]Leibniz - Institut für Analytische Wissenschaften - ISAS - e.V., Albert-Einstein-Str.9, D-12489 Berlin, Germany — [2]School of Chemistry, SFI Tetrapyrrole Laboratory, Trinity College Dublin, Dublin 2, Ireland — [3]Helmholtz-Zentrum Berlin for Materials and Energy GmbH, Institute for Silicon Photovoltaics, Kekuléstrasse 5, Berlin, 12489, Germany

Thin films of ethyne-bridged porphyrin dimers are investigated by means of spectroscopic ellipsometry in the NIR-Vis spectral range. The porphyrin films were prepared on silicon substrates covered by the native oxide. For a better understanding of the optical behaviour of the porphyrin dimers, their corresponding monomers are additionally characterized. The dielectric functions of the porphyrin monomers and dimers are derived from ellipsometrical measurements by employing a three-phase optical model. The optical response of the porphyrin dimers is mainly characterized by red-shifts of the first absorption structure, Q-band, as well as by strong changes in the Q/B ratios, compared to the corresponding porphyrin monomers.

DS 42.50 Wed 15:00 P1

Characterization of temperature-sensitive swelling behavior of PNIPAAm brushes via in-situ infrared ellipsometry — •Andreas Furchner[1], Dennis Aulich[1], Eva Bittrich[2], and Karsten Hinrichs[1] — [1]Leibniz-Institut für Analytische Wissenschaften - ISAS - e. V. — [2]Leibniz-Institut für Polymerforschung Dresden e. V.

Over the last years, polymer brushes have received growing attention owing to their stimuli-responsive surface properties. In particular, mixed brushes, consisting of at least two different polymers, are interesting, since they represent biofunctional surfaces for controlled protein and cell adsorption due to stimuli-responsive behavior on changes in, for example, temperature, pH, or solvent.

Infrared Spectroscopic Ellipsometry (IRSE), a method for studying film properties at the solid-liquid interface, allows to study the structural and chemical properties of polymer layers and therefore makes it possible to tune mixed brush systems to the specific needs.

As an intermediate step towards a better understanding of mixed temperature-sensitive brushes, poly(N-isopropyl acrylamide) (PNIPAAm) mono-brushes were investigated using ex-situ as well as in-situ SE. The information about optical and structural properties obtained by fitting SE data to an appropriate optical layer model were then used to characterize the temperature-sensitive swelling behavior of PNIPAAm brushes.

DS 42.51 Wed 15:00 P1

Vibrational Properties of Metal Phthalocyanine Thin Films — •Michael Ludemann[1], Iulia E. Brumboiu[1,2], Ovidiu D. Gordan[1], Vasile Chiş[2], and Dietrich R. T. Zahn[1] — [1]Semiconductor Physics, Chemnitz University of Technology — [2]Faculty of Physics, Babeş-Bolyai University, Cluj-Napoca

In this work experimental Raman spectra of several phthalocyanine (Pc) molecules with different central metal atoms (Cu, Co, Fe and Ni) are compared to DFT calculations. Besides symmetry aspects the calculated and measured relative shifts of the vibrational bands due to the different central metal atoms provide additional information utilized to assign the measured Raman modes.

All samples were prepared by organic molecular deposition (OMBD) in ultra-high vacuum conditions (UHV). The measurements are performed *in situ* during growth or stepwise at fixed film thicknesses. For a better comparison to single molecule calculations Raman spectra at ultra-low coverage were measured.

DS 42.52 Wed 15:00 P1

Broadband dielectric spectroscopic studies on 4- heptan - 4'- isothiocyanatobiphenyl (7BT) in confining geometry. — •Malgorzata Jasiurkowska[1], Emmanuel U. Mapesa[1], Ciprian Iacob[1], Periklis Papadopoulos[1], Friedrich Kremer[1], and Maria Massalska-Arodz[2] — [1]Institute of Experimental Physics I, University of Leipzig, 04103 Leipzig, Germany — [2]The Henryk Niewodniczanski Institute of Nuclear Physics Polish Academy of Sciences, Radzikowskiego 152, 31-342 Kraków, Poland

Band Dielectric Spectroscopy is employed to investigate 4-heptan-4'- isothiocyanatobiphenyl (abbreviated as 7BT) in one- and two-dimensional confinement (in the frequency range 0.1 Hz to 10-6 Hz). In bulk, only one liquid crystalline phase, the smectic E (SmE) phase with orthorhombic arrangement within the molecular layers is observed. The bulk dielectric properties of the nBT compounds are now well understood. For measurements under one-dimensional confinement, ultrathin films of 7BT prepared by spin-coating method are measured in the nanostructured-electrode configuration. In contrast to bulk dielectric spectra where only one process is observed in the low frequency regime, an additional process appears. Dynamic properties of 7BT are also studied in nanoporous silica membranes. It is observed that the crystallization temperature is significantly reduced in comparison to the value for bulk 7BT. Moreover, beside the relaxation around short axis, two extra processes are observed. The influence of pore size on molecular dynamics will be discussed.

DS 42.53 Wed 15:00 P1

Density-Dependent Reorientation and Rehybridization of the Strongly Chemisorbed Conjugated Molecule Hexaazatriphenylene-hexacarbonitrile (HATCN) on Ag(111) — •A. Vollmer[1], B. Bröker[2], O. T. Hofmann[3], G. M. Rangger[3], P. Frank[3], R.-P. Blum[2], R. Rieger[4], L. Venema[5], H. Glowatzki[2], K. Müllen[4], J. P. Rabe[2], A. Winkler[3], P. Rudolf[5], E. Zojer[3], and N. Koch[2,1] — [1]Helmholtz Zentrum Berlin für Materialien und Energie GmbH, Germany — [2]Institut für Physik, Humboldt-Universität zu Berlin, Germany — [3]Institute of Solid State Physics, Graz University of Technology, Austria — [4]MPI für Polymerforschung, Mainz, Germany — [5]Zernike Institute for Advanced Materials, Groningen, The Netherlands

Understanding the fundamental electronic and morphological properties of interfaces between metals and conjugated organic materials (COM) is crucial in the field of organic electronics. Hitherto, it has been commonly accepted that the orientation of a COM monolayer on a metal surface depends only on the strength of metal-molecule vs. intermolecular interactions. Here we show that a re-orientation of a face-on to an edge-on first layer can be triggered by increasing the amount of deposited molecules. We will report on the strong molecular acceptor HATCN on Ag(111), where this rearrangement is facilitated through the molecular cyano groups and accompanied by a rehybridization of molecular and metal electronic states, significantly modifying the interface and surface electronic properties. We will present UPS, $\Delta\Phi$, TDS, RAIRS, STM, and DFT. PRL,104,23,(2010), Nano Lett,8,11,(2008)

DS 42.54 Wed 15:00 P1

Chemical transformation of chloroaluminum phthalocyanine films upon post deposition annealing in magnetic field — Tamara Basova[1], Vladimir Plyashkevich[1], •Fotini Petraki[2], Heiko Peisert[2], and Thomas Chassé[2] — [1]Laboratory for chemistry of volatile and metallorganic compounds, Nikolaev Institute

of Inorganic Chemistry, Siberian Branch Russian Academy of Science, 630090, Lavrentiev ave.3, Novosibirsk, Russian Federation — [2]Universität Tübingen, IPTC, Auf der Morgenstelle 18, 72076 Tübingen, Germany

The annealing of chloroaluminum(III)phthalocyanine (AlClPc) thin films in air results in a chemical transformation to μ-(oxo)bis[phthalocyaninato] aluminum(III) ((AlPc)2O). A comparative analysis of the influence of post deposition annealing process without and under applied magnetic field of 1 T, on the composition and morphology of AlClPc films, has been carried out. The chemical transformation of AlClPc to (AlPc)2O on the substrate surface is studied using UV-vis and Infrared (IR) spectroscopies, Raman, X-ray photoelectron spectroscopy (XPS) as well as atomic force microscopy (AFM). Two interesting effects were observed upon heating the AlClPc films in magnetic field of 1 T: First, the temperature of the chemical transformation of AlClPc to (AlPc)2O decreases from 300 to 200 °C, when magnetic field was applied during post deposition annealing. Second, the formation of (AlPc)2O films with elongated crystallites with a preferential orientation was observed. The heating of (AlPc)2O films in the magnetic field at the same conditions did not demonstrate any effect on structure and morphology of these films.

DS 42.55 Wed 15:00 P1

Second-Harmonic Generation Spectroscopy of Magnesium Tetraphenylporphyrin Films

— •Jan Metje[1,2], Gerhard Lilienkamp[1], and Winfried Daum[1,2] — [1]Institute for Energy Research and Physical Technologies, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld — [2]NTH School for Contacts in Nanosystems

Porphyrins such as magnesium tetraphenylporphyrin (MgTPP) are widely known as energy harvester in biological energy cycles. More recently, their efficient conversion of photonic energy has triggered their use as sensitizers in solar cells. The strong absorption of light by porphyrin molecules in the blue-to-violet spectral range is due to the molecular $S_0 \rightarrow S_2$ excitation which gives rise to so-called Soret bands in absorption experiments. While the spectral position and width of these bands are rather insensitive to a substitution of the central atom (Mg, Zn, 2H), the spectra strongly depend on the local environment of the molecule. In this contribution we report on second-harmonic generation (SHG) experiments performed with MgTPP films evaporated on SiO_2 under ultra-high vacuum conditions. SHG spectra of MgTPP films in the spectral range of the Soret band show two bands with energies at 2.94 eV (422 nm) and 2.7 eV (460 nm). The spectral position of the former band agrees with that of individual MgTPP molecules dissolved in solutions whereas the large red shift of the latter band indicates strong intermolecular interactions. Results of SHG experiments with MgTPP films of different thicknesses will be presented to verify the surface and bulk character, respectively, of these molecular excitations.

DS 42.56 Wed 15:00 P1

Epitaxial Growth of Lead-Phthalocyanine on GaAs(001) Reconstructed Surfaces

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Heterostructures of semiconductors and metal substituted phthalocyanine (MPc) films have attracted growing scientific and industrial interest because of their application in opto- or electronic devices. An important aspect in this respect is the control of the molecular ordering within the organic layers since the electrical conductivity of these layer depends crucially on the orientation and ordering of the molecules. Here we report on Raman scattering experiments on lead phthalocyanine (PbPc) layers (up to 20nm thick) deposited on GaAs(001) with c(4x4), (2x4) and (4x2) reconstructed surfaces. The Raman intensity selection rules of the PbPc vibrational modes are analyzed with respect to the GaAs(001) substrate coordinate system by rotating the sample around its normal. We find that some Raman intensities of the PbPc molecular vibratonal modes, depending on the initial surface reconstruction, vary with a period exactly correlated with the GaAs(001) substrate phonons modes. These findings prove an epitaxial growth mode of the PbPc layers on the GaAs(001) substrate. The results are in agreement with scanning tunneling microscopy (STM) results on submonolayer coverages demonstrating a correlation between the initial GaAs(001) surface structure and the PbPc layer properties.

DS 42.57 Wed 15:00 P1

Tailoring defect structure in nano porous alumina templates

— •Hongdan Yan[1], Dirk Wulferding[1], Peter Lemmens[1], Jianmin Shi[2], Klaus Dieter Becker[2], Fatih Kalkan[3], Karina Morgenstern[3], Aidin Lak[4], and Meinhard Schilling[4] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]IPTC, TU-BS, Braunschweig, Germany — [3]IFP, LU Hannover, Germany — [4]EMG, TU-BS, Braunschweig, Germany

Self organized, nanostructured materials are interesting from both fundamental and applied point of view. Often their optical properties are deteriorated by fluorescence due to oxygen defects. In the present study we demonstrate how preparation conditions and a consequent annealing can be used to optimize both morphology and defect structure of templates. These templates are used to realize plasmonic devices by a electrochemical deposition of Au wires.

Work supported by DFG, IGSM and NTH.

DS 42.58 Wed 15:00 P1

Optical and electrical properties of nano-Si embedded in silica as novel solar cell semiconductor

— •David Friedrich, Karl-Heinz Heinig, and Bernd Schmidt — Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Germany

Silicon photovoltaic (PV) modules are based on monocrystalline, microcrystalline or thin film amorphous silicon. Nanostructured Si might be one approach to achieve lower costs of electricity (€/Wp) by higher PV cell efficiency without substantial increase of fabrication costs.

Here we present measurements of optical and electrical properties of Si nanocrystals and sponge-like nano-Si morphologies embedded in silica. These Si nanostructures are fabricated by sputter deposition of SiOx followed by thermally activated nucleation or spinodal decomposition, resulting in Si nanoclusters or Si nanosponge, respectively. Due to the nanoscale feature size of the obtained Si sponge its band gap is opened by quantum confinement. Compared to separated Si nanoclusters, the spongy morphology ensures a higher electrical conductivity due to percolation.

Optical absorption, reflection and transmission data of SiOx and phase separated Si nanostructures will be presented for different compositions, i.e. x-dependent. The SiOx composition has been measured by Rutherford Backscattering (RBS). Additionally, spectroscopic ellipsometry and photolumiscence studies have been performed. These results will be discussed together with electrical resistivity measurements.

DS 42.59 Wed 15:00 P1

Local elemental and surface chemistry analysis of laser-nanostructured thin Au films

— •Jürgen W. Gerlach, Marisa Mäder, Thomas Höche, Dietmar Hirsch, and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung, 04318 Leipzig

A regular arrangement of substrate-bound Au dots in fields of about 100 μm x 100 μm in size was obtained by structuring a thin Au film, which was deposited on a sapphire substrate, by Diffraction Mask Projection Laser Ablation (DiMPLA) [1]. Typical dot diameters of 150 nm to 200 nm resulted. Transmission electron microscopy revealed that during the structuring process with a single excimer laser pulse (KrF, 248 nm wavelength, 25 ns pulse length) the near-surface region of the single crystalline substrate melted and the Au dots were drawn partially or fully into the superficially molten substrate. Eventually, the Au dots were in parts embedded in the then amorphous near surface region of the substrate. In the present study, such fields of well-arranged Au dots on sapphire are investigated regarding the lateral elemental distribution as well as the surface chemistry by photoelectron spectroscopy. The results of elemental parallel imaging and small spot electron spectroscopy are compared with the actual distribution of Au dots in the structured fields as obtained by scanning electron microscopy. The presented results are discussed regarding localized charging effects or alternatively the formation of gold oxide. In the latter case, reaction of the Au dots with oxygen from the surrounding air during the laser structuring process has to be taken into account.

[1] M. Mäder et al., Phys. Stat. Sol. B, 247 (2010) 1372.

DS 42.60 Wed 15:00 P1

Mesostructured zinc oxide as basis material for dye-sensitized solar cells

— •Christoph Richter[1], Michael Schröder[2], Bernd Smarsly[2], and Derck Schlettwein[1] — [1]Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email:schlettwein@uni-giessen.de — [2]Institute of Physical Chemistry, Justus-Liebig-University Giessen, Germany

Polysterene (PS) spheres of a narrow size distribution were synthesized by mini-emulsion polymerization. Films (1 - 10 μm) of densely packed PS spheres were prepared from suspensions of the spheres on fluorine-doped tin oxide films on a carrier substrate. Macroporous ZnO films were electrodeposited into the free space between the polystyrene spheres. The PS template was removed by solvent or UV treatment leaving behind the macroporous ZnO matrix. In a subsequent deposition step, additional ZnO was electrodeposited into the macropores this time, however, using a molecular template and hence forming mesoporous ZnO filling the space which ad been occupied by the PS spheres before. The films were characterized and their applicability as hierarchical structures in dye-sensitized solar cells will be discussed.

DS 42.61 Wed 15:00 P1

Piezoresponse force measurements on hetero-epitaxially grown Sodium-Bismuth-Titanate (NBT) thin films deposited by MOCVD-technique — •Andreas Duk, Jutta Schwarzkopf, Günter Wagner, Saud Bin Anooz, and Roberto Fornari — Institute for Crystal Growth, Berlin, Germany

Epitaxially grown Sodium-Bismuth-Titanate (NBT) thin films deposited by the MOCVD-technique on SrTiO3, NdGaO3 and DyScO3 were investigated by local piezoresponse force measurements. Aurivillius phases with m = 3, m= 3.5 and m = 4 and the Na0.5Bi0.5TiO3 perovskite phase were realized by varying the substrate temperature and/or the Na/Bi ratio in the gas phase. It has been observed that the effective piezoelectric coefficient increases with increasing number of perovskite units between two (Bi2O2)2+ intermediate layers. The influence of the lattice strain in the films on the piezoelectric response and the ferroelectric properties were studied by using different oxide substrates and films with variable film thickness.

DS 42.62 Wed 15:00 P1

Combined Quasi-Magnetoresistive Magnetic Field Sensor utilizing Magnetostriction and Quantum Tunneling — Bodo Henkel[1], Amit Kulkarni[1], •Thomas Strunskus[1], Vladimir Zaporojtchenko[1], Christoph Bechtold[2], Eckhard Quandt[2], and Franz Faupel[1] — [1]Multicomponent Materials, Institute for Materials Science, University of Kiel, Kaiserstr. 2, 24143 Kiel, Germany — [2]Inorganic Functional Materials, Institute for Materials Science, University of Kiel, Kaiserstr. 2, 24143 Kiel, Germany

A new concept of magnetic field sensor was developed and characterized. It uses the combination of magnetostriction provided by a Terfenol-D substrate and quantum tunneling through a 2D gold cluster array which is in the regime near to percolation threshold. There already a small magnetically induced elongation of the Terfenol-D crystal will lead to a well measurable change of current through the cluster array. An additional feature of the specific design of the sensor is direction sensitivity with regard to external magnetic fields. The sensor was characterized in terms of sensor signal hysteresis, sensitivity, repeatability, aging behaviour and the effect of cluster embedding into the underlying polymer layer. A well defined repeatable hysteresis with a change in signal amplitude (current) of 5.50 % was achieved in first experiments. Designs for higher ratios are in progress.

DS 42.63 Wed 15:00 P1

Nanocomposites prepared by plasma polymerization and cluster deposition — •Tilo Peter[1], Maike Wegner[1], Thomas Strunskus[1], Vladimir Zaporojtchenko[1], Sven Bornholdt[2], Holger Kersten[2], and Franz Faupel[1] — [1]Institute for Materials Science, Kiel, Germany — [2]Institute of Experimental and Applied Physics, Kiel, Germany

Recently, there is much interest in nanocomposites consisting of metal nanoparticles dispersed in a dielectric matrix due to their novel functional properties [1,2]. In many cases the formation of metal clusters is affected by chemical reactions with the host matrix material during deposition. The integration of a magnetron cluster source into a plasma deposition process allows the pre formation of clusters in the gas phase and subsequent codeposition with the matrix material. Here we focus on the properties of Ag clusters and the subsequently obtained nanocomposites by embedding in a polymer matrix which is deposited by plasma polymerization of Hexamethyldisiloxane. Two possible deposition systems are investigated: In the first system the cluster formation and plasma polymerization take place in the same plasma region, while in the second system the cluster formation takes place in a separate atmosphere and at different plasma parameters. The cluster and nanocomposite film properties were investigated by x-ray photoelectron spectroscopy, transmission electron microscopy and UV/Vis spectroscopy.

[1] Faupel,F. et.al., Contrib. Plasma Phys. 47(2007), 537.

[2] Faupel,F. et.al., Adv. Eng. Mater. (2010) accepted.

DS 42.64 Wed 15:00 P1

Customized arrangements of a-Ge nanocolumns by glancing angle deposition — •Jens Bauer, Michael Weise, Chinmay Khare, Christoph Grüner, and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung, Permoserstrasse 15, D-04318 Leipzig, Germany

We present PVD investigations on self-organized a-Ge nanostructures by glancing angle deposition (GLAD). In particular, a Ge particle beam provided by ion-beam sputtering is directed under a flat angle to the substrate (glancing angle $< 5°$). As a result of shadowing inclined nanoneedles evolve competitively. By use of substrate rotation the nanostructure can be customized to vertical posts, screws or spirals. To improve nanostructure arrangement and uniformity patterned substrates with symmetrically ordered surface mounds were applied: square and hcp orders by electron beam lithography and honeycomb or hcp orders by nanosphere lithography. The temporal evolution is distinguished by three morphological stages: 1) Initially the shape and size of the pre-pattern mounds determine the GLAD structures' shape. The structure thickness successively broadens. 2) Following a columnar shape with parallel border planes is obtained reflecting the pattern symmetry: square cross-section for square order, three-fold for honeycomb, and hexagonal to round for hcp. Characteristic caps are formed at the nanostructures' tops. Both the size of the border planes and the cap size depend strongly on the glancing angle and the pattern periodicity. 3) Caused by increasing competition the formation of individual GLAD columns stops and the pre-pattern arrangement gets lost.

DS 42.65 Wed 15:00 P1

Reflectivity characterization of silicon ion-implanted PMMA for device application at 1.55 μm — •Bojana Florian[1], Ivan Stefanov[2], and Georgi Hadjichristov[3] — [1]Bulgarian Institute of Metrology, 2 Prof. P. Mutafchiev Str., 1797 Sofia, Bulgaria — [2]Dept.of Quantum Electronics, Faculty of Physics, Sofia University, 5 James Bourchier Blvd., 1164 Sofia, Bulgaria — [3]Institute of Solid State Physics, 72 Tzarigradsko Chaussee Blvd., 1784 Sofia, Bulgaria

Silicon ion-implanted poly(methyl methacrylate) (PMMA) ultrathin layers of thickness of 100 nm buried in a depth of 100 nm were characterized by means of their near-IR reflectivity. As a case of photonic application for an integrated optics purpose (in optical devices operating at the telecommunications wavelength of 1.55 μm), we will present here an ultrathin reflective-type beam splitter/coupler with a low absorption loss. Such an optical element was examined upon illumination with the output of a 1.55 μm CW laser source coupled to an optic fiber.

Specular reflectance-to-transmission ratio (R/T) of PMMA plates implanted with Si+ ions at an energy of 50 keV and ion fluence in the range from 10^14 to 10^17 cm^2 were analyzed as a function of the ion-implant fluence, as well as the angle of incidence, polarization and the power of incident laser beam. Diffuse reflectivity of the layers at 1.55 μm was also carefuly measured. The nanoclustered structure of the carbonaceous subsurface ion-implanted layer enhances R/T [1].

[1] G.B. Hadjichristov, I.L. Stefanov, Appl. Opt. 49 (2010) 1876.

Work supported by grants #FNI 098/2010 of the Sofia University and #DRNF 02/8-2009 of the National Science Fund of Bulgaria.

DS 42.66 Wed 15:00 P1

Growth and optimization of YBa$_2$Cu$_3$O$_{7-x}$-SrTiO$_3$-multilayers — •Alexander Guillaume, Frank Ludwig, Jan M. Scholtyssek, and Meinhard Schilling — Institut für Elektrische Messtechnik und Grundlagen der Elektrotechnik, Technische Universität Braunschweig, Hans-Sommer-Str. 66, D-38106 Braunschweig, Germany

YBa$_2$Cu$_3$O$_{7-x}$ (YBCO) is a commonly used high-T$_c$ superconducting material. Lattice matched insulating materials, such as SrTiO$_3$ (STO), are required for the fabrication of complex multilayer devices. We grow STO-YBCO multilayers on (100)-surfaces of STO-substrates via pulsed laser deposition (PLD). Here, the optimization of the PLD-parameters for the deposition of YBCO by using the technique of design of experiments (DOE) based on [1] is presented. Another DOE for optimizing the parameters of the insulating STO-films is currently carried out. The parameters varied are the energy density of the laser pulses, the oxygen partial pressure inside the recipient and the temperature of the substrate. The optimization took into account the morphological, electrical and superconducting properties of the films.

Atomic-force-micrographs are presented to illustrate the film morphology. Screening measurements were performed to investigate the superconducting transition characteristics and the homogeneity of the YBCO-layer while the van der Pauw-method was used to determine the thin film-resistivity.

[1] J.K. Heinsohn, D. Reimer, A. Richter, K.O. Subke, and M. Schilling, Physica C **299** (1998) 99-112.

DS 42.67 Wed 15:00 P1

Deposition of diamond-like carbon films on 3D substrates by liquid electrochemical technique — •Yangyang He[1], Guifeng Zhang[2], and Volker Buck[1] — [1]Thin Film Technology Group, Faculty of Physics, University Duisburg-Essen and CeNIDE, 47057, Duisburg, Germany — [2]School of Materials Science and Engineering, Dalian University of Technology, 116024, Dalian, China

Diamond-like carbon (DLC) films were simultaneously deposited on horizontally and vertically aligned stainless steel substrates by liquid electrochemical technique at low temperature. The applied potential and deposition time were 1000V and 2h. Isopropyl alcohol was chosen as electrolyte due to the advantages of high dielectric constant and small viscosity. SEM showed that the films deposited on horizontally aligned substrate were smooth and homogeneous. The films had uniform thickness on the whole surface of the horizontally aligned substrates. Raman analysis confirmed that typical DLC films were deposited on both substrates. The results showed that the films deposited on the horizontally aligned substrates had quite similar Raman spectra all over the surface. However, Raman spectra of the films deposited on the vertically aligned substrates appeared different depending on the position inside the solutions. The intensity of Raman spectra was supposed to correlate with the film thickness. It could be concluded that DLC films can be deposited on 3D substrates by liquid electrochemical technique which is of great importance in the industrial applications of DLC films.

DS 42.68 Wed 15:00 P1

Design and construction of an apparatus for the deposition of mass selected metal clusters — •Arne Fischer, Herbert Gleiter, and Horst Hahn — Karlsruher Institut für Technologie, Institut für Nanotechnologie, 76344 Eggenstein-Leopoldshafen, Germany

We report on the design and the construction of an apparatus for the non-destructive deposition of mass selected metal clusters. It will give us the opportunity to study clusters on various surfaces as well as clusters buried in matrices of other materials.

The clusters are provided by a magnetron sputter source installed in a liquid nitrogen cooled tube. The cold surrounding allows the sputtered atoms to condense to clusters, which are extracted by a helium stream. Depending on the mode of operation either anions or cations are accelerated and formed to an ion beam by electrostatic lenses. Downstream the beam gets mass separated in a 90° sector magnet (r = 500mm, resolution approx. 1/50), decelerated by an array of two einzellenses and finally soft landed on a cooled substrate (landing energy approx. 0.1 eV/atom). The matrix material can be optionally co-deposited via an integrated MBE.

DS 42.69 Wed 15:00 P1

Multiscale study of submonolayer growth for Fe/Mo(110) — •Martin Mašín[1], Mika O. Jahma[2], Tapio Ala-Nissila[2], and Miroslav Kotrla[1] — [1]Instute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, Prague, 18221, Czech Republic — [2]Department of Applied Physics, Aalto University School of Science, P.O. Box 11000 , FI-00076 Aalto, Espoo, Finland

We apply a multiscale approach to study growth during Molecular Beam Epitaxy (MBE) in submonolayer coverages for Fe/Mo(110). We compare results obtained for island size distributions from two methods – the Kinetic Rate Equation (KRE) approach and Monte Carlo (MC) simulations. The relevant energy parameters in MC are the activation energy for single–particle jumps, binding energy to the substrate, and attractive adatom interactions. In the second part we use the KRE approach combined with the Particle Coalescence Method to compute the island size distributions. KRE gives time evolution of the island size distributions for a system undergoing diffusion driven aggregation. Incoming parameters are diffusion coefficients, obtained from independent MC simulations, and aggregation kernels. For comparison we use the scaled island density function $g(x)$ as a function of the normalized island size $x = s/\bar{s}$. In the case of KRE we use adatom–island and island–island aggregation modes at two temperatures 500 K and 1000 K. In the case of MC we consider only 500 K due to computational demands. At this temperature we have good agreement for the scaling function between the MC and KRE adatom–island aggregation models.

DS 42.70 Wed 15:00 P1

PCMO thin film for resistive switching devices — •Anja Herpers, Chanwoo Park, Tobias Menke, Rainer Bruchhaus, Regina Dittmann, and Rainer Waser — Peter Gruenberg Institute (PGI-7), Electronic Materials, Forschungszentrum Juelich, 52425 Juelich, Germany

In many transition metal oxides the electrical resistance can be changed between two defined values by applying an electrical field. This effect can be used in resistive random access memories for non-volatile data storage.

In this work the material $\mathrm{Pr}_{0.48}\mathrm{Ca}_{0.52}\mathrm{MnO}_3$ (PCMO) as perovskite oxide and its interface to titanium and platinum is investigated. For the thin film preparation RHEED-assisted pulsed laser deposition is used. The material is epitaxially grown on SrTiO_3 substrates and SrRuO_3 films under different conditions. The deposition parameters have been optimized in regard of RHEED pattern (50 unit cell layers visible), surface roughness down to 2Å by AFM and crystal quality using XRD (FWHM of rocking curve down to 0.034°). We will compare devices having interfaces to metals with different work functions, as it is considered in literature that the Schottky barrier is changed during switching. We will present the corresponding I-V-curves and switching results.

DS 42.71 Wed 15:00 P1

Investigations of Thin Films Derived from Nanocrystalline Silicon Powder applying Raman, Infrared Spectroscopy, and Spectroscopic Ellipsometry — •Falko Seidel[1], Ovidiu D. Gordan[1], Roy Buschbeck[2], Alexander Jakob[2], and Dietrich R. T. Zahn[1] — [1]Semiconductor Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany — [2]Inorganic Chemistry, Chemnitz University of Technology, D-09107 Chemnitz, Germany

Thin film solar cells can have the advantage of being mechanically flexible and at the same time reducing material and production costs. At present, two main types of photovoltaic (PV) cells are found marketing applications: II-VI respectively II-III-VI compound semiconductors (CdTe, Cu(In,Ga)(S,Se)2 CIGS) and amorphous silicon (a-Si). The optical band gap of non-silicon CIGS PV cells can be tuned by changing the ratio of the incorporated elements. The most important advantage of Si is its availability. For application in solar cells it would be desirable to tune silicon properties as well. Thus, nanocrystalline silicon (nc-Si) is of great interest because of the band gap being tuneable with the particle size. The confinement effect leads to a shift of the optical band gap to higher energies. Additionally, the use of nanocrystalline powder makes price-efficient printing processes in the production feasible.

In this work optical characterisation of nc-Si powder and drop coated nc-Si films is presented using Raman Spectroscopy, Fourier Transform Infrared Spectroscopy (FTIRS), and Variable Angle Spectroscopic Ellipsometry (VASE).

DS 42.72 Wed 15:00 P1

Magneto-optical Kerr effect studies of copper oxide and cobalt thin films — •Michael Fronk[1], Steve Müller[2], Thomas Waechtler[2], Stefan E. Schulz[2], Dietrich R.T. Zahn[1], and Georgeta Salvan[1] — [1]Chemnitz University of Technology, Chemnitz, Germany — [2]Fraunhofer Research Institution for Electronic Nano Systems ENAS, Chemnitz, Germany

Copper oxide is supposed to be a model material for tunnel-magnetoresistance (TMR) structures together with cobalt as ferromagnetic electrode. Therefore the magnetic properties of copper oxide itself are of interest and under investigation by various techniques. This contribution will present spectroscopic magneto-optical Kerr effect (MOKE) studies of thin films of this material. The films are produced by atomic layer deposition based on a Cu(I) β-diketonate precursor at a process temperature of 120°C. The copper oxide films turned out to be magneto-optically active both in the spectral range around 2 eV and above 4 eV. Besides the experimental MOKE data the material-intrinsic magneto-optical Voigt constant extracted from optical model calculations will be presented. Cobalt, the ferromagnetic counterpart in the TMR structures, was prepared by magnetron sputtering as thin films with different thicknesses. The Voigt constant of Co can be deduced from measurements on thick films (˜ 120 nm). It is investigated whether these data can be used to predict the magneto-optical response of thinner Co layers (~ 10 nm).

DS 42.73 Wed 15:00 P1

Deep Trap Analysis using QTS and DLTS on Schottky Diodes with Gold Implanted Silicon — •Markus Arnold, Axel Fechner, Susann Müller, and Dietrich R.T. Zahn — Chemnitz University of Technology, Semiconductor Physics, 09107 Chemnitz, Germany

Charge transient spectroscopy (QTS) and deep-level transient spectroscopy (DLTS) measurements of Silicon Schottky diodes are presented revealing the influence of gold implantation into n-doped silicon on the charge carrier transport and trapping properties.

Charge transient spectroscopy (QTS) developed originally by Kirov et al. [1] is an electrical measurement method related to deep-level transient spectroscopy (DLTS) developed originally by Lang et al. [2]. Especially using QTS it is possible to measure high ohmic structures like Metal-Oxide-Semiconductor (MOS) capacitors with a high sensitivity. Due to the leakage current in the reverse bias region of Schottky diodes it is very challenging to measure QTS. So the results obtained using QTS are compared to current-voltage, capacitance-voltage, and DLTS measurements on the same samples. The compatibility of these techniques and their differences are discussed.

[1] K. I. Kirov, K.B. Radev, Phys. Stat. Sol. (a) 63 (1981) 711

[2] D. V. Lang, J. Appl. Phys. 45 (1974) 3023

DS 42.74 Wed 15:00 P1

Spectroscopic Investigations of DC Magnetron Sputtered Amorphous Silicon Thin Films — •Philipp Schäfer[1], Frank Nobis[2], Markus Arnold[1], 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

Spectroscopic techniques were used to provide an in-depth analysis of dc magnetron sputtered hydrogenated amorphous silicon (a-Si:H) layers for photovoltaic applications. The complex optical dispersion in the range from 0.7 eV to 5.0 eV was determined using variable angle spectroscopic ellipsometry. A shift of the absorption onset to higher energies for samples sputtered at increased hydrogen flow rates is related to less defect states within the mobility gap. In order to calculate the hydrogen content of the deposited layers, the absorption due to silicon-hydrogen stretching vibrations was evaluated employing Fourier transformed infrared (FTIR) spectroscopy. A linear relationship between the absorption onset and the hydrogen concentration is observed. Raman spectroscopy confirms the purely amorphous nature of the silicon network. A deeper understanding of the states within the mobility gap is obtained from electrical spectroscopic techniques. Charge deep level transient spectroscopy measurements at various temperatures probe the defect level energy and concentration. Furthermore, a comparison with densities estimated by drive level capacitance profiling is provided.

DS 42.75 Wed 15:00 P1

Mechanical dissipation in thermally grown silica at low temperatures — •Julius Komma[1], Christian Schwarz[1], Gerd Hofmann[1], Daniel Heinert[1], Ronny Nawrodt[1], Giles Hammond[2], and Paul Seidel[1] — [1]Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 5, D-07743 Jena, Germany — [2]Glasgow University, G12 8QQ Glasgow, UK

Silica (SiO_2) is a common material as low index material in thin optical layers. Its mechanical loss is of great interest since the thermal noise of a surface layer is directly related to its mechanical loss by means of the fluctuation dissipation theorem. It is well known that bulk silica shows a very large dissipation peak at cryogenic temperatures between 30 and 40 K.

We present a detailed analysis of the mechanical loss of thin silica layers with a thickness between 0.1 and $3\,\mu$m in a temperature range from 5 to 300 K. The measurements have been performed in a ring-down technique. The layers have been produced by thermal oxidation of thin silicon flexures.

The dependence of the mechanical loss of the layer thickness is discussed and a possible transition of the micro-structure from a thin layer to a thick layer model is presented. The comparison of the activation energy of the dissipation process reveals differences between the bulk silica and thin layer silica samples.

This work is supported by the German Science Foundation (DFG) within the SFB Transregio 7.

DS 42.76 Wed 15:00 P1

Enhancement of growth and structure properties of $YBa_2Cu_3O_{7-\delta}$ thin layers by in situ incorporation of gold nano-clusters — •Ralf Erlebach[1], Michael Hübner[1], Sandra Christke[1], Veit Grosse[1], Frank Schmidl[1], Jürgen Kräusslich[2], Markus Rettenmayr[3], and Paul Seidel[1] — [1]Friedrich-Schiller-University Jena, Institute of Solid State Physics, Helmholtzweg 5, 07743 Jena, Germany — [2]Friedrich-Schiller-University Jena, Institute of Optics and Quantum Electronics, Max-Wien-Platz 1, 07743 Jena, Germany — [3]Friedrich-Schiller-University Jena, Institute of Materials Sciene and Technology, Löbdergraben 32, 07743 Jena, Germany

For most hetero-epitactic growth techniques, structural defects due to the lattice misfit, namely tilts, precipitates or holes, turn out to be limiting factors for the succesful fabrication of multilayer systems. A new approach of an in situ growth technique dealing with this problem by incorporation of gold nano-clusters is examined. Therefore, pulsed laser deposition (PLD) of a high-T_C $YBa_2Cu_3O_{7-\delta}$ (YBCO) layer onto a strontium titanate (STO) template with a temporary interlayer of gold with a well-defined film thickness is investigated. Within this process, the gold interlayer shows nano-clustering behavior.

Effects on the properties of structure like crystallographic or surface features of the ablated YBCO layer by variation of the film thickness of the gold and YBCO layers are presented. Moreover, distribution and clustering behavior of the crystallized gold nano-particles as well as the basic superconducting properties of the layer system are analyzed.

DS 42.77 Wed 15:00 P1

Investigation of improvements of electrical and optical properties of reactively sputtered ZnO:Al thin films upon post-deposition thermal annealing — •Patrick Ries, Dominik Köhl, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

Aluminium-doped zinc oxide (ZnO:Al) has gained significant scientific and industrial interest during the past decade. Particularly, ZnO:Al films have become the material of choice in the fabrication of transparent electrodes for silicon thin film solar cells, which offer a low-cost alternative to wafer-based highly-efficient but more expensive modules. ZnO:Al films exhibit high optical transparency. The electrical conductivity is only by a factor of 3 smaller than the one of ITO films. ITO is the most commonly used but more expensive Transparent Conducting Oxide. Consequently, efforts are presently focused on improving film properties to improve the electrical conductivity of ZnO:Al to potentially replace ITO in the near future. To accomplish this goal, post-deposition annealing of the specimens to cure defects is investigated in the present study. The aim is to thoroughly understand the principle scattering mechanisms. The electrical and optical properties as a function of annealing temperature are investigated by Ellipsometry, FTIR & UV/VIS spectroscopy, van der Pauw and Hall measurements. Conclusions on the dominant scattering channels and their temperature dependence are drawn.

DS 42.78 Wed 15:00 P1

Photocatalysis in sputtered TiO_2 thin films: Measurement of the surface work function to correlate structural features with photocatalytic activity — •Alexandra Yatim, Dominik Köhl, and Matthias Wuttig — I. Physikalisches Institut IA, RWTH Aachen, Germany

Titanium dioxide (TiO_2) is known for its very unique physical properties. Specifically, TiO_2 provides a large refractive index and a pronounced photocatalytic activity. Therefore it has become the material of choice in the fabrication of anti-reflective or self-cleaning coatings in architectural glazing. Interestingly, although products already exist on the market, little is known about the underlying mechanism governing the strong photocatalysis. This particularly includes insufficient knowledge about the influence of the specific coating process on the activity of the films. In the architectural glazing industry, magnetron sputtering is preferably utilized since it provides both, homogeneity of the coating on large area substrates and flexibility in the choice of materials. Hence, it is the aim of the present work to investigate the photocatalytic properties of sputtered TiO_2 thin films. Kelvin Probe measurements to determine the surface photovoltage of the specimens under UV illumination are utilized. The data is compared and correlated with data of structural properties from XRD and AFM measurements and with the specific deposition conditions. The major goal of the study is to explain the photocatalytic activity of the specimens on a microscopic scale and hence to find criteria that allow for the fabrication of highly active coatings.

DS 42.79 Wed 15:00 P1

Improved lateral conductivity of a two phase SiO:ucSi[n] intermediate reflective layer in thin film solar cells — Burkhard Gilles[1], Ulrich Heinzmann[1], Helmut Stiebig[2], Stefan Gruss[2], and •Florian Maier[2] — [1]Univ. of Bielefeld, Faculty of Physics, Molecular & Surface Physics — [2]Malibu GmbH Co. KG

Increasing the efficiency of thin film solar cells is a crucial requirement for competing with other technologies in the field of solar energy conversion. After the introduction of thin film tandem solar cells, light management has become an important issue to achieve this end. The application of intermediate reflective layers is a promising approach for the optimisation of the light distribution between top and bottom cell. Numerous works on this field have been carried out so far. However, a major problem is the poor conductivity of those films which lead to an increase of the series resistance. The application of a layer of doped silicon oxide containing a phase of microcrystalline silicon (μc-SiOx:H <n>) can overcome this problem. The experiments were carried out on samples of industrial scale (1.1 m x 1.3 m). A number of possibilities for the suppression of the lateral resistivity have been examined. A substantial increase of conductivity has been achieved. The correlation of growth conditions, thickness and conductivity will be discussed.

DS 42.80 Wed 15:00 P1

Thin SiO films condensed at different substrate temperatures studied by infrared spectroscopy — •Steffen Wetzel[1], Hans-Peter Gail[2], and Annemarie Pucci[1] — [1]Kirchhoff-Institut für Physik, INF 227, 69120 Heidelberg — [2]Institut für Theoretische Astrophysik, Albert-Ueberle-Str. 2, 69120 Heidelberg

Silicon oxides are not only of basic scientific interest but also of great importance in microelectronics and of considerable relevance in astronomy as building blocks of silicates, the most abundant minerals in space. Their spectral features can reveal the chemical composition and inform on formation conditions as gas pressure or temperature. To look into the origin of IR spectral changes, the growth of thermally evaporated silicon monoxide (SiO) on silicon substrates was studied in situ by infrared spectroscopy under ultra-high vacuum conditions. Previous studies on the growth of ultrathin films on clean Si(111) showed a thickness dependent shift of the main vibrational line of up to 120 cm^{-1} compared to the bulk value of 984 cm^{-1} [1, 2] at 300 K substrate temperature. In our recent study we investigated the influence of different substrate temperatures on the condensation process. Measurements at temperatures between 40 K and 500 K reveal a clear shift of the vibrational peak position from 960 cm^{-1} to 1000 cm^{-1} with increasing temperature. Details on the experimental setup and explanations for the observed peak shift will be presented.

[1] M. Klevenz et al. Phys. Status Solidi B, 247(9), 2179-2184 (2010)

[2] M. Klevenz et al. Applied Spectroscopy, 64(3), 298-303 (2010)

DS 42.81 Wed 15:00 P1

The effect of gold nanoclusters on the growth and properties of homoepitaxial strontium titanate layers — •Sandra Christke[1], Ralf Erlebach[1], Frank Schmidl[1], Jürgen Kräusslich[2], Markus Rettenmayr[3], and Paul Seidel[1] — [1]Friedrich-Schiller-University Jena, Institute of Solid State Physics, Helmholtzweg 5, 07743 Jena, Germany — [2]Friedrich-Schiller-University Jena, Institute of Optics and Quantum Electronics, Max-Wien-Platz 1, 07743 Jena, Germany — [3]Friedrich-Schiller-University Jena, Institute of Materials Science and Technology, Löbdergraben 32, 07743 Jena, Germany

We use pulsed layer deposition (PLD) to fabricate single crystal thin films and layer systems which can be epitaxially deposited. Here we present analysis regarding the growth of strontium titanate (STO) layers on single crystal STO substrates. The specific characteristic of these experiments is the deposition of the STO layer through PLD. Therefore, during the formation of the STO layer onto the substrate the initial gold layer is transformed into nanoclusters. We show the dependence of crystallographic and optical properties as a function of gold and STO layer thicknesses as well as surface parameters.

DS 42.82 Wed 15:00 P1

Investigation of optical and electrical properties of magnetron sputtered ZnO:Al films for in-line characterization — •Regina Nowak, Benedikt Schumacher, Daniela Rogler, Karsten von Maydell, and Carsten Agert — NEXT ENERGY, EWE-Forschungszentrum für Energietechnologie e.V.

Due to cheaper and easier processing, thin film solar cells promise a substantial cost reduction potential compared to conventional crystalline silicon solar cells. The front electrode of these devices consists of a transparent conducting oxide (TCO) layer. In the case of hydrogenated amorphous (a-Si:H) and microcrystalline (μc-Si:H) silicon thin film solar cells, aluminum doped zinc oxide (ZnO:Al) is widely used as TCO.

In this study, the influence of the variation of the process parameters on the optical and electrical properties of ZnO:Al has been analyzed. Therefore ZnO:Al layers on glass were deposited under varying conditions using magnetron sputtering. The ZnO:Al films were characterized by spectroscopic ellipsometry, raman spectroscopy, four-point probe and AFM. The aim of these investigations is to find measurable values which can be used for cheap process control. This shall later on be involved in an in-line characterization of the whole solar cell.

DS 42.83 Wed 15:00 P1

Significant stress reduction of cBN layers upon ion irradiation at elevated temperatures — •Stefan Weidner[1], Sebastian Geburt[1], Jian Ye[2], Sven Ulrich[2], and Carsten Ronning[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena — [2]Institut für Materialforschung, Forschungszentrum Karlsruhe

Cubic boron nitride (cBN) is the hardest materials beneath diamond and exceeds the properties in terms of chemical resistivity, making it a promising candidate for ultra-hard coatings in extreme environments. Due to the ion assisted growth process, the cBN layers suffer from an intrinsic stress, which limits the layer thickness and therefore possible industrial applications.

To investigate new approaches for the synthesis of low stress cBN layers, we applied ion irradiation with various ion species (O, Ne, Kr) and at different temperatures between 300 to 600 K to cBN:O layers [1]. The intrinsic stress and the cBN content were monitored by profilometer and FTIR after each implantation step. As expected, ion irradiation at room temperature leads to a stress reduction with constant cBN content upon an ion induced damage up to 0.5 dpa [2], but a severe damage is introduced to the layer above this value resulting into a phase transition to hBN. However, irradiation at elevated temperatures results in a significant stress reduction without decrease of the cBN quality even up to 4.3 dpa.

[1] Ye at al. Thin Solid Films 517(3), 2008, p.1151-1155

[2] Widmayer et al., Diamond and Related Materials 6, 1997, p. 621-625

DS 42.84 Wed 15:00 P1

Interdiffusion and Magnetic Properties of Buried Fe-Layers in Planar Cavities Containing C-matrix — •Balaram Sahoo[1], Ralf Roehlsberger[1], Kai Schlage[1], Ulrich von Hoersten[2], Werner Keune[2], Heiko Wende[2], Hans-Christian Wille[1], Wolfgang Calibe[1], Joern Donges[1], Roman Chernikov[1], Edmund Welter[1], and Andre Rothkirch[1] — [1]Deutsches Elektronen Synchrotron DESY, Notkestr. 85, 22607, Hamburg, Germany — [2]Universität Duisburg-Essen, Lotharstr. 1, D-47048 Duisburg, Germany

We report on the preparation of planar wave guides by DC magnetron sputtering with buried 57Fe-probe layers of varied thickness and the characterization of their interfaces and magnetism via X-ray diffraction (XRD), X-ray reflectivity (XRR), extended X-ray absorption fine structure (EXAFS) spectroscopy and 57Fe conversion-electron Mössbauer spectroscopy (CEMS). XRD, EXAFS and CEMS results suggests the amorphous nature of the diffused interface. CEMS results demonstrate that the Fe layers are paramagnetic at RT, when the Fe layer thickness was below 1.1 nm. A paramagnetic to ferromagnetic phase transition has been observed for increasing Fe layer thicknesses. In addition, intermixing between Fe and C atoms at the interfacial region has been observed as a distribution of magnetic hyperfine field in the CEM spectrum. The intermixing was estimated to be extended to about 1.2 nm on either side of the Fe layers; however, this is expected to be strongly dependent on the preparation method.

DS 42.85 Wed 15:00 P1

Characterization of lattice defects by X-ray absorption spectroscopy in ferromagnetic pure ZnO films — •Jörg Haug[1], Angelika Chassé[1], Stephan Borek[1], Manfred Dubiel[1], Muhammad Khalid[2], and Pablo Esquinazi[2] — [1]Department of Physics, University of Halle-Wittenberg, Von-Danckelmann-Platz 3, D-06120 Halle — [2]Division of Superconductivity and Magnetism, University of

Leipzig, D-04103 Leipzig

ZnO films were grown on graphite substrates by pulsed laser deposition under different nitrogen pressure (0.01 - 1.0 mbar) using a KrF excimer laser. The film thickness was between 60 and 500 nm. X-ray diffraction experiments of (100) and (112) reflections demonstrate the a-plane orientation of pure ZnO films. The line broadening of reflection peaks yield crystallite sizes of approximately 50 nm. The comparison of XRD lattice parameters and Zn-O and Zn-Zn distances as determined by EXAFS experiments at the Zn K edge indicates a mismatch to the structure of ZnO single crystals as well as a slight dependence on nitrogen pressure. X-ray absorption experiments of the near edge region (XANES) show an orientation dependence of signals on x-ray polarization and a correlation between the intensity of 1s to 4p transition with the defect concentration. XANES simulations of Zn K edge by means of a multiple-scattering approach demonstrate the sensitivity to vacancy defects. With that structural models of defect centers has been developed to interpret the experimental data.

DS 42.86 Wed 15:00 P1

Picosecond-Pulsed Laser Deposition of $Ge_2Sb_2Te_5$ — •Julia Benke, Erik Thelander, and Bernd Rauschenbach — Leibniz Institute of Surface Modification, Leipzig

The chalcogenide compound $Ge_2Sb_2Te_5$ (GST) is a commonly used material for phase change applications like PC-RAM and optical data storage [1]. Here, we present thin films of GST synthesized by Pulsed Laser Deposition (PLD) using a picosecond laser. The use of ultra-short pulses drastically changes the ablation mechanism compared to conventional PLD and hence another type of film morphology is to be expected [2]. Samples have been deposited on glass and SiO_2 in an UHV-chamber in different inert gas environments. The influence of substrate temperature and target-to-substrate distance on the surface topography has been investigated and characterized with SEM and AFM whereas structural information has been obtained with XRD, XPS and RBS.

[1] Raoux S., Annu. Rev. Mater. Res., **48**, (2009), 39:25

[2] Teghil et al., Appl. Surf. Sci., **210** (2003), 307

DS 42.87 Wed 15:00 P1

Ultimate soft x-ray microspectroscopy for chemical analysis — •Andreas Späth[1], Jörg Raabe[2], Christian Hub[1], Stephan Wenzel[1], Benjamin Watts[2], and Rainer H. Fink[1] — [1]Friedrich-Alexander Universität Erlangen-Nürnberg, Physikalische Chemie II and ICMM, Erlangen, Germany — [2]Swiss Light Source (SLS), Paul Scherrer Institut, Villigen, Switzerland

Zone-plate based x-ray microscopes offer a wide range of potential applications in fundamental and applied science, in physics, chemistry and material science or in the imaging of biosamples. The present PolLux scanning transmission x-ray microspectroscope is installed at a bending magnet beamline of the Swiss Light Source (SLS) operating from 260 - 1200 eV [1]. Using the latest zone-plate technology, imaging of lateral structures with 12 nm periods was achieved [2]. The available energy range is ideally suited for soft matter investigations. We will present spectromicroscopic results from various organic based materials, like organic hybrid materials, polymer films, organic nanocrystals or biosamples. The recent extension of the detection setup by an electron multiplier offers additional surface-enhanced detection. Thus, we are able to combine bulk and surface sensitivity. In addition, differential phase-contrast imaging offers another detection scheme to improve image contrast. The complementary use of the various detection schemes offers improved knowledge on the investigated soft matter samples. The project is funded by the BMBF under contract 05 KS7WE1.

1. J. Raabe, et al., Rev. Sci. Instrum. 79, 2008, 113704.
2. K. Jefimovs, et al., Phys. Rev. Lett. 99, 2007, 264801.

DS 42.88 Wed 15:00 P1

Mechanical properties of thin sputtered a-C and CNx multilayers on polymer substrates — •Zdenek Stryhal[1], Martin Dubau[1], Arndt Schumann[1], Dieter Schneider[2], and Frank Richter[1] — [1]Chemnitz University of Technology,Reichenhainer Straße 70, D-09126 Chemnitz, Germany — [2]Fraunhofer IWS Dresden, Winterbergstrasse 28, 01277 Dresden, Germany

The aim of this work was to investigate the formation of carbonaceous layers on polymer substrates and to characterize the friction and wear behavior of those layers. Amorphous (nearly hydrogen free) carbon and nitrogen doped carbon films have been grown by pulsed DC magnetron sputtering from a graphite target in argon and argon/nitrogen gas mixture. Single films of these two materials as well as multilayers composed of them have been investigated. Our layer were deposited on various polymer substrates (polybutylene terephthalate – PBT and polyamide – PA66) that are used in industrial conveying systems. Following methods have been used to characterize deposited layers: stylus profilometer (intrinsic stress, compressive 0.1–5.5GPa), adhesion (pull-out test, >14MPa), reciprocating tribometer (wear resistance and friction coefficient, μ=0.15–0.35), bending test(deformation resistance), SAW (elastic modulus, 50–250GPa) and SEM (surface topography). Friction and wear tests were made at conditions similar to those we expect in real transport systems.

DS 42.89 Wed 15:00 P1

Resonant Photoelectron Spectroscopy of epitaxial Fe-doped $SrTiO_3$ — •Annemarie Köhl[1], Christian Lenser[1], Jacek Szade[2], Dariusz Kajewski[2], Jurek Kubacki[2], Regina Dittmann[1], Kristof Szot[1], and Rainer Waser[1] — [1]Peter Grünberg Institut (PGI-7), Forschungszentrum Jülich, Germany — [2]A.Chelkowski Institute of Physics, University of Silesia, Katowice, 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 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.

Therefore the electronic structure of epitaxial Fe-doped $SrTiO_3$ was studied by photoelectron spectroscopy. Thin film samples with Fe concentration of 1 at.% and 2 at.% as well as undoped references are prepared by pulsed laser deposition and checked for surface quality by AFM. Core-level photoelectron peaks are analysed regarding the chemical shift and valence state. 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 42.90 Wed 15:00 P1

Influence of growth conditions on the crystallization behaviour of reactively magnetron sputtered amorphous molybdenum oxide films — •Sven C. Liepertz, Gomathi Natarajan, Dominik Köhl, Peter Zalden, and Matthias Wuttig — Institute of Physics IA, RWTH Aachen University

The objective of the present work is the synthesis and characterization of meta-stable crystalline phases of group IV and VI transition metal oxides. To grow such specimen, amorphous films are deposited by reactive magnetron sputtering of the elemental transition metal target. Crystallization is induced by thermal annealing and studied by XRD (phase information), SEM and optical microscopy (morphology). Special emphasis is put on the influence of specific features of the amorphous matrix on the crystallization behaviour. Particularly, the stoichiometry of the precursor is tailored by adjusting the deposition process parameters. The elemental composition of such specimen is deduced from RBS measurements. The optical properties of amorphous and crystalline films are investigated by spectroscopic ellipsometry and reflections/transmittance measurements in the UV/VIS spectral region. The optical data is modelled to determine the dielectric function which has been related to the crystallization behaviour. The focus of the present study is on the investigation of MoO_3 films. It will be shown that films with different crystallization behaviour and corresponding crystalline phases can be fabricated by tailoring film deposition and subsequent annealing.

DS 42.91 Wed 15:00 P1

H_2 plasma modification of polydimethylsiloxane thin films investigated by infrared reflection absorption spectroscopy — •Vladimir Danilov, Hans-Erich Wagner, and Jürgen Meichsner — Ernst Moritz Arndt University of Greifswald, Germany

Plasma modification of polydimethylsiloxane (PDMS) thin films was studied by means of Fourier-Transform-Infrared-Reflection-Absorption-Spectroscopy. The spin-coated PDMS films with the thickness between 10 nm and 400 nm were prepared on Al-coated glass substrates and were treated by direct contact with H_2 plasma as well as by the H_2 plasma radiation, only. In direct plasma treatment the substrates were positioned on the powered electrode of an asymmetric capacitively coupled RF discharge in H_2 at low pressure. The influence of the plasma radiation was studied in different spectral ranges due to the screening of the thin film from the bulk plasma by selected window characterized by different cut-off wavelength: soda-lime glass (300 nm), quartz glass (160 nm) and MgF_2 (115 nm). The strong modification effect was observed in experiments with the MgF_2 window, only. The evolution of IR spectra was monitored, and the changes of PDMS characteristic absorption bands as well as the formation of new bands are discussed. It was found that the films consist of methyl-free SiO_x top layer (10-30 nm), followed by partially methyl-free region, and an underlying non-modified PDMS layer in the case of thin films prepared with initial thickness exceeding 350-400 nm.

Funded by the Volkswagen Foundation, Plasma Hybrid Coating, grant no. I/83275.

DS 42.92 Wed 15:00 P1

Low Energy SEM - High Resolution, Low Charging, Low Damage — •Philipp Tonndorf, Steffen Schulze, and Michael Hietschold — Chemnitz University of Technology, Reichenhainer Straße 70, D-09126 Chemnitz, Germany

With the usage of slow primary electrons in the scanning electron microscope it is possible to achieve more valueable images with respect to resolution, charging and damage. The primary electrons are accelerated as usual with some kV. Then after the last lens they are slowed down to some hundreds of eV through an opposing field. So the interaction volume shrinks and one gets higher resolution and better signal-noise-ratio. Another effect is a higher surface sensitivity. Through the smaller landing energy the SE and BSE yield changes. If the total yield is 1 no charging occurs. So it is possible to investigate insulators with no metal coating. With very slow primary electrons ($<$ 50 eV) the damaging of organics and the carbon contamination decreases. At about 25 eV there is no more damage observed through ionisation. At this energy backscattering becomes inversely proportional to the local density of states. Carbon contamination stops at about 4 eV.

DS 42.93 Wed 15:00 P1

Trends in crystallization behavior of phase-change materials under high external pressure — •Matthias Kaes[1], Peter Zalden[1], Julia van Eijk[1], Giuliana Aquilanti[2], Sakura Pascarelli[2], and Matthias Wuttig[1] — [1]I. Physikalisches Institut (1A), RWTH Aachen University, D-52056 Aachen, Germany — [2]European Synchrotron Radiation Facility, Grenoble, France

Phase-change materials (PCMs) exhibit a rapid crystallization of their amorphous phase and a related change in electrical conductivity of several orders of magnitude. There have been estimations that high pressures (6 GPa) might occur in a phase-change random access memory (PCRAM)-cell due to thermal expansion, which could influence the switching mechanism in small PCRAM-cells. Moreover, PCMs show surprising pressure-dependent behavior, as the prototypical PCM $Ge_2Sb_2Te_5$ has been observed to amorphize under increasing pressures (10-20 GPa) [1].

Here, we present in-situ EXAFS experiments at the Ge K absorption edge by which we have investigated the pressure-induced changes in short-range order in $Ge_2Sb_2Te_5$ and $Ge_4Sb_1Te_5$.

While both materials show similar crystallization behavior under ambient pressure, it is found that the crystallization is influenced or even suppressed by applied external pressures. We compare our results with previous findings and derive stoichiometric trends, from which we propose that the reliability of PCRAM-devices could benefit from the use of PCMs with high content of GeTe.

[1] A.V. Kolobov et al. Physical Review Letters 035701, p. 2-5 (2006).

DS 42.94 Wed 15:00 P1

Preparation and X-Ray standing Wave Measurements of STO/LAO films — •Christoph Schlueter and Jörg Zegenhagen — ESRF, 6 rue Jules Horowitz, BP 220, 38043 Grenoble, CEDEX 9, France

The formation of a quasi-2dimensional electron gas at the interface of $SrTiO_3$ (STO) and $LaAlO_3$ (LAO) attracted considerable attention in recent years.[1] A X-ray standing wave (XSW) and X-Ray Photoelectron Spectroscopy (XPS) experiment is expected to help elucidate details of the electronic and atomic structure at the interface. Samples of high crystallographic quality are needed for these experiments. Samples were grown on (001) oriented STO single crystal substrates. TiO_2 termination was obtained by standard methods.[2] The thin films were deposited in a UHV compatible pulsed laser deposition (PLD) chamber using a UV laser (λ=248nm) at sample temperatures of 750 - 820°C in an oxygen atmosphere of $5*10^{-5}$ mbar. For samples held at elevated temperatures for longer times (tempering and/or slow cooling rate) steps were found to bunch by atomic force microscopy (AFM). This is indicative on a significant surface diffusivity at these temperatures. Faster cooling times (1-1.5h) resulted in smooth surfaces with unit cell height steps. AFM and reflectivity data are in reasonable agreement. For even higher cooling rates powder rings prove that parts of the film are badly oriented. Diffraction and XSW experiments indicate the formation of fully strained films.

1. 1. A. Ohtomo et al., Nature 427, no. 6973, (2004): 423-426.
2. G. Koster et al., Appl. Phys. Lett. 73, no. 20 (1998): 2920-2922.

DS 42.95 Wed 15:00 P1

Anisotropic structural and electrical properties of strained SrTiO3 films on sapphire — •Thomas Grellmann, Kyrylo Greben, Eugen Hollmann, Rolf Kutzner, and Roger Wördenweber — Institute of Bio- and Nanosystems (IBN), Forschungszentrum Jülich, D-52425 Jülich

The electronic properties of oxide films strongly depend on the composition, structure and structural imperfections. Since lattice constants and thermal expansion coefficient of substrate and films are usually different, mechanical strain is imposed on the growing films. In this work we examine the strain of epitaxially grown SrTiO3 films on sapphire and its impact on the ferroelectric properties of the film. The lattice mismatch of about 10% between SrTiO3 and sapphire is reduced via a buffer layer, CeO2. The strain induced modification of the structure is determined via XRD measurements. High-resolution Pole-figure measurements demonstrate the anisotropic and thickness dependent (i.e., relaxation) distortion of the SrTiO3 lattice. Electronic characterization of the dielectric properties reveal the resulting anisotropy of the polarizability of film. Furthermore, it demonstrates that ferroelectric can be induced via strain in the originally incipient ferroelectric SrTiO3 up to high temperatures well above 200K.

DS 42.96 Wed 15:00 P1

In-Situ SEM Investigation Of Swift Heavy Ion Induced Dewetting — •Daniel Garmatter, Michael Haag, Redi Ferhati, Sankarakumar Amirthapandian, and Wolfgang Bolse — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart

Recently we have found that swift heavy ion (SHI) irradiation of thin oxide films on Si results in restructuring [1] similar to the dewetting patterns formed when melting polymer films on Si [2]. However, in these ex-situ experiments we could only investigate the average development of the surface structure, since a new sample had to be taken for each irradiation fluence. With our new in-situ SEM/EDX at the UNILAC accelerator of GSI [3] we are now able to follow the history of individual objects from the first ion impact until their final state. The nucleation and growth mechanisms of SHI induced dewetting can now be easily studied, since the irradiation process can be controlled in very small fluence steps and dewetting stops as soon as the ion beam is switched off. This allows to immediately freeze the actual state of dewetting for careful analysis, which is hardly possible in case of liquid films. After the next irradiation step, one and the same spot can be analyzed again and such the nucleation and growth kinetics of individual dewetting holes can be determined. We will report our first results on SHI induced dewetting of iron-oxide layers with varying film thicknesses and artificial defect concentrations. [1] T. Bolse, et al., Nucl.Instr.Meth. 245 (2006), [2] S. Herminghaus, et al., Science 282 (1998), [3] S. Amirthapandian, et al., Rev.Sci.Instr. 81, (2010)

DS 42.97 Wed 15:00 P1

Model calculations for XRD at polycrystalline thin films — •Susanne Hahne, Thomas Weisemoeller, and Joachim Wollschlaeger — Department of Physics, University of Osnabrück, Barbarastr. 7, D-49069 Osnabrück, Germany

The evaluation of x-ray diffraction (XRD) data is an important method for structure determination. Regarding thin films the theoretical description of XRD is commonly based on an ideal lateral and vertical structure without defects to determine lattice constants and the film thickness. This contribution introduces a new 2D model, which includes defects of the thin film. It replaces the ideal layer with a distribution of crystallites, which cover the substrate surface completely. Their sizes are randomly distributed according to a Γ-distribution. The new model is primarily characterized by the additional dimension, which allows the reproduction of in-plane and out-of-plane data. Two types of crystallite distributions are implemented. For one type the crystallite positions are fixed to certain substrate atoms. The other type assumes a floating film. A first survey verified that the influence on the diffraction pattern of every parameter in the model is correctly reproduced. This includes a variation of the vertical lattice constant, which changes the diffraction peak position. The peaks out-of-plane are broadened, if the vertical crystallite size is decreased. For scattering vectors, which do not coincide with crystal truncation rods, strong fringes are observed. Their oscillation is strongly attenuated with a growing variance of the crystallite height distribution. Similar results are obtained with respect to the lateral crystallite sizes.

DS 42.98 Wed 15:00 P1

Surface analysis of Li-ion battery model anodes — •Andreas Seemayer, Philipp Bach, and Frank Uwe Renner — Max Planck Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf

Lithium ion batteries are the most promising power source for future electromobility applications. Research on the battery systems aims to achieve higher rate capability, cycle life, or better safety. To achieve necessary further improvements a better understanding of the basic processes is needed. Following a surface science approach we focus on the investigation of simple model systems (like single crystals or thin film electrodes) of relevant anode materials.

We report investigations of the electrochemical insertion of Lithium in Au, Ag, Al, Mg and Si model surfaces, i.e. alloying and dealloying of Lithium alloys. As electrolyte we use the ionic liquid 1-Butyl-1-methylpyrrolidinium bis(trifluoromethanesolfonyl)imide (PYR14TFSI) with 0.3M LiTFSI. The electrochemical characterisation is performed by Cyclic Voltammetry (CV). The surface and film characterisation regarding its geometrical structure is investigated by means of Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM). The chemical composition is characterised ex-situ by Photoelectron Spectroscopy (PES) and Secondary Ion Mass Spectrometry (SIMS).

DS 42.99 Wed 15:00 P1

Picosecond-Pulsed Laser Deposition of $LaAlO_3$ — •Erik Thelander and Bernd Rauschenbach — Leibniz Institute of Surface Modification, Leipzig

The perovskite material $LaAlO_3$ is a dielectric with a permittivity of around 25 and a beneficial conduction band offset towards Si. Therefore it is an interesting candidate to be used as the next generation gate oxide in CMOS technology if it ever were to be grown epitaxially on Si. Here we present findings made on thin films of $LaAlO_3$, synthesized with a Pulsed Laser Deposition (PLD) process using ultrashort laser pulses, deposited both on Si and lattice matched $SrTiO_3$. Using suitable filtering techniques, we show that it is possible to avoid the incorporation of nanoparticles in the growing films which is normally a most troublesome feature of ultrashort PLD [1,2]. Film topography has been investigated with SEM and AFM, which show low particle density and smooth surfaces with RMS-values between 0.3 and 1 nm. XRD and XPS have been used to obtain structural information of the samples whereas TOF-SIMS have been employed to gain information about the diffusion in the interface as well as the elemental distribution within the films.

[1] Teghil et al., Appl. Surf. Sci., **210** (2003), 307

[2] Amoruso et al., Appl. Phys. Lett., **84** (2004), 4502

DS 42.100 Wed 15:00 P1

Contamination and Cleaning of Multilayer Mirrors with X-ray Photoelectron Spectroscopy — •Sina Gusenleitner[1,2], Marius Ernst[1,2], Dirk Ehm[2], and Friedrich Reinert[3] — [1]Universität Würzburg, Experimentelle Physik VII, D-97074 Würzburg, Germany — [2]Carl Zeiss SMT GmbH, Rudolf Eber StraSSe 2, D-73447 Oberkochen, Germany — [3]Karlsruhe Institut für Technologie (KIT), Gemeinschaftslabor für Nanoanalytik, D-76021 Karlsruhe, Germany

Extreme Ultraviolet Lithography is a promising next generation lithography technology. In this radiation regime (wavelength 13.5 nm) advanced multilayer mirrors (MLM) are used as collector and illuminator optics. The mirrors consist of a stack of alternating molybdenum and silicon layer, coated with a dedicated capping material such as Si, Ti, Mo, Pd, Ru, or their oxides. Various contamination dynamics in the lithography tool lead to formation of hydrocarbon layers on the mirror surface. In order to understand these contamination processes the adsorption, bonding and chemical environment of carbonaceous layers on MLM surfaces are investigated with X-ray Photoelectron Spectroscopy (XPS). A clean reference surface can be obtained by exposing a contaminated mirror surface to reactive species. The influence of these species on the chemical structure of the MLM surface and adsorbed carbonaceous layers was monitored with XPS. Variation of the take-off angle in XPS measurements provided information about the influence of the cleaning process on the structure of the surface, such as intermixing of the underlying layers with the capping layer material.

DS 42.101 Wed 15:00 P1

growth, characterization and bio-functionalization of cubic boron nitride thin films — •hong yin[1], lianchen shan[1], marc saitner[1], lars grieten[1], sylvia wenmackers[1], veronique vermeeren[2], fabian wilbers[1], marcel ameloot[2], luc michiels[2], marc d'olieslaeger[1,3], patrick wagner[1,3], and hans-gerd boyen[1] — [1]institute for materials research, hasselt university, wetenscharpspark 1, 3590 diepenbeek, belgium — [2]biomedical research institute, hasselt university, agoralaan buiding c, 3590 diepenbeek, belgium — [3]IMEC, division IMOMEC, wetenscharpspark 1, 3590 diepenbeek, belgium

Beside their applications as superhard coatings, in high-temperature electronics, or UV-photonics, cubic boron nitride (c-BN) thin films are also promising candidates for biological applications due to their bio-compatibility and chemical inertness. In this work, we will demonstrate that c-BN films have the potential to be used as new transducer material for biosensor applications. Impurity-free c-BN films are synthesized by means of radio frequency (r.f.) magnetron sputtering under UHV conditions. In-situ XPS and ex-situ FTIR are used as analytical tools to collect information about both, the surface and the volume parts of the films, respectively. Hydrogen-terminated films are successfully functionalized for the subsequent attachment of (amino-terminated) DNA. The successful attachment of single-stranded DNA and the subsequent hybridization to form double-stranded DNA is confirmed by supernatant fluorescence microscopy.

DS 42.102 Wed 15:00 P1

Monte Carlo Simulations for a focusing neutron guide at TOFTOF — •Roxana Valicu[1,2], Giovanna Simeoni[1,2], Peter Böni[2], Wienfried Petry[1], and Gunther Borchert[1] — [1]Forschung Reaktor München, Neutronenquelle, Lichtenbergstrasse 85747 Garching — [2]Physik-Department E21 James-Franck-Strasse 85748 Garching

TOFTOF is a direct-geometry multi-disc chopper time-of-flight spectrometer, installed at the neutron source Heinz Maier-Leibnitz FRM II. For further studies of magnetic systems and for investigation of samples under extreme conditions (high-pressure cells, electromagnetic and electrostatic levitator devices, magnetic fields) Monte Carlo simulations were performed for focusing the neutron beam and increasing the neutron flux . The gains in flux as well as the expected profile of the beam resulting from the simulations will be presented.

DS 42.103 Wed 15:00 P1

Thermal interface resistance of metal films on insulator and semi-conductor substrates measured by thermal wave techniques — •Puchong Kijamnajsuk[1], Mihai Chirtoc[2], Marc Möller[1], David Schäfer[3], Christoph Eisenmenger-Sittner[3], Detlef Spoddig[1], Ralf Meckenstock[1], and Josef Pelzl[4] — [1]Experimental Physics, University Duisburg-Essen, Germany — [2]Université de Reims Champagne-Ardenne, GRESPI-CATHERM, Reims, France — [3]Vienna University of Technology, Institute of Solid State Physics, Wien, Austria — [4]Institute of Experimental Physics, Ruhr-University, Bochum, Germany

Thermal interfaces are essential for the application of modern composites in electronic devices. The thermal interface resistance in Cu/C and Fe/GaAs flat model systems was studied by novel approach, which relies on the frequency dependence of the photothermal signal phase and amplitude at intermediate frequencies and thermo-reflectivity. Cu-films (1 μm) were deposited by magnetron sputtering and Fe (100nm) was grown by molecular beam epitaxy. The influence of thin bonding layers (5 nm) and subsequent heat treatment on the thermal interface resistance was investigated. The bonding layer were based on B with additions of the carbide forming metals Mo, Ti and Cr. These measurements were complemented by secondary ion mass spectroscopy, scanning electron microscopy and atomic force microscopy. No correlation was found with respect to the bonding layer. A correlation was observed between adhesion strength and thermal interface resistance as well as the heat treated samples.

DS 42.104 Wed 15:00 P1

Oxidation Of Thin Metal Films For Low-cost Vacuum Quality Monitoring

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Ultrathin metal films are investigated in terms of resistance changes, caused by the decrease of the electrical conductive cross section, for their application as vacuum quality sensors. Almost any pure metal is not stable in an oxygen-rich atmosphere and reacts to a metal oxide. In general, this oxide has a some orders of magnitude higher resistivity and so the growth of an oxide layer reduces the conductive path of the metal layer. For modeling the kinetics of these sensors an extended theory of metal oxidation [1,2] is used where the pressure dependence is explicitly considered. The application field of these sensors is as Vacuum Insulation Panels (VIP), which are good thermal insulators at sufficiently low inside pressure. Aluminum in the thickness range of some up to 20 nm is investigated as a metal with a compact oxide layer wherefore limiting oxide thickness and hence a long lifetime of the sensor is expected. In contrast copper is studied as a metal with a porous oxide structure, in order to yield a great resistance change in short time and therefore a better sensor response.

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[2]Boggio, J. E.; Plumb, R. C.; Surface Science **44** 3 (1966).

DS 42.105 Wed 15:00 P1

Optical switching properties and durability of a Mg-Fe alloy based thin film hydrogen sensor

— •Marc K. Dietrich, Gunther Haas, André Portz, Andreas Laufer, Angelika Polity, and Bruno K. Meyer — I. Physikalisches Institut, Giessen, Germany

Mg-Fe alloy based hydrogen gas sensors were produced by a RF sputtering process. By exposure to a hydrogen containing gas mixture the Mg-metal alloy switches from the metal phase into a hydride phase, thereby the optical reflection shows a change. A Pd top layer acts as hydrogen catalyst. The degradation of the hydrogenation speed (sensor reaction) and the switching durability are well known problems of such Mg-metal based switching mirrors. Furthermore, there is a delay of sensor reaction after some weeks of storage (in air).

In order to solve these problems, we added a Ti buffer layer between MgFe and Pd layer. The buffer layer inserted sensor system featured an improvement of sensor reaction and switching durability. A polytetrafluoroethylene (PTFE) covering coat was added and reduced the sensor degeneration after the storage. Furthermore, there was an additional improvement of switching durability. Samples of PTFE/Pd/Ti/MgFe achieved over 1000 switching cycles (with 4 % hydrogen in air) without a significant performance reduction.

DS 42.106 Wed 15:00 P1

Nonvolatile bipolar resistive switching in Au/BiFeO3/Pt

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Nonvolatile bipolar resistive switching has been observed in an Au/BiFeO3/Pt structure, where a Schottky contact and an 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 with a resistance ratio larger than two orders of magnitude. Based on a systematic investigation of its electrical properties with an emphasize on its transport characteristics, a model associated with the redistribution of OVs and electron hopping process is proposed, which agrees well with our experimental observations. It is known that electron hopping usually occurs in BFO thin films and causes large leakage current, which is undesirable in traditional ferroelectric or multiferroic applications. However, it is found in the present work that the electron hopping can be controlled and utilized to realize bipolar resistive switching, which is promising for future high density memory devices.

DS 42.107 Wed 15:00 P1

The Influence of Oxygen on the Potential Distribution of Operating Zinc Oxide FETs

— •Daniel Walker — TU Darmstadt, FB Materialwissenschaften, FG Elektronische Materialeigenschaften, Petersenstr 23, 64287 Darmstadt

Zinc Oxide has been studied extensively over the past 40 years and remains a material of interest for many applications including flexible electronics due to its n-type semi-conducting properties, printability from solution, transparency and wide band gap. One well known factor that has to be mitigated before commercial ZnO based electronics can be implemented is its very strong sensitivity to oxygen. This work discusses the effects of oxygen on the surface potential of an operating transistor with a highly granular ZnO film, fabricated by spin coating from solution. An ultra high vacuum Scanning Kelvin Force Microscope is used to examine at which parts of the device oxygen alters the potential distribution along the channel. It is shown that the oxygen strongly influences the behaviour of the device at the source and drain contacts and these effects are then interpreted in a qualitative model depicting the mode of operation of the transistor. The results are then related back to the conventional current-voltage characteristics.

DS 42.108 Wed 15:00 P1

Fabrication and characterization of YSZ microstructures

— •Osman Khalil, Markus Piechotka, Martin Fischer, Torsten Henning, and Peter J. Klar — 1. Physikalisches Institut, Justus-Liebig-Universität, 35392 Giessen

Yttria-stabilized zirconia (YSZ) is known for its ion-conducting behaviour due to oxygen vacancies in its anion-lattice. To extract these ions from the surface a three-phase-boundary between air, YSZ and platin is desirable. Thus the conductance of an YSZ sample can be reduced by the use of thin films or by an increase of the three-phase boundary-surface. Therefore we investigated the fabrication of free-standing YSZ membranes grown on silicon by anisotropical etching of (100)-Si-wafers as well as the microstructuring of the YSZ-surface. The treatment of the samples was performed with photolithography, KOH-etching and Ar^+-ion-beam-etching. The samples were then investigated using AFM, SEM and optical microscopy.

DS 42.109 Wed 15:00 P1

Improvement and investigation of the emission behaviour of YSZ samples using nanostructuring and thin film technology

— •Markus Piechotka, Martin Fischer, Torsten Henning, Davar Feili, and Peter J Klar — 1. Physikalisches Institut, Justus-Liebig-Universität, 35392 Giessen

We developed nano-structured free-standing YSZ-membranes for electrospray applications as well as for ion emitting purposes. YSZ is a well known solid electrolyte used widely in the production of solid oxide fuel cells (SOFC) as well as as electroceramics and possible ion emitter. Especially in the field of micro-thrust space engines, new techniques of ion emission have to be developed.

100 nm to 2 microns thin YSZ films were grown on double-side polished and thermally oxidized 2 inch silicon wafer using PLD. Subsequently photolithography structuring and wet etching with BHF and KOH were performed to lay the membrane bare. Afterwards needle structures were transferred into the YSZ-membranes using electron beam lithography followed by ion-beam etching with an Ar^+-beam.

The surfaces of the structured samples were investigated using AFM as well as SEM. The samples were then mounted into an integrated sample holder with multiple high voltage grids in front of the sample. This assembly functions as a solid state ion emitter with a heater as well as an oxygen supply beneath the sample. Furthermore we emitted oxygen ions from the YSZ-surface and measured the temperature dependence of the emission current as well as the ion energy distribution with Faraday cups and with a retarding potential analyser.

DS 42.110 Wed 15:00 P1

Zelladhäsive Plasmapolymerschichten aus Ethylendiamin

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Dünne Plasmapolymerschichten mit einer Schichtdicke zwischen 50 und 100 nm wurden in einer asymmetrischen, kapazitiv gekoppelten Hochfrequenzentladung in einem Gemisch aus Argon und Ethylendiamin (EDA) hergestellt. Die plasmachemischen Stoffwandlungsprozesse wurden mit der optischen Emissionsspektroskopie, FTIR Spektroskopie und Massenspektrometrie untersucht. Die Charakterisierung der Schichteigenschaften erfolgte mittels Ellipsometrie, IRRAS und XPS. Die optische Emission des Plasmas ist neben charakteristischen Ar-Linien durch eine zunehmende Intensität von CN-Banden bestimmt. Stabile gasförmige Reaktionsprodukte sind insbesondere NH3, HCN und H2. Die dünnen plasmapolymerisierten Schichten aus EDA besitzen einen hohen Stickstoffanteil (N/C ca. 40%) und zeigen charakteris-

tische IR-Absorptionsbanden der N-H, C-H und C-N Molekülschwingungen. Eine Lagerung an Luft führte zu einer Alterung der Schichten, wobei insbesondere sauerstoffhaltige Gruppen nachgewiesen wurden. Die Beschichtung von biomedizinisch relevanten Substraten (Implantate) führte zu einer signifikanten Erhöhung der Adhäsion und Ausbreitung von humanen Knochenzellen. Gefördert im Campus PlasmaMed, Nr.13N9774.

DS 42.111 Wed 15:00 P1

Attosecond pulse-shaping including control of the attochirp by aperiodic extreme ultraviolet multilayer mirrors — •Michael Hofstetter[1,2], Alexander Guggenmos[1,2], Eleftherios Goulielmakis[1], Martin Schultze[1,2], Elisabeth Magerl[1], Stefan Neppl[3], Elisabeth Bothschafter[1,3], Markus Fiess[1], Benjamin Dennhardt[3], Justin Gagnon[1,2], Vladislav Yakovlev[1,2], Reinhard Kienberger[1,3], Adrian Cavalieri[1], Ralph Ernstorfer[1,3], Ferenc Krausz[1,2], and Ulf Kleineberg[1,2] — [1]MPQ, Garching, Germany — [2]LMU, Garching, Germany — [3]TUM, Garching, Germany

Attosecond physics allow to reveal the dynamics of elementary electronic processes with never before enterable precision. Multilayer XUV mirrors are the key components to shape all attosecond pulse parameters as its central energy, spectral bandwidth, pulse length and attochirp with a high degree of freedom. This allows us to investigate and compare resonant and non-resonant electronic transitions in solids, surfaces, molecules and gases, as each experiment requires its perfectly synchronized pulse and test current physical models. We will present our latest results on shaping attosecond pulses in the spectral range between 80 and 140 eV from gas high harmonics, characterized via FROG analyses of electron streaking. We will present explicit examples of dispersion control using chirped XUV multilayers. We will further present ideas on attosecond spectral cleaning that enable experiments with high temporal (few 100 as) and high spectral (few eV) resolution and clearly reduced noise.

DS 42.112 Wed 15:00 P1

Simulation of the ultrafast nonlinear optical response of metal slabs — •Mathias Wand, Torsten Meier, and Jens Förstner — Department Physik and CeOPP, Universität Paderborn, 33098 Paderborn, Germany

With the current rise of interest in plasmonic nanostructures [1], it has become apparent that the nonlocal and nonlinear optical properties of such systems can only be described properly by theoretical models beyond the classical free-electron Drude model.

We present a nonequilibrium ab initio method for calculating nonlinear and nonlocal optical effects in metallic slabs with a thickness of several nanometers. The numerical analysis is based on the full solution of the time-dependent Kohn-Sham equations [2] for a jellium system and allows to study the optical response of metal electrons subject to arbitrarily shaped intense light pulses. We find a strong localization of the generated second-harmonic current in the surface regions of the slabs [3].

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2. A. Castro, M.A.L. Marques, and A. Rubio, J. Chem. Phys. 121, 8 (2004).
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DS 42.113 Wed 15:00 P1

A study on nanocomposites made of a conducting polymer and metallic nanoparticles — •rania mohammed ahmed khalil[1,2], ramzy abdelaziz mahmoud abdelaziz[1], thomas strunkus[2], franz faupel[2], and mady elbahri[1,3] — [1]Nanochemistry and Nanoengineering, Institute for materials science, Faculty of engineering, Christian-Albrechts-University of Kiel — [2]Multicomponent materials, Institute for materials science, Faculty of engineering, Christian-Albrechts-University of Kiel — [3]Helmholtz-Zentrum Geesthacht GmbH, Institute of Polymer Research, Nanochemistry and Nanoengineering

Conducting polymers offer a unique combination of properties that makes them attractive materials for many electronic applications. PEDOT:PSS is one of the most successful conductive materials which is considered to be highly stable and resisting degradation under typical ambient conditions. In this study, we have prepared two sets of conducting polymer nano-composites. The first set is composed of PEDOT:PSS doped with different aspect ratios of gold nanorod and the other one is PEDOT:PSS doped with different sizes of gold nanosphere. The chemical reduction method was used for preparing the nano-particles. Indeed, gold nanorods and nanosphere which exhibit tunable absorption as a function of their size and aspect ratio, respectively, have tuned the absorption coefficient for PEDOT: PSS. The nature of the dopant as well as the degree of doping has played a significant role in the improvement of the electrical conductivity of conducting polymer.

DS 42.114 Wed 15:00 P1

Mueller matrix ellipsometry on large area split ring resonator arrays — •Bruno Gompf, Barbara Krausz, Bettina Frank, Harald Giessen, and Martin Dressel — Physikalisches Institut and Research Center SCOPE, Universität Stuttgart

The workhorse of the metamaterial community is the split ring resonator (SRR). It represents the top-down approach to tailored effective optical parameters in the sense that it is essentially a miniature inductive-capacitive resonant circuit. Arranging many of these nanocircuits, sometimes called photonic atoms, together, it is assumed that they merge into a material with effective optical parameters. The problem is that in general the optical response is k-dependent, only in the special case when the regular building blocks of a material (molecules, unit cells, nanostructures, etc.) are small compared to the wavelength, spatial dispersion can be neglected. Surprisingly the complete k-dependent optical response of SRR-arrays was not measured up to now. We present Mueller matrix spectroscopic ellipsometry on large area SRR arrays in transmission at various angles of incidence and azimuthal orientations in the energy range of 0.73 to 4.6eV. To visualize the experimental results, we plot the matrix elements in polar coordinates. From the off-diagonal elements, it becomes obvious that the SRR-array is birefringent, but with strongly k-dependent optical axes. Closed ring structures, fabricated in the same way, do not exhibit this behaviour. The results clearly show that the optical response of the SRR array cannot be described by purely dielectric effective parameters.

DS 42.115 Wed 15:00 P1

Theory of the Spatiotemporal Control of Optical Excitations in Metal Nanostructures — •Felix Schlosser[1], Mario Schoth[1], Sven Burger[2], Frank Schmidt[2], Andreas Knorr[1], Shaul Mukamel[3], and Marten Richter[1,3] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Germany — [2]Zuse-Institut Berlin, Germany — [3]Department of Chemistry, University of California, Irvine, USA

Spatiotemporal control of electronic excitations with subwavelength precision is a useful technique in modern experiments. It can be achieved by combination of pulse shaping techniques for ultrashort laser pulses with nanoplasmonics [1]. In order to describe the linear and nonlinear excitation and response of metal nanostructures on a fundamental level, a microscopic material model is combined with a Maxwell solver (JCMwave, Zuse-Institut Berlin) to simulate the spatiotemporal control caused by shaped pulses [2] including phase control optimized by a genetic algorithm. As a first application, we demonstrate that the precise control of excitations in coupled semiconductor quantum dots opens new possibilities for coherent spectroscopy: In particular, we discuss a double quantum coherence (DQC) method [3] enhanced by the additional spatial control, which will reveal more information about the delocalized excitonic wave functions in coupled nanostructures compared to DQC without spatial control.

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[2] M. Reichelt and T. Meier, Opt. Lett. **34**, 2900-2902 (2009)
[3] L. Yang and S. Mukamel, Phys. Rev. Lett. **100**, 057402 (2008)

DS 42.116 Wed 15:00 P1

Silver on nanostructured quartz as reusable SERS-active substrates — •Henrik Schneidewind[1], Karina Weber[2], Matthias Zeisberger[1], Uwe Huebner[1], Dana Cialla[2], Roland Mattheis[1], and Juergen Popp[1,2] — [1]Institute of Photonic Technology Jena (IPHT), Albert-Einstein-Strasse 9, 07745 Jena, Germany — [2]Institute of Physical Chemistry, Friedrich-Schiller-University Jena, Helmholtzweg 4, 07743 Jena, Germany

We investigated reusable substrates for Surface Enhanced Raman Spectroscopy (SERS) comprising of nanostructured gratings in quartz coated with silver films. The contribution involves the ED modelling of suited structures, there preparation, and some exemplary SERS results. Although the shown structures were prepared by means of electron lithography they offer the opportunity for easy and economical fabrication using e.g. imprint techniques. We show the influence of technological parameters as well as of thin film properties on the SERS enhancement of the structures. A homogeneous enhancement exceeding 10^5 is possible across large areas. The SERS enhancement is clearly caused by surface plasmons generated in consequence of the periodic structures and not by surface roughness.

DS 42.117 Wed 15:00 P1

Femtosecond pump-probe spectroscopy of the dielectric function of a polymer matrix with embedded gold nanoparticles — •Mareike Kiel[1], Steffen Mitzscherling[1], and Matias Bargheer[1,2] — [1]Institut für Physik, Universität Potsdam, Germany — [2]Helmholtz Zentrum Berlin, Germany

We investigate a well characterized multilayered compound system [1] of polyelectrolytes and gold nanoparticles with femtosecond pump-probe spectroscopy. The transient absorption A(t) and reflection R(t) after heating the electrons with an intense femtosecond laser pulse are measured simultaneously. We test the well known theoretical model that ascribes the observed signals to the smearing of the Fermi-edge of the conduction electrons by a quantitative comparison to the simultaneously measured A(t) and R(t). In a separate evaluation scheme we directly derive the real and imaginary part of the dielectric function of the composite material from the experiment. A detailed comparison of the two approaches is given.

[1] M. Kiel et al., Langmuir 26, 18499 (2010)

DS 42.118 Wed 15:00 P1

Plasmon-Polariton modes of dense Au nanowire arrays — •Hongdan Yan[1], Peter Lemmens[1], Dirk Wulferding[1], Mehmet Fatih Cetin[1], Sabine Tornow[2], Gertrud Zwicknagl[2], Ulrich Krieg[3], Herbert Pfnür[3], Winfried Daum[4], Gerhard Lilienkamp[4], and Meinhard Schilling[5] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]IMP, TU-BS, Braunschweig, Germany — [3]IFP, LU Hannover, Germany — [4]IEPT, TU Clausthal, Germany — [5]EMG, TU-BS, Braunschweig, Germany

Using optical absorption and other techniques we study plasmon-polariton modes of dense Au nanowire arrays as function of geometrical parameters and coupling to molecular degrees of freedom. For this instance we electrochemically deposit Au nanowires in porous alumina with well controlled morphology and defect concentration. Transverse and longitudinal modes are observed in the absorption spectra resulting from the anisotropic plasmonic structure. The longitudinal mode shows a blue shift of energy with increasing length of the wires due to the more collective nature of this response. We compare our observations with model calculations and corresponding results on 2D Ag nanowire lattices.

Work supported by IGSM and NTH.

DS 42.119 Wed 15:00 P1

Simulation of Plasmonic Microcavities — •Sven Burger, Lin Zschiedrich, Jan Pomplun, and Frank Schmidt — Zuse Institute Berlin, Berlin, Germany

Plasmon-based waveguiding structures allow for transport and storage of light at subwavelength scales. Fast and accurate 3D Maxwell solvers are needed for designing structural parameters of, e.g., hybrid plasmonic waveguides. Due to the multi-scale nature of the corresponding field distributions, accurate computation of the properties of such devices can be numerically challenging.

We have developed finite-element method (FEM) based solvers for the Maxwell eigenvalue and scattering problems. The method is based on higher order vectorial elements, adaptive unstructured grids, and on a rigorous treatment of transparent boundaries. The method has been applied to plasmonic devices like plasmonic antennas, gratings and waveguides [1-5]. Here we present 3D simulations of light propagation in plasmonic waveguides and plasmon laser cavities. We investigate the accuracy of the simulations in a convergence analysis of the numerical results.

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DS 42.120 Wed 15:00 P1

Fabrication of diffractive XUV optics and plasmonic nanostructures by e-beam lithography — •Christian Späth[1], David Kronmüller[1], Jürgen Schmidt[1], Soo Hoon Chew[1], Michael Hofstetter[2], Alexander Guggenmos[2], Mihael Kranjec[1], and Ulf Kleineberg[1,2] — [1]Fakultät für Physik, Ludwig-Maximilians-Universität München, 85748 Garching, Germany — [2]Max-Planck-Institut für Quantenoptik, 85748 Garching, Germany

E-beam lithography is one of the premier choices for fabricating artificial structures on the nanometer scale and is widely used in the field of electronics and nanophotonics. We are reporting about our latest results in the development of diffractive nanostructures for sub-μm focusing of coherent XUV high harmonic radiation at around 95 eV photon energy. Zone Plate patterns (D=120 μm, N = 120) have been written in PMMA and HSQ resist on Si(100) wafer and have subsequently been coated with a Mo/Si multilayer resulting in a reflective nanofocusing device. These structures have been characterized by means of atomic force and scanning electron microscopy. Furthermore bow-tie nanostructures for local near field enhancement of ultrashort femtosecond laser pulses have been fabricated in PMMA and were transferred in 30 nm Ag by Lift-Off. These silver nanostructures were investigated by AFM as well as 1P-PEEM and 2P-PEEM.

DS 42.121 Wed 15:00 P1

Electrical and structural properties of SrTiO3 / Sr-based conducting films on microwave suitable carriers — •Kyrylo Greben[1], Eugen Hollmann[1], Thomas Grellmann[1], Rolf Kutzner[1], Oleksandr Prokopenko[2], Vladimir Pan[3], and Roger Wördenweber[1] — [1]Institute of Bio- and Nanosystems (IBN), Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]Radiophysics Faculty of Taras Shevchenko National University of Kyiv, 2, Acad. Glushkov Ave., building 5, 03127, Kyiv, Ukraine — [3]Institute for Metal Physics, National Academy of Sciences of Ukraine, 36 Vernadsky Street, Kiev, 03142, Ukraine

The aim of this work is the preparation of microwave suitable thin film devices consisting of a conducting base layer covered by a high-k oxide layer. Different systems are considered. Here we mainly report on the system consisting of r-cut sapphire or LaAlO3, SrRuO3 or Nb:SrTiO3, and SrTiO3 as a substrate, conductor, and high-k layer, respectively. In order to achieve epitaxial growth, the sapphire is covered with a (002) CeO2 buffer layer. Bottom electrodes and high-k SrTiO3 are deposited via rf magnetron sputter technique. Depending on the choice of parameters various phases and structural orientations are obtained for the base layer resulting in a large variation in the specific resistance. Finally, SrTiO3 layers are deposited onto the bottom electrodes layers. The resulting structural and electronic properties of both layers are determined via RBS, XRD analysis and cryoelectronic analysis, respectively.

DS 42.122 Wed 15:00 P1

Dielectric function of ultra-thin high-k films grown by atomic layer deposition — •Li Ding[1], Lin Chen[2], Marion Friedrich[1], Ovidiu Gordan[1], Wei Zhang[2], and Dietrich Zahn[1] — [1]Semiconductor Physics, Chemnitz University of Technology, D-09107, Germany — [2]State Key Laboratory of ASIC and System, Department of Microelectronics, Fudan University, Shanghai 200433, China

High-k dielectrics are intensively studied to replace the conventionally used SiO2 as gate dielectrics in various electronic devices [1]. Hafnium dioxide (HfO2) is one of the candidates due to a high k value, a wide band gap around 6.4 eV, and a good thermal stability [2]. HfO2 usually forms crystalline structures, but amorphous films are preferred to minimize leakage currents through dielectric layers. It is possible to obtain amorphous films by growing HfO2 together with another compound, such as Al2O3, which stays amorphous at much higher temperatures.

Two series of samples were prepared by atomic layer deposition (ALD). One series consists of alloy films with different component ratios between HfO2 and Al2O3, while the other consists of bilayer films with various layer thicknesses. In order to investigate the influence of the film thickness and layer structure on the band gap, a vacuum ultraviolet (VUV) ellipsometer (4.0-9.8 eV) is employed using synchrotron radiation as a light source. Moreover, a laboratory spectroscopic ellipsometer (0.7-5 eV) is used to determine the film thickness.

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DS 42.123 Wed 15:00 P1

Admittance spectroscopy to characterize interface traps in MOS structures containing high-k materials — •Markus Hippler[1], Jan Lehmann[1], Varun John[1], Wolfgang Skorupa[1], Manfred Helm[1], Heidemarie Schmidt[1], Marcelo Lopes[2], Jür-

gen Schubert[2], and Siegfried Mantl[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01314 Dresden — [2]PGI-9 and JARAFIT, Research Centre Jülich, 52425 Jülich

Today‘s planar metal-oxide-semiconductor field-effect transistor (MOSFET) technology with silicon dioxide (SiO2) as the gate dielectric has reached its limit of scaling, because the leakage currents through 1nm SiO2 are unacceptable. For an ongoing down-scaling process, the gate dielectric has to be exchanged by a material with a higher relative dielectric constant k. Two of those candidates are lanthanum lutetium oxide (LLO) and lanthanum scandate oxide (LSO) with relative dielectric constants of k(LSO)=24 and k(LLO)=32, respectively. Here we characterize the properties of the interface traps, i.e. the trap density and time constant of MOS diodes based on those materials by admittance spectroscopy. For this purpose 6 and 20nm thick layers of LLO and LSO layers have been grown by molecular beam deposition (MBD) on RCA-cleaned p-Si.The admittance measurements were performed in the frequency range from 50 Hz to 20 kHz with an AC test bias amplitude of 10mV under variation of the DC ground voltage. Measured data have been analyzed by a numerical fitting program with respect to the serial resistance Rs and oxide capacitance Cox.

DS 42.124 Wed 15:00 P1

Ab initio study of the silylation mechanism of OH-groups with different Silazanes — •Oliver Böhm[1,2], Roman Leitsmann[1], Philipp Plänitz[1], Christian Radehaus[1], Michael Schreiber[2], and Matthias Schaller[3] — [1]GWT-TUD GmbH, Material Calculations, Chemnitz, Germany — [2]Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz — [3]Globalfoundries Dresden Module Two GmbH & Co. KG, Germany

The decreasing feature size of integrated circuits results in a smaller distance between the conduction layers, which is accompanied by an increasing resistance capacitance delay. Therefore, the usage of materials with an ultra low dielectric constant is necessary. However, the application of such ultra low k (ULK) materials is connected to several problems, like the formation of OH-groups after the etch process. This results in moisture uptake and a strongly increasing dielectric constant. To restore the k-value, a post-etch treatment is necessary. In this study we investigate the silylation of OH-groups with different silazanes. In particular we use density functional theory to study the different reaction mechanisms. For the silylation reaction of Hexamethyldisilazane (HMDS) and Trimethylaminosilane (TMAS) with Silanol, the minimum energy paths as well as the transition states are discussed in detail.

DS 42.125 Wed 15:00 P1

Thermal stability of BaSrO thin films and the influence of Al intermediate layers to the electrical properties of high-k Si(001)/BaSrO/Au MOS diodes — •Shariful Islam[1], Dirk Müller-Sajak[1], Alexandr Cosceev[2], Herbert Pfnür[1], and Karl R. Hofmann[2] — [1]Leibniz-Universität Hannover, Inst. f. Festkörperphysik — [2]Leibniz-Universität Hannover, Bauelemente der Mikro- und Nanoelektronik

MOS diodes with crystalline $Ba_{0.7}Sr_{0.3}O$ gate oxide and Au gate metal on n- and p-Si(001) were produced, which have a dielectric constant of $\epsilon_r \approx 28$. The oxides were grown on structured Si(001) in a UHV chamber by MBE in oxygen ambient conditions and capped with 100nm Au for ex-situ electrical measurements. I-V measurements show low leakage currents compared to SiO_2 with the same EOT. From C-V measurements we extracted with the Terman method a density of interface states, D_{it}, of only $\approx 10^{10}eV^{-1}cm^{-2}$.
We tested the thermal stability of these oxides and investigated them with X-Ray Photoelectron Spectroscopy (XPS). They are fully stable up to 450°C but convert to other chemical species, most likely silicates, at higher temperatures. But even at 700°C no formation of SiO_2 at the interface to Si was detectable.
To improve the adhesion between the Au gate metal and the oxide we evaporated a thin layer of Al at the Au/oxide interface. This causes a thickness dependent shift of the flatband voltage. We will present our XPS measurements of the chemical origin of this shift.

DS 43: Poster II: Thin Film Chalcogenide Photovoltaics; Thermoelectric Materials, Thin Films, and Nanostructures

Time: Wednesday 15:00–17:30 Location: P2

DS 43.1 Wed 15:00 P2

Aspects of designing an optimized molybdenum back contact in CIGS-technology — •Michael Oertel, Stefan Götz, Jakob Haarstrich, Heinrich Metzner, Udo Reislöhner, Carsten Ronning, and Werner Wesch — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, 07743 Jena, Germany

In $Cu(In,Ga)Se_2$(CIGS)-solar cell and module production, the sputtering of the molybdenum back contact is the first step in nearly all process lines. We present our results of experiments to elucidate the different aspects which have to be kept in mind when depositing the molybdenum back contact by dc-magnetron sputtering. These aspects include: I) The adhesion of the molybdenum to the glass substrate as well as the adhesion of the CIGS-layer to the molybdenum, II) electrical conductivity, III) sodium diffusion and IV) the specific contact resistance of the molybdenum to the aluminium doped zinc oxide (Al:ZnO) window layer. We present our three layer design of the back contact which combines an optimized adhesion to both the substrate and the absorber and also a high electrical conductivity. X-ray diffraction measurements (XRD) are employed to characterize each single layer. We also discuss I-U-measurements of $CuInSe_2$-solar cells made in a sequential absorber layer process in order to study the sodium transport behaviour of molybdenum back contacts sputtered at different argon sputter pressures. The sodium content in the absorber and the different back contact layers is measured by secondary ion mass spectroscopy (SIMS). A lowest value of the specific contact resistance between the Mo and the Al:ZnO of $(1.37 \pm 0.14) \cdot 10^5 \Omega cm^2$ was determined.

DS 43.2 Wed 15:00 P2

Characterisation of Cu_2ZnSnS_4 — •Jan E. Stehr[1], Detlev M. Hofmann[1], Bruno K. Meyer[1], Folker Zutz[2], Christine Chory[2], Ingo Riedel[2], and Jürgen Parisi[2] — [1]1st Physics Institute, Justus-Liebig-University Gießen, Heinrich-Buff-Ring 16, 35392 Gießen, Germany — [2]Institut für Physik, Carl von Ossietzky Universität Oldenburg, Carl-von-Ossietzky-Straße 9-11, 26129 Oldenburg, Germany

Cu_2ZnSnS_4 (CZTS) is an interesting material for thin film photovoltaic applications. It has a band gap energy in the required range (~ 1.5 eV) and avoids the cost intensive Indium being part of the solar-cell-absorbers based in $CuInS_2$. We investigated CZTS nanoparticles prepared by wet chemistry and deposited in the form of thin films on glass substrates by optical absorption and magnetic resonance spectroscopies. Optical absorption starts at about 1.3 eV which indicates that some centres causing sub-band-gap absorption are present in the material. Low temperature EPR spectra reveal the presence of Cu^{2+} by the observation of the typical 4 line spectrum caused by the hyperfine splitting. Regarding the precursors used for synthesis one expects copper to be in the valence state of 1 (Cu^+) thus the result may give a first experimental hint on the origin of the intrinsic p-type conductivity of the material.

DS 43.3 Wed 15:00 P2

Modeling the Thermal Conductance of Silicon Phononic Crystal Plates — •Stefanie Thiem[1] and Joel Moore[2] — [1]Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany — [2]Department of Physics, University of California, Berkeley, CA 94720, USA

Silicon phononic crystal plates with void pores have been found to posses enhanced figures of merit ZT, which make them potentially interesting for the construction of thermoelectric devices. We developed a method to compute the phonon thermal conductivity for these materials using the Landauer formula. This requires the calculation of the complete dispersion relation for the holey silicon plates. Thereby, we determine the elastic band structure by a plane-wave expansion method with a supercell approach.

DS 43.4 Wed 15:00 P2

Thermal conduction in correlated multilayer structures — •Stefanie Wiedigen[1], Kodanda R. Mangipudi[1], Manuel Feuchter[2], Christian Jooss[1], Cynthia A. Volkert[1], and Marc Kamlah[2] — [1]Institut für Materialphysik, Georg-August-Universität Göttingen, Germany — [2]Institut for Materials Research II, Karlsruhe Institute of Technology, Germany

High-efficient thermoelectric devices require effective methods of suppressing thermal conductivity, e.g. by complex materials, multilayer structures or nanoscale patterning to enhance the figure of merit Z. The goal of this collaborative work is to understand the anisotropic and size dependent thermal conductivity in multilayer structures. Because of correlation effects, e.g. perovskite oxides are promising new thermoelectric materials. Thin films of these materials are measured with the 3ω method which is a common and reliable measurement technique for thin film and multilayer thermal conductivity. However, measuring complex geometries requires an extension of the standard method. Improvement of the experimental setup is related to new heater concepts and patterned layer configurations. This needs support by finite element simulations with respect to the detailed thermal and electric conditions due to lack of analytical solutions. Another important requirement is the selection of multilayer materials and their geometry. We study phonon dispersion in a two component singly-periodic infinite multilayer system using continuum finite element models. The results will be presented in terms of the effect of the elastic constants and thickness on the phonon band gap variation.

DS 43.5 Wed 15:00 P2

Nb Substitution in Zr0.5Hf0.5NiSn based Compounds. — •Schwall Michael and Benjamin Balke — Johannes-Gutenberg University Mainz

This work reports about the structural and physical properties of the Heusler alloy (Zr0.5Hf0.5)1-xNbxNiSn with varying Nb concentration. The structure of the(Zr0.5Hf0.5)1-xNbxNiSn solid solution was investigated by means of X-ray diffraction. It is found that the alloys exhibit the C1b structure for all Nb concentration. The physical properties were studied using the PPMS from low temperature to room temperature. It was shown that the thermoelectric properties like the dimensionless Figure of Merit is increased 5 times by substituting(Zr0.5Hf0.5) with Nb to 0.09 at 300 K and the Powerfactor is increased 10 times to 1.8 mW/K2m at 300K.

DS 43.6 Wed 15:00 P2

The potential of phase change materials for thermoelectric applications - An investigation of alloys along the pseudo binary line from GeTe to SnTe — •Felix Lange, Hanno Volker, Karl Simon Siegert, and Matthias Wuttig — 1. Physikalisches Institut IA, RWTH Aachen University

Thermoelectric generators make use of the Seebeck effect which is an intrinsic property of any non dielectric solid. Materials with a high conversion efficiency are characterized by a high figure-of-merit $ZT = \sigma S^2/\kappa$, where σ is the electrical conductivity, S the Seebeck coefficient and κ the thermal conductivity.

We have recently shown that phase change materials employ resonant bonding [1] which results in a delocalization of carriers and an anharmonic potential [2]. The delocalization of carriers leads to high electrical conductivity while the anharmonic potential enhances the probability for phonon-phonon interactions such as umklapp processes. Hence, phase change materials are promising candidates for thermoelectric applications.

Therefore alloys along the pseudo binary line from GeTe to SnTe are investigated. It is shown, that the electrical conductivity can be tailored by gradually adding Sn. The disorder on the Ge-Sn sublattice causes a low thermal conductivity which develops a minimum for $Ge_2Sn_2Te_4$.

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

[2] D. Lencer *et al.*, Nature Materials **7**, 972-977 (2008)

DS 43.7 Wed 15:00 P2

Laser-induced electronic transport through electrochemically-fabricated point-contacts — •Bastian Kopp, Daniel Benner, Markus Schmotz, Zhiwei Yi, Johannes Boneberg, Paul Leiderer, and Elke Scheer — Universität Konstanz

Aim of this work is to study the effects of laser illumination on electrochemically-fabricated metallic point-contacts. By electron-beam lithography we pattern nanoscale metallic electrodes separated by a gap of roughly 500nm. This gap is then closed by electrochemical deposition of a second metal [1]. After removal of the electrolyte solution atomic-size contacts with conductance in the range of 10 to 100 G_0 are obtained. We present results measured on contacts consisting of various metal combinations including Au, Ag and Pt. We observe a distinct change of the conductance of these contacts upon laser irradiation. We study the spatial and wavelength dependence of the conductance change. The amplitude and sign of the signal depend on both the position of irradiation and the applied voltage. Our results can qualitatively be explained by thermoelectric effects with corrections for small conductance values.

[1] F.-Q. Xie, Phys. Rev. Lett. **93**, 128303 (2004)

DS 43.8 Wed 15:00 P2

A set-up for 3ω measurements on semiconductor nanowires and the role of electron-phonon decoupling — •Johannes Gooth[1,2], Phillip Wu[1], Sofia Fahlvik Svensson[1], Johannes Kimling[2], Kornelius Nielsch[2], and Heiner Linke[1] — [1]Division of Solid State Physics, Lund University, Sweden — [2]Applied Physics and Microstructure Research Center Hamburg, University of Hamburg, Germany

To characterise the performance of thermoelectric materials, the so called "figure of merit" ZT is an important value. We present a device for ZT measurements in semiconductor nanowires by using a microheater for the thermopower measurement and use of the the 3ω method to measure the thermal conductivity. A double-resist technique is used to suspend CBE-grown InAs nanowires wires above a substrate. Whereas near room temperature the 3ω method is very well established, questions arise about the coupling of electrons and phonons during the self-heating process at lower temperatures. To obtain a better understanding, we model the situation using a two temperature model, and we aim to compare our experimental results to a measurement method which is not based on self heating.

DS 43.9 Wed 15:00 P2

Ab initio investigations of inter atomic force constants and phonon dispersion relations at ZnO interfaces — •Michael Bachmann, Saeideh Edalati Boostan, and Christian Heiliger — I. Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany

ZnO/ZnS nanostructures are a promising material for thermoelectric applications due to the expectation of a strong phonon scattering at the interface but a high transmission of electrons through the interface. Since the heat conductance due to phonons reduces the efficiency of thermoelectric elements the understanding of phonon transport across interfaces is an important feature to improve thermoelectric devices. We present ab initio calculations of the inter atomic force constants for ZnO/ZnO interfaces. From these force constants we calculate the dynamic matrix and the dispersion relation as well as the phonon density of states. These calculations help us to first understand the thermal transport in sputtered ZnO films which is the basis for further investigations of the ZnO/ZnS nanostructure.

DS 43.10 Wed 15:00 P2

Reduction of the Lattice Thermal Conductivity in One-Dimensional Quantum Dot Superlattices due to Phonon Filtering — Denis L. Nika[1], Evghenii P. Pokatilov[1], Alexander A. Balandin[2], Vladimir M. Fomin[3], •Armando Rastelli[3], and Oliver G. Schmidt[3] — [1]Laboratory PMSMM, Department of Theoretical Physics, Moldova State University, MD-2009 Chisinau, Republic of Moldova — [2]Nano-Device Laboratory, Department of Electrical Engineering, University of California–Riverside, CA 92521 Riverside, U.S.A. — [3]Institute for Integrative Nanosciences, IFW-Dresden, D-01069 Dresden, Germany

One-dimensional quantum-dot superlattices (1D-QDS) consisting of acoustically mismatched materials Si/Ge, Si/plastic, Si/SiO_2 and Si/SiC are shown to possess sub-1 W $m^{-1}K^{-1}$ thermal conductivity in a temperature range from 50 K to 400 K. The phonon energy spectra are calculated in the framework of the molecular dynamic Face-centered Cubic Cell model. A significant reduction of the lattice thermal conductivity in 1D-QDS structures in comparison with homogeneous rectangular Si quantum wires is explained by the fact that the 1D-QDS structures act as effective phonon filters eliminating a significant number of phonons from thermal transport. The work was supported by the IB BMBF Project MDA 09/007 and ASM-BMBF Project 10.820.05.02GA.

DS 43.11 Wed 15:00 P2

Thermal conductivity measurements on nano air gaps. — •Thorben Bartsch, Matthias Schmidt, Christian Heyn, and Wolfgang Hansen — Institut für Angewandte Physik, Universität Hamburg, 20355 Hamburg, Germany

Nano air gaps in thermoelectric devices are an attempt to enlarge the efficiency of thermoelectric devices by drastically lowering of the thermal conductivity [1]. We present thermal conductivity measurements on GaAs based nano air gap heterostructures. The investigated structure is grown by molecular beam epitaxy. It is composed of a 50 nm GaAs layer which quasi hovers above the underlying GaAs substrate. The GaAs layers are held in position by GaAs nanopillars. Two samples have been studied with an air gap of 4 and 6 nm thickness, respectively. The measurements were performed for temperatures between 20 K and 300 K via the 3ω - method. The thermal conductivity values are up to three orders of magnitude smaller than the corresponding bulk thermal conductivity. [1] T. Zeng, Appl. Phys. Lett. 88, 153104 (2006).

DS 43.12 Wed 15:00 P2

3ω-measurements on ZnO/ZnS thin film structures — •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 of rf-sputtered ZnO/ZnS thin film layer structures. For this purpose a 3ω measurement system has been set up. It is based on a passive bridge circuit to eliminate the 1ω voltage component to facilitate a reliable measurement of the 3ω component. The samples can be heated as well as cooled, so that measurements can take place in a temperature range from 80 K to 400 K. In addition to the experimental setup, first measurements on ZnO/ZnS thin film layers will be presented. These will be carried out in a heater on top configuration and with different heater lengths on the same samples. The different ΔT curves are compared and the cross-plane thermal conductivities of the films will be evaluated for different temperatures.

DS 43.13 Wed 15:00 P2

Thermal conductivity and thermoelectric properties of a suspended GaAs/AlGaAs heterostructure — •Matthias Schmidt, Andrea Stemmann, and Wolfgang Hansen — Institut für Angewandte Physik, Universität Hamburg, 20355 Hamburg, Germany

We study low-temperature magnetothermoelectric properties of two-dimensional electron systems (2DEGs) embedded in a thin suspended membrane consisting of a modulation doped GaAs/AlGaAs heterostructure grown by molecular beam epitaxy. Electron-beam lithography is used to pattern the top of the membrane featuring a micro-scaled Hall bar, thermometers, and a Joule heater on top. The heater at the central region of the membrane generates a strong thermal gradient between the hot and the cold end side of the 34 μm long Hall bar including the 2DEG. A temperature difference of more than 5 K can be achieved at a mean temperature well below 10 K. We present heat conductivity and magnetothermopower measurements. The results show that the specific thermal conductivity of the membrane is qualitatively and quantitatively different with respect to the bulk value. Observed magnetothermopower is similar to results of earlier publications on GaAs/AlGaAs heterostructures. However, in contrast to previous results our measurements of the zero-field thermopower reveal that thermodiffusion is the main source of the thermopower at temperatures up to 3 K until the phonon drag dominates the run of the thermopower. This value is significantly higher than reported for non-suspended heterostructures [1].

[1] R. Fletcher et al., *Phyical Review B* 14991 (1994)

DS 43.14 Wed 15:00 P2

In-plane transport of artificially structured CVD ZnO/ZnO:Ga and ZnS/ZnO:Ga barstructures with different interface design — •Gert Homm, Steve Petznick, Sebastian Eisermann, Torsten Henning, Martin Eickhoff, Bruno K. Meyer, and Peter J. Klar — I. Physikalisches Institut, Justus-Liebig Universität, Heinrich-Buff-Ring 16, 35392 Gießen, Germany

Series of different bar-shaped samples consisting of lateral arrangements of either alternating ZnO:Ga and ZnO stripes or ZnO:Ga and ZnS stripes were fabricated from rf-sputtered layers or epitaxial layers. Photolithography techniques and wet-chemical or ion-beam etching followed by a second sputtering process were used to transfer the pattern. The bar-shaped structures have dimensions of a few micrometers and are oriented parallel to the applied temperature gradient and thus to the transport direction. The structure of the interfaces is varied to create controlled interface roughnesses. This enables one to gain information about the extension of the interface region and the transport mechanisms along the interfaces by measuring the Seebeck coefficient and the electrical conductivity of series of samples with different interface structures.

DS 43.15 Wed 15:00 P2

Doping of hydrogenated a-Si and a-Ge nanostructures — •Christoph Grüner, Jens Bauer, Chinmay Khare, and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung, Permoserstrasse 15, D-04318 Leipzig, Germany

Nanostructured semiconductor thin films promise high performance in future thermoelectric applications. Glancing angle deposition (GLAD) is a recent technique to fabricate self-organized nanostructures. Based on shadowing at oblique incidence angle separated nanocolums evolve, which can be shaped by substrate rotation about its normal. As a result vertical nanospirals, nanoscrews, or nanocolumns are formed. By variing the incidence angle the deposition can be further customized. Amorphous hydrogenated silicon and germanium layers and nanostructures were grown by electron-beam evaporation at room temperature. Antimony and boron were used for in-situ doping by effusion cells. Hydrogenation is done with a hydrogen atom beam source. Hydrogen passivates the dangling bonds of the amorphous materials and thus it is used to enhance the electrical properties of doped a-Si and a-Ge films. We will present the influence of hydrogen on the dopant concentration and the electrical resistivity in a-Si and a-Ge thin films. The effect of Sb and B segregation will be discussed with respect to the hydrogen flux. The chemical composition is investigated by SIMS profiles. Furthermore, rapid temperature annealing experiments were performed for electrical activation of the dopants. Also the influence of hydrogenation and doping on the appearance and distribution of nanostructures is shown.

DS 43.16 Wed 15:00 P2

Measurements of the in-plane thermal conductivity of thin films using a microstructured heater and sensor arrangement — •David Hartung, Achim Kronenberger, Steve Petznick, Torsten Henning, Bruno K. Meyer, and Peter J. Klar — I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Germany

The aim of this work is to characterise the lateral heat flow in a thin semiconductor layer on a glass substrate. Cover-glass is used for the heater and sensor arrangement. The masurement area is 0.5 mm × 0.5 mm where sensor and heater are deposited. A broad Au wire along the middle axis of this measurement area serves as the electric heater, three narrow Au wires at different distances from, but parallel to the heater wire, serve as temperature sensors. The arrangement was defined by photolithography on to the grass-substrate. Thin films of insulating ZnS and ZnO are deposited on to the measurement by RF-sputtering. First results of the measurements will be presented.

DS 43.17 Wed 15:00 P2

Thermal properties of phase change materials — •Karl Simon Siegert, Carl Schlockermann, Peter Zalden, and Matthias Wuttig — 1. Physikalisches Institut IA, RWTH Aachen University, 52064 Aachen

Many chalcogenic alloys such as GeTe or $Ge_1Sb_2Te_4$ offer unique physical properties which justify their classification as so called phase change materials (PCM). All of these materials share the following attributes: high contrast between the amorphous and the crystalline state in both electrical resistivity and optical reflectivity combined with fast crystallization speed in the order of ns [1]. This special combination of properties make PCMs favorable for modern data storage applications. As the switching between states is induced by temperature, detailed knowledge of the thermal properties is needed for further improvement of PCM based data storage devices.

This work contributes to the thermal characterization of phase change materials. Several PCM thin films were sputter deposited on silicon substrates. Using different experimental techniques, the specific heat (DSC measurements) and the cross plane thermal conductivity (differential 3ω) of the films were measured. Further data processing revelead the thermal diffusivity and the main heat conduction channels of the materials. Additionally, the influence of thermal interface resistances within a PC-dielectric dual-layer system was determined by thickness series.

[1] Bruns et al., Nanosecond switching in GeTe phase change memory cells, APL 2009

DS 43.18 Wed 15:00 P2

Investigation of thermal and electrical properties of individual nanostructures using specially designed microchips — •Daniel Huzel[1,2], Heiko Reith[1,2], Matthias C Schmitt[1,2], Friedemann Völklein[1], Roland Sachser[2], and Michael Huth[2] — [1]Institut für Mikrotechnologien (IMtech), Hochschule RheinMain, Am Brückweg 26, D-65428 Rüsselsheim — [2]Physikalisches Institut, Goethe-Universität, Max-von-Laue-Str. 1, D-60438 Frankfurt am Main

Our work focuses on the determination of thermal and electrical transport properties of individual thermoelectric nanostructures, in particular single nanowires. The Seebeck coefficient, electrical and thermal conductivity depend strongly on material, composition, crystallinity and geometric structure. To measure these coefficients, specially designed microchips have been developed and employed. FEM simulations demonstrate that the temperature profiles of the microchips show appropriate temperature gradients for Seebeck effect measurements and heat sink conditions for thermal conductivity investigations. Results of measurements on bismuth, bismuth-telluride and -antimonide nanowires are presented. The microchips have also been used for thermoelectric measurements on nano-granular metals prepared by focused electron beam induced deposition (FEBID).

DS 44: Invited – Yarmoff

Time: Thursday 10:15–11:00 Location: GER 37

Invited Talk DS 44.1 Thu 10:15 GER 37

Electronic Properties of Metal Nanoclusters Measured by Low Energy Ion-Surface Charge Exchange — •Jory Yarmoff — Department of Physics and Astronomy, University of California, Riverside, CA 92521 USA

Due to the quantum nature of their localized electronic states, small metal nanoclusters have great potential for use in diverse applications. We use low energy ion scattering (LEIS) to interrogate metal clusters by measuring the neutralization of backscattered alkali ions. Charge exchange during alkali ion scattering provides a unique probe of surface electronic properties and is acutely sensitive to the quantum states in nanomaterials. The sensitivity results from electrons that resonantly tunnel between the projectile ionization level and overlapping states in the clusters.

Nanomaterials were produced by deposition of metals onto oxide substrates and by sputtering a thin metal film with noble gas ions. The shapes of the scattered energy spectra provide information on the atomic structure of the clusters, while the neutralization depends on electronic states that are a function of cluster size. The sputtering of a thin film is a novel means for nanomaterial fabrication, as the interplay between curvature dependent roughening and diffusion-induced smoothing can produce clusters with quantum confinement. Future efforts will include investigations of other supported nanocrystals, chemically synthesized nanoparticles, and nanomaterials in diverse media.

DS 45: Ion Interactions with Nano Scale Materials I (Focused Session – Organisers: Diesing, Facsko)

Time: Thursday 11:00–13:00 Location: GER 37

DS 45.1 Thu 11:00 GER 37

Electron emission in the interaction of slow ions and electrons with nanostructured surfaces — Pierfrancesco Riccardi, Michele Pisarra, and •Antonio Sindona — Università della Calabria and INFN, Cosenza, Italy

We will discuss some case studies showing that secondary electron spectroscopy of nanomaterials reveals important electronic properties of the targets. Early studies [1] showed that a submonolayer Sodium film grown on Metal substrates can be converted into two-dimensional patches by ion bombardment. Spectroscopy of electrons, emitted by autoionization of projectiles excited in collisions with target atoms, reveals the coexistence of surface regions with very different work functions which are relatively adsorbate rich and adsorbate depleted. More recently, studies of of ion- and electron-induced electron emission have been carried out on carbon based nanomaterials [2]. Here, we will report on the energy distributions of electrons ejected by the impact keV He ions and electrons on graphene adsorbed on a Ni surface [3]. We use secondary electron spectroscopy to probe the excited states of graphene adsorbed on a Ni surface. A fine structure directly related to the empty bands above the vacuum level of the sample is resolved in the spectra excited by electrons. Ion-induced spectra reveal a high energy feature that is consistent with electron promotion from valence to conduction band states. References [1] P. Riccardi et al. Thin Solid Film 289 (1996) 177 [2] M. Commisso et al. Surface Science 601 (2007) 2832 [3] P. Riccardi et al. Applied Physics Letters 97 (2010) at press

Topical Talk DS 45.2 Thu 11:15 GER 37

Energy dissipation in the scattering of N_2 from W(110) — •J. Inaki Juaristi — Departamento de Física de Materiales, Facultad de Químicas, UPV/EHU, San Sebastián, Spain — Centro de Física de Materiales (CSIC-UPV/EHU), San Sebastián, Spain

Motivated by the measurements reported in [1], we study the scattering of N_2 from W(110) with classical dynamics calculations on a multi-dimensional potential energy surface (PES). In this talk, I will show the results of our simulations for the rotational state distributions and discuss the possible mechanisms involved in the energy dissipation measured in the experiments. The potential energy surface is obtained by the interpolation of an extended ab-initio data set calculated within density functional theory over a broad six-dimensional configuration space. Regarding the energy dissipation mechanisms we analyze the relative importance of electron-hole and phonon excitations. The former are incorporated through a friction force with the aid of a model developed in our group. Briefly, the friction coefficient is calculated within a local density approach, for an ion embedded in an electron gas [6]. Phonon excitations are included via a Generalized Langevin Oscillator model [7].

[1] Hanisco T F, Kummel A C, J. Vac. Sci. Technol. A, 11, 1907 (1993)

[6] Juaristi J I, Alducin M, Díez Muiño R, Busnengo H F, and Salin A, Phys. Rev. Lett., 100, 116102 (2008)

[7] Busnengo H F, Dong W, and Salin A, Phys. Rev. Lett., 93, 236103 (2004)

DS 45.3 Thu 11:45 GER 37

Internal Electron Emission detected in Metal-Insulator-Metal Thin Film Tunnel Devices bombarded with keV Cluster Projectiles — •Mario Marpe[1], Christian Heuser[1], Detlef Diesing[2], and Andreas Wucher[1] — [1]Fakultät für Physik , Universität Duisburg-Essen, D-47048 Duisburg, Germany — [2]Fakultät für Chemie, Universität Duisburg-Essen, D-45117 Essen, Germany

The electronic excitation of a solid surface bombarded by energetic ions manifests in the production of hot electrons, which can be either emitted from the surface (”kinetic electron emission”) or remain within the solid. We use Metal-Insulator-Metal (MIM) tunneling junctions to detect and investigate hot charge carriers (electrons and holes) produced during bombardment of a metal surface with keV rare gas (Ar+) ions. The sample consists of a top metal film of about 20 nm thickness (the actual bombarded target surface), an underlying thin (2-3 nm) oxide film deposited and another metal electrode underneath. With such a device, excitations below the vacuum level can be detected as an internal electron emission current between the two metal electrodes.

By combining the information obtained from external and internal emission, it is possible to gain information regarding the depth distribution of the generated excitation as well as the transport mechanism distributing the excitation away from its initial point of generation. We demonstrate this by varying the impact angle of the projectile ion beam. It is found that external and internal emission currents vary exactly in opposite direction when going from normal to oblique incidence.

DS 45.4 Thu 12:00 GER 37

Time resolved transport of alkali ions through ultra-thin films — •Susanne Schulze and Karl-Michael Weitzel — Philipps-Universität Marburg, Fachbereich Chemie, 35032 Marburg

In this study, we report on the transport of K^+ through poly(*para*-xylylene) films of 200 to 3000 nm thickness. The experiments are performed in an ultra-high vacuum chamber where an ion beam is generated by thermionic emission of K^+ from aluminosilicates [1]. In one experiment the film is bombarded by a c.w. K^+ ion beam. Individual ions transmitted through the film are detected by two microchannel plates. The analysis of the pulse-pair correlation function of successive ion detection events reveals a sharp drop in the width of the probability distribution between impact energies of 1300 and 1400 V. This variation is interpreted as an indication of a change in the underlying transport mechanism connected to an electrical breakdown induced by space charge zones as a consequence of the ion bombardment [2]. In a second experiment the film is bombarded by a pulsed ion beam. Ions passing through the film are analysed in a time of flight (TOF) spectrometer. The TOF is measured through the film as a function of the impact energy and is compared to the one in the absence of the film. For low impact energies the ions are delayed by the film, which is not the case for high impact energies. These results will be discussed in terms of the transition from diffusive to space-charge driven transport. [1] T. Kolling, A. Schlemmer, C. Pietzonka, B. Harbrecht, J. Appl. Phys., 107, 014105, (2010). [2] K. Schröck, S. Schulze, A. Schlemmer, K.-M. Weitzel, J. Phys. D Appl. Phys., 43, 025501, (2010).

DS 45.5 Thu 12:15 GER 37

Monitoring particle and photo induced electronic excitations by metal–insulator–semiconductor devices — •Kevin Stella[1], Domocos A. Kovacs[1], Wolfgang Brezna[2], Jürgen Smoliner[1], and Detlef Diesing[1] — [1]Fakultät für Chemie, Universität Duisburg-Essen, D-45117 Essen, Germany — [2]Institut für Festkörperelektronik, TU Wien, A-1040 Wien, Austria

Excited charge carriers in and on thin metal-insulator-semiconductor devices (MIS) are released either by internal photoemission or by exposing the device surface with argon ions. Photons (visible and near infrared) penetrate all three layers of the MIS device and excite carriers in the semiconductor as well as in the metal. Excited carriers by low energy argon ions ($E_{kin} = 200\,\mathrm{eV}$) are released only in the first atomic layers of the top metal film. Photon induced carrier transport shows a strong bias dependence with saturation values of up to 0.1 for the photoyield in reverse bias. The voltage necessary for reaching the saturation value is a clear function of the interstitial oxide layers thickness. With forward bias the photoyield decreases to 10^{-4}. Ion induced carrier transport exhibits an opposed bias dependence with a suppression of the signal in reverse biasing.

DS 45.6 Thu 12:30 GER 37

Ion Beam Irradiation of Nanostructures - A 3D Monte Carlo Simulation Code — •Christian Borschel and Carsten Ronning — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena

We have developed a computer program for the simulation of ion beam irradiation of nanostructures. The code uses a Monte Carlo algorithm to simulate the transport of energetic ions through matter, similar to the often used SRIM code. When irradiating nanostructures, which are of the same size as the ion range or the dimension of the damage cascade, new effects occur as compared to bulk. Our code can account for these effects by allowing almost arbitrary 3-dimensional target structures as opposed to the layered target structures used in SRIM. Thus, more accurate 3D distributions of implanted ions and implantation damage for nanostructures can be obtained. The functionality of the code is demonstrated by comparing simulations with experimental results from ion beam implantation into nanowires.

DS 45.7 Thu 12:45 GER 37

Production and design of quantum dot lattices by ion beam irradiation — •Maja Buljan[1], Iva Bogdanović-Radović[1], Nikola Radić[1], Marko Karlušić[1], Goran Dražić[2], Sigrid Bernstorff[3], and Holy Vaclav[4] — [1]Rudjer Bošković Institute, 10000 zagreb, Croatia — [2]Jožef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia — [3]Sinchrotrone Trieste, 34102 Basovizza, Italy — [4]Faculty of Mathematics and Physics, Charles University in Prague, 12116 Prague, Czech Republic

Quantum dot (QD) based materials are widely investigated nowadays due to their interesting properties and numerous possible applications. Especially interesting are semiconductor quantum dots embedded in amorphous wide-bandgap matrices due to strong confinement effects. However, the production of such materials with controllable size, composition and arrangement properties remains a challenge. Here we demonstrate a method for the production of a well-ordered three-dimensional array of semiconductor quantum dots in amorphous silica matrix. The ordering is achieved by ion beam irradiation and annealing of a multilayer film. Structural analysis shows that the quantum dots nucleate along the direction of the ion beam, while the mutual distance of the dots is determined by the diffusion properties of the multilayer material rather than by the distances between the traces of the irradiating ions. In addition, we present the effects of a post-irradiation annealing on the internal structure of the quantum dots.

[1] M. Buljan, et al. Appl. Phys. Lett. 95, 063104 (2009). [2] M. Buljan, et al. Phys. Rev. B 81 085321 (2010).

DS 46: Invited – Bell

Time: Thursday 14:00–14:45 Location: GER 37

Invited Talk DS 46.1 Thu 14:00 GER 37

Structuring Graphene with He Ions — •David C. Bell — School of Engineering and Applied Sciences and Center for Nanoscale Systems, Harvard University, USA

Helium Ion Microscopy (HeIM) has been introduced as an ultra high-resolution imaging technology for a variety of materials applications, with a probe size in the order of 0.5 nm. However, being a charged ion beam instrument it is also possible to perform milling and sputtering tasks similar to conventional gallium ion beam systems (FIB). The combination of these features has the capability to make this instrument one of the most precise direct fabrication tools currently available for materials. We demonstrate etching of graphene devices with a helium ion beam, including in situ electrical measurement during lithography. The etching process can be used to nanostructure and electrically isolate different regions in a graphene device, as demonstrated by etching gaps of about 10 nm into graphene devices. Graphene on silicon dioxide (SiO_2) substrates etches with considerably lower He ion doses compared to suspended graphene.

DS 47: Ion Interactions with Nano Scale Materials II (Focused Session – Organisers: Diesing, Facsko)

Time: Thursday 14:45–15:45 Location: GER 37

Topical Talk DS 47.1 Thu 14:45 GER 37

Trails of kilovolt ions created by subsurface channeling — •Thomas Michely[1], Alex Redinger[1], Sebastian Standop[1], Yudi Rosandi[2], and Herbert Urbassek[2] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Fachbereich Physik und Forschungszentrum OPTIMAS, Universität Kaiserslautern, Germany

Using scanning tunneling microscopy, we observe the damage trails produced by keV noble-gas ions incident at glancing angles onto Pt(111). Surface vacancies and adatoms aligned along the ion trajectory constitute ion trails. Atomistic simulations reveal that these straight trails are produced by nuclear (elastic) collisions with surface layer atoms during subsurface channeling of the projectiles. In a small energy window around 5 keV, Xe$^+$ ions create vacancy grooves that mark the ion trajectory with atomic precision. The asymmetry of the adatom production on the two sides of the projectile path is traced back to the asymmetry of the subsurface channel. For ripple pattern formation through grazing incidence ion bombardment trail formation is of decisive importance for the regularity and alignment of the resulting erosion morphology.

Topical Talk DS 47.2 Thu 15:15 GER 37

The impact of fast ions in pulsed laser deposition — •Michael Schmid — TU Wien, Institut für Angewandte Physik, Wien, Austria

Pulsed laser deposition (PLD) is a method for growing thin films that combines nonthermal particle energies (typically 30 to 300 eV) with ultrahigh-vacuum compatibility. This allows us to study the effects of energetic ions on growth of ultrathin films by high-resolution scanning tunneling microscopy [1]. Ions with energies above 100 eV can create adatoms or small adatom clusters by "failed sputtering", which increases the number of nucleation centers and, thus, the island density. Ion implantation in the surface is possible already at lower energies. In heteroepitaxy, ion implantation creates a chemically inhomogeneous surface, which modifies surface diffusion and again leads to an increased island density. High island densities, combined with facile implantation near steps, result in improved layer-by-layer growth. We propose that the same mechanisms are effective in sputter deposition.

[1] M. Schmid et al., Phys. Rev. Lett. 103, 076101 (2009).

DS 48: Ion Interactions with Nano Scale Materials III (Focused Session – Organisers: Diesing, Facsko)

Time: Thursday 16:00–17:30 Location: GER 37

Topical Talk DS 48.1 Thu 16:00 GER 37

Ion beam doping of semiconductor nanowires — •Carsten Ronning — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena

Semiconductor nanowires are of major importance within the area of nanotechnology, and are usually synthesized using the so-called vapor-liquid-solid (VLS) mechanism. Controlled doping, a necessary issue in order to realize device applications, is an unsolved problem and an extremely difficult task if using such a growth mechanism. We use an alternative route for modifying the electrical, optical and magnetic properties of semiconductor nanowires: low-energy ion implantation within the keV range. The structural impact to the nanowires was investigated, and several effects due to the fact the ion range matches the diameter of the nanostructures had to be considered. A new simulation tool was therefore developed. This together with several independent studies on optical and electrical doping of semiconductor nanowires will be presented.

DS 48.2 Thu 16:30 GER 37

Structural investigations of ion beam doped silicon nanowires — •Jörg Grenzer[1], Olga D. Roshchupkina[1], Reinhard Kögler[1], Pratyush Das Kanungo[2], and Peter Werner[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf , Bautzner Landstraße 400, 01328 Dresden — [2]Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle

For the development of nano-optical devices nano wires (NW) are of emerging interest. One of the most important steps in the fabrication of Si devices is doping using ion beam implantation. However, this may lead to a distortion of the NW's crystalline structure or even to an amorphization. A subsequent annealing procedure is necessary to recover the crystalline structure. The advantage of implanted Si NW's is that the electrical conductivities are significantly higher than MBE-grown in-situ doped ones [1]. NW's of about 100nm in diameter and 100..400 nm in length, nominally undoped, were MBE grown on Si(111) using Au as a growth-initiator. We followed the structural changes of the NW's caused by implantation and annealing. We used rapid thermal annealing up to a temperature of 1100°C of about 30 seconds to remove a possible damage induced by implantation. Diffraction experiments were carried out at the ID01 ESRF beamline using a microfocused X-ray beam in combination with a 2D detector to obtain 3D diffraction patterns. Our experiments have shown that defect structure and form of the investigated NW's change after implantation and annealing. [1] X.Ou, P. Das Kanungo, R. Koegler, P. Werner, U. Gosele, W. Skorupa, and X. Wang, Nano Letters 10, 171 (2010).

DS 48.3 Thu 16:45 GER 37

Evolution of surface topography of Si(001) during ion beam erosion — •Martin Engler[1], Sven Macko[1], Frank Frost[2], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Leibniz-Institut für Oberflächenmodifizierung e. V., Leipzig, Germany

We investigated the evolution of surface topography of Si(001) during 2 keV Kr$^+$ ion beam erosion with in-situ STM under UHV conditions for fluences up to $1 \times 10^{22}\,\mathrm{ions\,m^{-2}}$. At room temperature and for an ion incidence angle of $\vartheta = 75^\circ$ with respect to the surface normal the flat surface rapidly destabilizes. The observed topography changes qualitatively with ion fluence. We have identified a sequence of distinct phases in the surface evolution: a stochastically roughened surface transforms into a ripple pattern and finally into a faceted surface. These phases are governed by different processes. At low fluences the stochastic nature of ion bombardment dominates. With increasing fluence ripples with constant wavelength are selected by an interplay of roughening and smoothening. At high fluences non-linear effects like the gradient dependence of sputtering yield and reflection of ions lead to a faceted topography which coarsens and looses homogeneity in structure size. A similar sequence was observed for impurity induced pattern formation at $\vartheta = 30^\circ$ although the mechanisms of pattern formation are different.

DS 48.4 Thu 17:00 GER 37

Shadowing in metal assisted ion beam patterning on Si(001) — •Sven Macko[1], Martin Engler[1], Frank Frost[2], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Leibniz-Institut für Oberflächenmodifizierung e. V., Leipzig, Germany

At grazing incidence low energy ion beam erosion of Si surfaces gives rise to nanoscale surface patterning. Co-sputterdeposition of stainless steel expands the angular range of pattern formation also to non-grazing and normal directions of incidence. Here we employ co-evaporation instead of co-sputterdeposition and a 2 keV Kr$^+$ ion beam under UHV conditions. Due to the thermal energy and well defined angle of incidence of the co-evaporated species the experiments provide a more direct insight to pattern formation mechanisms. In dependence of the atom-to-ion arrival ratio we find the flat surface as well as dot and ripple patterns. Fluence dependent experiments show that the type of pattern is already selected in the early stages of pattern formation. A key parameter for pattern formation is the angle α between the impinging ion beam and the co-deposition flux. For $\alpha > 90°$ we observe rapid formation of a faceted and rough pattern while for small angles $\alpha \approx 30°$ pattern formation diminishes. We conclude that shadowing is of decisive importance for the formation of local impurity concentration inhomogeneities which in turn cause local sputtering yield variations and thus the destabilization of the surface.

DS 48.5 Thu 17:15 GER 37

Nanohole Pattern Formation on Ge by Focused Ion Beam and Broad Beam — •Monika Fritzsche, Stefan Facsko, and Kilian Lenz — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, P.O. Box 510119, 01314 Dresden, Germany

The morphology of surfaces strongly influences optical, electrical, and magnetic properties of thin films. Using low energy ion beam sputtering different self-organized periodic patterns can be obtained. These are ripple patterns with periodicities in the nanometre range for oblique ion incidence and hexagonal dot patterns on compound materials for normal incidence. Low energy ion beam sputtering of Ge at normal incidence using a 5 keV Ga^+ focused ion beam (FIB) produces periodic nanohole patterns [1]. In this work we studied the flux dependence of nanohole formation using FIB technique and compared the results with patterns produced by broad Ga^+ beam sputtering with a six orders of magnitude smaller ion flux. In both cases Ga^+ ions with an energy of 5 keV at normal incidence were used. Obtaining the same results shows that nanohole formation is independent of flux over a few orders of magnitude and that rastering of the FIB does not add extra contributions.

[1] Q. Wei, X. Zhou, B. Joshi, Y. Chen, K. Li, Q. Wei, K. Sun, and L. Wang, *Adv. Mater.* **21**, 2865 (2009).

DS 49: Ion Interactions with Nano Scale Materials IV (Focused Session – Organisers: Diesing, Facsko)

Time: Thursday 17:45–19:15 Location: GER 37

Topical Talk DS 49.1 Thu 17:45 GER 37

Nano-scale surface modifications produced by highly charged ion impact — •Friedrich Aumayr — TU Wien, Inst. für Angewandte Physik

The large amount of potential energy stored in highly charged ions (HCI) is liberated during the interaction with a solid surface within a few femtoseconds into a nanometer size volume close to the surface. It is therefore not astonishing that severe surface modifications with nanometer dimensions have been demonstrated for the impact of individual slow HCI on various surfaces, similar to the impact of individual swift heavy ions. Depending on the type of material, nanohillocks, nano-pits or caldera-like nano-craters have been found at the ion impact site.

Present research tries to control the production of material modifications on surfaces and thin films (including 2D carbon-nanosheets and graphene) with well-defined size in the nanometer region by a variation of the HCI potential energy. The current status of this rather new field will be presented.

DS 49.2 Thu 18:15 GER 37

Nanostructures induced by slow highly charged ions on KBr(001) surfaces — •Richard Wilhelm, René Heller, and Stefan Facsko — Helmholtz-Zentrum Dresden - Rossendorf – Institut für Ionenstrahlphysik und Materialforschung – Bautzner Landstraße 400 - 01328 Dresden

Highly charged ions carry a large amount of potential energy (up to 100 keV) which is defined as the sum of all binding energies of all missing electrons. This energy can be used to modify surfaces on the nano-scale and due to very low kinetic energies (less than 100 eV) significant bulk damage can be avoided. The production of nanometer sized pit-like structures on KBr(001) surfaces by the impact of single highly charged ions was studied in detail previously. The investigation of high fluence effects of highly and lowly charged ions is important to clearly identify the mechanism of defect mediated desorption as the driving force for the creation of pit-like nanostructures on ionic crystals like KBr. Results of high fluence compared to low fluence irradiations will be shown and kinetic and potential energy effects will be discussed.

DS 49.3 Thu 18:30 GER 37

Surface patterning by ion bombardment: predictions of large-scale atomistic simulations — •Bartosz Liedke, Karl-Heinz Heinig, Stefan Facsko, and Wolfhard Möller — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany

Despite of intense studies in recent years, atomistic understanding of surface evolution during ion irradiation is still under discussion. Continuum models, like the Bradley and Harper theory, cannot explain microscopic processes during ion irradiation. So far, atomistic simulations could not describe pattern dynamics on spatiotemporal scales of experiments.

We present a novel program package that unifies the simulation of collision cascades with kinetic Monte-Carlo simulations. The 3D atom relocations were calculated in the Binary Collision Approximation (BCA), whereas the thermally activated relaxation of energetically unstable atomic configurations as well as diffusive processes were simulated by a very efficient bit-coded kinetic 3D Monte Carlo code.

Our studies show that: (i) bulk defects continuously created within the collision cascade are responsible for local surface topography fluctuations and induce surface mass currents. These currents smooth the surface from normal incidence up to $\theta = 40°$, whereas at $\theta > 40°$ ripple patterns appear; (ii) sputtering is not the dominant driving force for the ripple formation at non-grazing incidence angles. Surface patterning is caused by processes like bulk and surface defect migration, recombination, bulk and surface diffusion and ion induced diffusion.

DS 49.4 Thu 18:45 GER 37

Temporally resolved track creation in dielectrics after swift heavy ion irradiation. Part I: Monte-Carlo simulation — •Nikita Medvedev[1,2], Orkhan Osmani[1,3], Marika Schleberger[3], and Baerbel Rethfeld[1] — [1]Technical University of Kaiserslautern, Germany — [2]CFEL at DESY, Hamburg, Germany — [3]University of Duisburg-Essen, Germany

The dynamics of structural modifications of dielectrics irradiated with swift heavy ions (SHI, with energies E > 1 MeV/u and masses M > 20 proton mass) are investigated theoretically. We developed a combination of Monte-Carlo method (MC), used to describe SHI penetration and following excitation and relaxation of the electronic subsystem, with Two Temperature Model (TTM) describing the heating of the lattice [1,2].

In part I of this report we describe the MC method and its main results: the thermalization time of electrons in track, the distribution of energies of electrons, holes, and lattice. That gives a physical background, limits of validity, initial conditions and parameters necessary for the subsequent TTM calculations, presented in the part II.

[1] N.Medvedev, A.E.Volkov, N.Stcheblanov, B.Rethfeld, Phys. Rev. B **82**, 125425 (2010)

[2] N.Medvedev, O.Osmani, B.Rethfeld, M.Schleberger, Nucl. Instrum. and Meth. B **268**, 3160 (2010)

DS 49.5 Thu 19:00 GER 37

Temporally resolved track creation in dielectrics after swift heavy ion irradiation. Part II: Two Temperature Model — •Orkhan Osmani[1,2], Nikita Medvedev[1], Bärbel Rethfeld[1], and Marika Schleberger[2] — [1]University of Duisburg-Essen, Germany — [2]Technical University of Kaiserslautern, Germany

The dynamics of structural modfications of dielectrics irradiated with swift heavy ions (E>1MeV/u and masses M>20 proton mass) are investigated theoretically. In part II of this report on our combined Monte Carlo–Two Temperature description we show that the results obtained from the MC calculations determine the conditions at which the TTM can be applied. Out of these results material parameters for the electron system, such as the specific heat capacity and the electron-phonon coupling, can be extracted. These parameters are necessary for the final track radii calculations within the TTM [1] and are often not accessible by experiments. It will be demonstrated how to couple the (kinetic) MC results with the (continuum) TTM simulation. Finally the computed track radius will be compared with experimental observations [2].

[1] O. Osmani, A. Duvenbeck, E. Akcöltekin, R. Meyer, H. Lebius and M. Schleberger, New J. Phys. 10, 053007 (2008)

[2] P. Kluth, C. S. Schnohr, O. H. Pakarinen, F. Djurabekova, D. J. Sprouster, R. Giulian, M. C. Ridgway, A. P. Byrne, C. Trautmann, D. J. Cookson, K. Nordlund, and M. Toulemonde, Phys. Rev. Lett., 101 175503 (2008)

DS 50: Organic Electronics and Photovoltaics I (jointly with CPP, HL, and O)

Time: Thursday 10:15–11:45 Location: GER 38

DS 50.1 Thu 10:15 GER 38

Structuring of Organic Conductors by Laser Ablation — •Alexander Esser, Moritz Schaefer, Jens Holtkamp, and Arnold Gillner — Fraunhofer ILT, Steinbachstraße 15, 52074 Aachen

PEDOT:PSS is a transparent organic polymer with a sheet resistivity of about 200ohm/sq. These attributes make it an ideal candidate for substituting ITO in organic LEDs and organic photovoltaic cells: making them fully organic, flexible, lightweight and cheap to produce. Organic thin-film photovoltaics are a low cost alternative to state of the art silicon and other inorganic semiconductor-based solar cells. OLEDs can be made more flexible without the use of transparent conducting oxides.

We present structuring of organic conductors by laser ablation from spin coated films of PEDOT:PSS. We have investigated ablation characteristics of PEDOT:PSS depending on laser wavelength in the deep UV and required fluence. The smallest structuring resolution by UV laser patterning has been found.

In further measurements we have determined the conductivity depending on layer thickness and structure size. Especially the influence of laser radiation on conductivity and electrical properties in the vicinity of the ablated area has been studied. Therefor we have performed AFM measurements as well as four-point probing.

DS 50.2 Thu 10:30 GER 38

Investigation of the origin of the memory effect in devices based on C_{60} — •Philipp Sebastian, Alexander Zakhidov, Björn Lüssem, and Karl Leo — Institut für Angewandte Photophysik, George-Bähr-Straße 1, 01069 Dresden, Germany

Besides their application in organic solar cells and organic light emitting diodes, organic semiconductors also show much potential in the field of flexible and lightweight electronics, such as organic memory. In particular, the development of organic memory devices has turned out to be challenging. So far, many different approaches for organic memory devices have been reported in literature [1].

In this contribution, we report on an organic memory device comprising SiO_2 layer on top of a indium tin (ITO) ground contact, followed by electron accepting C_{60} layer, a n-doped (Cs) 4,7-diphenyl-1,10-phenanthroline (BPhen) layer and an Al top electrode. IV measurements reveal a reproducible hysteresis of our devices with a maximum ON-OFF ratio of about one order of magnitude. The memory devices also demonstrate a remarkable switching cycle durability of more than 10^4 successfully applied write read erase read cycles, whereas the ON-OFF ratio remains constant at about 10. Retention times of several weeks underline a reasonable non-volatility. Further, the memory mechanism has been investigated by impedance spectroscopy. A hysteresis in capacitance-voltage measurements expresses the accumulation of electrons in the C_{60} and at the interface to the SiO_2 layer.

[1] J. Scott, L. Bozano, Advanced Materials 19, 1452 (2007)

DS 50.3 Thu 10:45 GER 38

Growth and morphology of aluminium contacts on P3HT films — •Gunar Kaune[1,2], Robert Meier[1], Ezzeldin Metwalli[1], Volker Körstgens[1], Kai Schlage[3], Sebastien Couet[3], Stephan V. Roth[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Straße 1, 85747 Garching — [2]Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, Fachgruppe Photovoltaik, Von-Danckelmann-Platz 3, 06120 Halle — [3]HASYLAB at DESY, Notkestraße 85, 22603 Hamburg

The characteristics of organic electronic devices are strongly influenced by the type and structure of the metal electrodes needed to inject or extract charge carriers. Therefore understanding of the metal growth process and its relation to the interactions at the metal-organic interface are necessary. We investigate the growth of an aluminium layer on the surface of a P3HT thin film by in-situ application of grazing incidence small-angle X-ray scattering (GISAXS). By subsequent modelling of the scattering data the structural parameters of the growing film are extracted and a growth process is found, which proceeds two-dimensional by stacking single atomic layers on top each other. This process results in a homogeneous film with a large contact area to the polymer and is explained by a strong chemical interaction between aluminium and P3HT, which suppresses clustering of the metal on the polymer surface. The diffusion of single aluminium atoms into the P3HT and the formation of an intermixing layer is revealed by X-ray reflectivity measurements.

DS 50.4 Thu 11:00 GER 38

Effect of high-k substrates on the photocurrent of organic semiconductors: Tailoring the Coulomb interaction — •Miriam Engel[1], Doru C. Lupascu[2], Niels Benson[1], and Roland Schmechel[1] — [1]Nanostrukturtechnik, Universität Duisburg-Essen, 47057 Duisburg — [2]Institut für Materialwissenschaft, Universität Duisburg-Essen, 45117 Essen

A major difficulty for organic photovoltaic cells is the dissociation of excitons into free charge-carriers. This is caused by high exciton binding energies, due to the low permittivity of the organic material. There are approaches to use acceptor-donator systems in the form of bulk-heterojunctions, which leads to successful exciton dissociations per volume. However, re-trapping may occur even after efficient charge-carrier separation due to Coulomb interaction (CI). Our aim is to use inorganic high-k materials to increase the exciton dissociation and to lower CI. In our proof of principle experiments devices are based on substrates with different permittivities. Pentacene is deposited as the active organic layer on them. Silver electrodes are used as top-contacts. For the electrical characterization we performed I(V) measurements in the dark and under illumination. Because of the known influence of the pentacene morphology on the mobility of the charge-carriers, we corrected the current under illumination by the dark current to obtain the pure contribution from the photo-effect. We obtained an improvement of the photocurrent using high-k substrates. The final goal is to transfer the layered system into an organic-inorganic composite system with high-k nanoparticles embedded in a photoactive organic matrix.

DS 50.5 Thu 11:15 GER 38

Organic pin-Diodes with Adjustable Current-Voltage Performance Applicable at Ultra-High-Frequencies — •Hans Kleemann, Christoph Schünemann, Paul Pahner, Alexander A. Zakhidov, Björn Lüssem, and Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Straße 1, 01069 Dresden, Germany

Organic diodes have been intensively studied during the past years and great progress has been achieved in the field of organic light-emitting diodes (OLEDs) and organic solar cells (OSC). Moreover, the development of other organic devices like thin film transistors, vertical transistors, memory arrays, and high-frequency diodes which are required for an electronic circuitry will allow the design and integration of complete organic electronics. In this contribution we present organic *pin*-diodes with adjustable forward and reverse current-voltage performance applicable in the ultra-high-frequency region. Key parameters to design these diodes are the doping concentration, the intrinsic interlayer thickness and the material properties. In this way the reversible backward breakdown can be shifted from $-3V$ to more than $-20V$ independently of the forward performance [1]. Due to the high rectification ratio (10^5) and since the diodes contain high mobility materials like pentacene and C_{60} we present high-frequency properties of these pin-diodes above 13.56MHz required for RFID-tags.

[1] H. Kleemann et al., Organic Zener Diodes: Tunneling across the Gap in Organic Semiconductor Materials, Nano Letters 2010, pub-

lished online.

DS 50.6 Thu 11:30 GER 38

Photoinduced degradation process of Fir6 emitter molecules: a laser desorption/ionization time-of-flight mass spectrometry investigation — •Ines Rabelo de Moraes[1], Ruben Seifert[1,2], Sebastian Scholz[1,3], Björn Lüssem[1], and Karl Leo[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Str. 1, 01062 Dresden, Germany — [2]Von Ardenne Anlagentechnik GmbH, Plattleite 19/29, 01324 Dresden, Germany — [3]Fraunhofer-Institut für Keramische Technologien und Systeme, Winterbergstraße 28, 01277 Dresden, Germany

Phosphorescent Organic Light Emitting diodes (OLEDs) have attracted much interest for their potential application in the field of full color displays and as next generation of lighting sources. One of the major problems related to the OLED technology is the short lifetime of the blue phosphorescent emitters. For improving the lifetime of the OLEDs a deep understanding of the intrinsic chemical degradation is required. Our work is focused on the photoinduced degradation process of single layer of the Fir6 molecule used as blue phosphorescent emitter by laser desorption/ionization time-of-flight mass spectrometry (LDI-TOF-MS). The LDI-TOF spectra collected at the laser intensity of 114 μJ/pulse indicate that the Fir6 molecule dissociates into [Ir(F2ppy)2]+ and [Fir6-(pyrazole)1]+. The reaction between the Fir6 fragments and the Fir6 molecule itself resulting in the formation of [Fir6+(pyrazole)1]+, and [Fir6-(pyrazole)1+Ir(F2ppy)2]+ could be observed as well. Additionally, the degradation processes of full processed OLEDs based on Fir6 emitter will be presented.

DS 51: Organic Electronics and Photovoltaics II (jointly with CPP, HL, and O)

Time: Thursday 12:00–13:00 Location: GER 38

DS 51.1 Thu 12:00 GER 38

Improving the performance of phosphorescent light-emitting electrochemical cells without sacrificing stability — •Sebastian Meier[1,2], Wiebke Sarfert[2], David Hartmann[2], and Albrecht Winnacker[1] — [1]University of Erlangen-Nuremberg, Department of Materials Science, Chair VI: Materials for Electronics and Energy Technology, Martensstr. 7, 91058 Erlangen, Germany — [2]Siemens AG, Corporate Technology, GTF ORE, Günther-Scharowsky-Str. 1, 91058 Erlangen, Germany

Within the past few years a novel class of solution-processable solid-state organic light-emitting devices referred to as light-emitting electrochemical cells (LECs) has attracted considerable interest. Key feature of these devices is the existence of mobile ions within the active layer, which enable in-situ electrochemical doping with subsequent formation of a light-emitting p-n-junction. Due to their simple architecture and the use of air-stable electrodes LECs are regarded as an attractive approach for flexible large area lighting applications.

To compete with state of the art lighting technologies, however, the overall device performance of LECs has to be improved. For this purpose, an optimization of the device configuration and processing conditions as well as the use of a proper driving mode can be helpful. We show that the performance can be significantly enhanced due to modifications in the stack configuration (e.g. interfaces, layer thickness, cathode), processing conditions and by an adequate mode of operation without any losses in the device stability.

DS 51.2 Thu 12:15 GER 38

OLEDs under high current densities – transient electroluminescence turn-on dynamics and singlet-triplet quenching — •Daniel Kasemann, Hartmut Fröb, and Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany

Organic solid state lasers have been intensively studied during the last decade due to the promising combination of versatile organic materials with the advantages of solid state emitters. Even though various optically pumped devices comprising different resonator types and material combinations have been shown, direct electrical pumping has not been achieved yet. The high excitation density needed in the active layer to achieve inversion is easily created by pulsed optical pumping, but additional losses prevent the excitation to reach the critical point when driven electrically.

To estimate the dimensions of these additional losses, we investigate full pin-OLEDs comprising the singlet emitter system DCM doped into Alq3 under high current densities. With the OLED active area reduced to $100x100\mu m^2$, these devices sustain current densities in the order of kA/cm^2 in pulsed operation. The results of time resolved electroluminescence (EL) measurements as well as power dependent emission spectra give promising insight into the behaviour of OLEDs under these extreme excitation conditions. Intense EL transient turn-on peaks on the nanosecond time scale can be explained by modelling the singlet and triplet population taking into account singlet-triplet and triplet-triplet quenching in the emission layer.

DS 51.3 Thu 12:30 GER 38

Investigation of the chemical and electronic structure of F_{16}CoPc from Monolayer to thick films by photoemission spectroscopy — •M. Grobosch and M. Knupfer — IFW Dresden, D-01069 Dresden, Germany

We have grown F_{16}CoPc with different film thickness under ultra high vacuum conditions on polycrystalline Au surfaces. By means of combined X-ray and ultraviolet photoemission spectroscopy (XPS, UPS) we have investigated the chemical and electronic structure of the F_{16}CoPc films. Within the first monolayers we could identify a charge transfer from the substrate on the F_{16}CoPc molecules. Our results indicate a clear difference in the valence band spectra for sub-monolayer thin and several nm thick F_{16}CoPc films. Furthermore, for F_{16}CoPc the ionization potential can be changed by the fluorination of the molecules from 4.8 eV for CoPc to 6.5 eV for F_{16}CoPc. The investigated heterointerface CoPc/F_{16}CoPc can be characterized as free from chemical reactions.

DS 51.4 Thu 12:45 GER 38

Influence of sample geometry and contact metal on the characterictics of organic field-effect transistors — •Dominik Klaus, Christopher Keil, Jan Hartel, and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email:schlettwein@uni-giessen.de

Thin films of $F_{16}PcCu$ were prepared by physical vapor deposition on μ-structured electrode arrays of different contact metals. I/V-measurements of structures with various channel lengths showed a nonlinear injection of charge carriers for low Source-Drain-Voltages V_{DS}. Such behavior was especially found for μ-structures of small channel length indicating an influence of the contact behavior at the interface between metal electrode and organic semiconductor channel. A model was developed based on different aspects of an injection barrier, channel resistance and a parameter characterizing the geometry of the conducting channel which were separately used in the literature before. The model was used to determine the charge carrier mobility also for low values of V_{DS} and consistent values with those from typically evaluated large V_{DS} in the saturation regime were obtained. Implications for technical applicability of such transistors and general validity of such model are discussed.

DS 52: Organic Electronics and Photovoltaics III (jointly with CPP, HL, and O)

Time: Thursday 14:00–16:00 Location: GER 38

DS 52.1 Thu 14:00 GER 38

Influence of the thickness dependent structural order on the electrical potential distribution in the channel of OFET's — Richa Sharma, Benedikt Gburek, •Torsten Balster, and Veit Wagner — School of Engineering and Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen

Soluble organic semiconductors often exhibit a charge carrier dependent mobility and energetic disorder, which typically vary with layer thickness. In this study, organic field effect transistors (OFET) with different thicknesses of regio-regular P3HT as semiconductor and PMMA as gate-insulator on PET foils are investigated and analyzed statistically.

The mobility, which is very low for layers up to 10 nm, increases with the thickness over two orders of magnitude and saturates after 30 nm. This behavior is analyzed according to the Vissenberg-Matters model (VM) of the charge carrier density dependent mobility $\mu = \mu_0((V_{GS} - V_{th})/V_{aa})^\gamma$, where the disorder parameter γ decreases from 1.7 to 0.8 over the examined thicknesses proving the higher energetic disorder for thinner films. Increasing domain sizes in phase contrast AFM pictures confirm these findings.

The potential distribution within the channel, which has been measured by additional sense electrodes, is used to determine the potential steps at source and drain contact applying the VM model. The influence of the disorder parameter on the potential distribution is elucidated.

DS 52.2 Thu 14:15 GER 38

Local analysis on organic field effect transistors — •Harald Graaf[1], Franziska Lüttich[1], Daniel Lehmann[2], Dietrich R.T. Zahn[2], and Christian von Borczyskowski[1] — [1]Optische Spektroskopie und Molekülphysik, Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz — [2]Halbleiterphysik, Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz

Within the last decade the interest on organic electronics increased tremendously and reaches even industrial applications. Nevertheless, there are still a lot of open questions concerning e.g. the charge transport in the organic materials especially on a local scale. Here the focus is on the influence of trap states at interfaces and within the bulk provided e.g. by grain boundaries. By the combination of diverse measurement techniques a deeper insight and a better understanding of the local properties of the materials can be obtained.

We will present recent results on organic materials gained by electrical DC-measurements, Kelvin probe force microscopy on operating devices, optical and topographical investigations. By the results one obtain on the one hand information about the orientation and the coupling of the chromophoric systems (which is responsible also for the charge transport) within the film. On the other hand the electrical and electronical characterizations permit insight in the properties especially at the relevant interfaces (electrode/semiconductor and semiconductor/isolator) and on the local transport characteristics of the charges.

DS 52.3 Thu 14:30 GER 38

Dynamics of optically induced instabilities in P3HT field-effect transistors — •Lorenz Kehrer, Christian Melzer, and Heinz von Seggern — Electronic Materials Department, Institute of Materials Science, TU Darmstadt, Petersenstr. 23, 64287 Darmstadt

The development of stable printed organic electronic circuits for everyday use remains a great challenge. Under ambient conditions electrical instabilities may be driven by external influences such as gases, humidity or light. Here, we report on a light induced instability of state of the art poly(3-hexylthiophene) field-effect transistors under ambient atmosphere. By illuminating p-type, top-gate poly(3-hexylthiophene) field-effect transistors in depletion mode with visible light a substantial shift of the threshold-voltage and an increase in the off-current by three orders of magnitudes has been observed. Both phenomena, the threshold-voltage shift and the increase of the off-current, require the presence of oxygen and are persistent for days at room temperature. The origin of this long lasting instability is attributed to traps which are induced in the semiconductor by oxygen incorporation and subsequent optical filling of these traps by electrons. This charge trapping shifts the threshold voltage and increases the doping level. The temporal evolution of the optically induced changes in the OFET characteristics under different thermal conditions will be highlighted. Such an instability is crucial for logic elements where OFETs are normally hold in the off-state, thus in depletion. Under these operational conditions light induces the aforementioned change in the OFET characteristics affecting the functionality of the employed logic circuit substantially.

DS 52.4 Thu 14:45 GER 38

Towards a biosensing device based on pentacene transistors — •Martin Göllner, Martin Huth, and Bert Nickel — Department für Physik und CeNS, Ludwig-Maximilians-Universität, Geschwister-Scholl-Platz 1, 80539 München, Deutschland

Organic semiconductors can be processed on flexible, biocompatible plastic substrates and offer a soft and non-toxic ambience to living cells (e.g. neurons). Therefore organic thin film transistors (OTFTs) are considered as promising candidates for the next generation of biosensing devices. However, most high mobility organic semiconductors have a limited lifetime in physiological aqueous conditions. For a stable device operation it is necessary to suppress redox reactions with the electrolyte and so called leakage currents.

For this purpose we recently used a thin alkane layer to passivate a pentacene thin film transistor, enabling the operation in an aquatic environment for many hours [1]. A transducer based on a capped OTFT should be sensitive to subtle changes of the charges at the interface to the electrolyte. Ongoing measurements indicate that it is possible to change the source-drain current of the transistor by changing the electrochemical potential of the electrolyte by a few mV. This suggests that the device should also be sensitive to the adsorption of charged molecules and the activity of cells. The sensing mechanism is discussed.

[1] M. Göllner, M. Huth, B. Nickel, Advanced Materials 22, 4350-4354 (2010)

DS 52.5 Thu 15:00 GER 38

Electronic properties of spiro-compounds: A combined photoelectron spectroscopy and energy-loss spectroscopy study — •B. Mahns[1], M. Grobosch[1], T. Saragi[2], J. Salbeck[2], and M. Knupfer[1] — [1]IFW Dresden, Helmhotzstrasse 20, 01069 Dresden, Germany — [2]Macromolecular Chemistry and Molecular Materials, Institute of Chemistry, Department of Science and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Strasse 40, 34132 Kassel, Germany

The electronic properties of three different spiro-compounds have been investigated using a combination of photoelectron spectroscopy and electron energy-loss spectroscopy. The compounds are characterized by parts with different electron affinity, and we demonstrate their variation in ionization potential and optical gap. Moreover, our data give a measure of the occupied density of states as well as the dielectric properties in a wide energy range.

DS 52.6 Thu 15:15 GER 38

Spatially resolved photoresponse of pentacene thin film transistors: slow component by trap release — •Christian Westermeier, Matthias Fiebig, and Bert Nickel — Department für Physik und CeNS, Ludwig-Maximilians-Universität München

Organic thin film transistors (OTFTs) have witnessed continuous improvement over the past years and become suited for widespread application. Small organic molecules, such as pentacene, are often used for OTFTs, since their ordered thin-film structures result in high charge carrier mobilities. Although pentacene has attracted high interest of research, the electronic transport and photoresponse mechanisms and their relation to the morphology and trap densities of the polycrystalline film are not well understood.

We perform spatially and time resolved photoresponse measurements of pentacene TFTs using a laser scanning setup for local illumination with varying laser frequencies and a photon energy of 1.96 eV. The excitation corresponds to the upper Davydov component of the S_1 state of pentacene. Besides the absorption in the 50 nm pentacene film, a significant fraction of the laser light is absorbed in the Si wafer upon reflection. Since the excitons in pentacene decay mostly radiationless, both contributions result in local heating. We argue that heat assisted detrapping results in the release of holes from trap states, thus the effective charge carrier mobility increases locally. These bolometric effects are associated with a slow contribution to the photoresponse on a millisecond timescale and with an inhomogeneous structure presumably corresponding to the trap density distribution in pentacene.

DS 52.7 Thu 15:30 GER 38

Contact properties of organic PCBM field effect transistors analyzed by combined photoemission spectroscopy and electrical measurements — •M. Grobosch[1], I. Hörselmann[2], J. Bartsch[2], S. Scheinert[2], M. Knupfer[1], and G. Paasch[1] — [1]IFW Dresden, D-01069 Dresden, Germany — [2]Technical University Ilmenau, D-98684 Ilmenau, Germany

Source/drain contacts in OFETs based on a solution prepared modified PCBM were characterized by combined X-ray and ultra violet photoemission spectroscopy (XPS, UPS) and electrical measurements of the OFET. Thereby the sample preparation for the different measuring principles has been realized in parallel, differing only in the layer thickness of the polymer. By means of UPS a reduced work function could be demonstrated for differently prepared, sputtered, and as-received Au and Al contacts in agreement with previous publications [1]. On top of the Al contacts a natural AlO_x layer could be identified. For both the PCBM/Au and PCBM/Al systems from UPS a hole injection barrier of 1.8 eV has been determined. Considering the gap of 2.0 eV [2] the electron injection barrier would be the same of 0.2 eV. In contrast to these identical barriers as following from UPS, the OFET currents with Au and Al contacts differ by more than two orders of magnitude. A possible origin of this striking discrepancacy will be presented. [1] M. Grobosch et al., Adv. Mater. 19 (2007) 754. [2] Z.-L. Guan et al., Organic Electronics 11 (2010) 1779.

DS 52.8 Thu 15:45 GER 38

Dye directed changes in ZnO matrices in organic/inorganic photovoltaic systems — •Harald Graaf[1], Franziska Lüttich[1], Mirko Kehr[1], Christian Dunkel[2], and Torsten Oekermann[2] — [1]Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz — [2]Institut für Physikalische Chemie und Elektrochemie, Leibniz Universität Hannover, 30167 Hannover

Dye-sensitized photovoltaic cells with zinc oxide (ZnO) as the inorganic semiconductor and organic dye molecules as the sensitizer are well-known devices with high efficiency. Such cells are prepared by electrochemical deposition of an aqueous zinc salt solution including dye molecules. After deposition the dye is desorbed to obtain a porous ZnO network followed by re-adsorption of the dye as a sensitizer. The dye molecules influence the crystal orientation of the ZnO as they tend to physisorb on different crystal surfaces.

We will present recent results on as-deposited and desorbed dye/ZnO films obtained by different analytic methods: X-ray investigations, Scanning Electron Microscopy, Atomic and Kelvin probe force microscopy and optical spectroscopy. This allows a deep insight into the dye/semiconductor system, which is necessary to improve the efficiency of such devices. Here the focus is on crystal orientation, morphology and work function of the ZnO matrix. Also the arrangement of the dye molecules in as well as on top of the as-deposited films and the band edge of the zinc oxide is accessible.

DS 53: Organic Electronics and Photovoltaics IV (jointly with CPP, HL, and O)

Time: Thursday 16:15–17:45 Location: GER 38

DS 53.1 Thu 16:15 GER 38

Energy level alignment at polymer/PCBM heterojunctions under operating conditions in an organic photovoltaic cell structure — •Johannes Frisch[1], Andreas Wilke[1], Patrick Amsalem[1], Jens Niederhausen[1], Antje Vollmer[2], and Norbert Koch[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Brook-Taylor-Str. 6, D-12489 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie - Speicherring BESSY II, Berlin, Germany

For heterojunction organic photovoltaic cells (OPVCs) generally vacuum level alignment at the donor/acceptor interface is assumed. In contrast, it has been shown that interface dipoles might occur at organic/organic heterojunctions, which questions the assumption of vacuum level alignment at OPVC interfaces. Therefore, we investigated the energy level alignment at the poly(3-hexylthiophene)/1-(3-methoxycarbonyl)propyl-1-phenyl[6.6]C61 (P3HT:PCBM) heterojunctions with ultraviolet photoelectron spectroscopy (UPS). The valence band of P3HT shifted to higher binding energy by 0.45 eV after deposition of PCBM, while vacuum level alignment was found. This observation would imply an increase of the P3HT ionization energy upon interface formation, which is usually not considered in simple models. The observed phenomenon can be explained either by a structural rearrangement of the donor polymer layer upon acceptor deposition or by surface photovoltage effects that occur during photoemission, which charges the P3HT layer positively whereas negative charges are collected in the PCBM layer.

DS 53.2 Thu 16:30 GER 38

New Imaging Approach for Organic Bulk Heterojunction Solar Cells Using Selective Dissolution — •Bettina Friedel, Bruno Ehrler, and Neil C. Greenham — University of Cambridge, Cavendish Laboratory, JJ Thomson Avenue, CB30HE Cambridge, United Kingdom

Morphology in organic photovoltaic devices is one of the most vital and most studied issues for optimum functionality, especially concerning bulk heterojunctions. However, it is always a challenge to control its microscopic structure towards improved exciton dissociation and charge transport. To get an insight into this microstructure usually a combination of various imaging techniques together with spectroscopic methods is used. Unfortunately imaging on all-organic structures is rather challenging since the high similarity of the carbon-based materials gives low contrasts and makes them hard to distinguish. We will present a new imaging approach for organic blends, based on a temperature controlled selective dissolution technique. We will demonstrate on two systems (polymer-polymer and polymer-PCBM) that this technique allows to selectively remove one of the components from a bulk heterojunction, leaving a scaffold of the other component, which can be easily characterized by high resolution imaging, due to the higher air-material contrast. Further the technique allows us to quantify the disordered fraction of semicrystalline components in a blend structure, which is valuable information for matters of charge transport. These new structural insights help understanding the changes in PV performance e.g. following thermal treatments or using solvent additives.

DS 53.3 Thu 16:45 GER 38

improvement of the CdSe/P3HT solar cells efficiency due to surface modification of the CdSe nanoparticles by alkylamine treatments — •nikolay radychev, irina lokteva, holger borchert, joanna kolny-olesiak, and jürgen parisi — institute of physics, energy and semiconductor research laboratory, university of oldenburg,oldenburg,germany

Semiconductor quantum dots (QDs) continue to attract immense attention because of their size-dependent optical, physical, and chemical properties which causes them to be a promising material for hybrid solar cell applications. Meanwhile QDs in a polymer matrix have to be stabilized by organic ligands that show significant influence on the charge transport and charge separation processes. Surface modification procedures such as stabilizing ligand exchange or crosslinking the QDs can enhance the efficiency of the hybrid blends. In the present work, as-synthesized QDs, initially capped with oleic acid, were subjected to ligand exchange procedures with the intention to obtain nanoparticles capped by butylamine ligands. Detailed characterisations of the butylamine stabilized QDs based on thermogravimetric analysis, nuclear magnetic resonance and transmission electron microscopy are shown. Laboratory solar cells with blends of the butylamine capped CdSe QDs and poly-3-hexylthiophene (P3HT) as active layer were prepared and investigated by current-voltage and external quantum efficiency measurements. Energy conversion efficiency of about 2% was obtained. The fundamental reasons of the efficiency enhancement were analyzed

DS 53.4 Thu 17:00 GER 38

Comparison of the operation of standard and inverted P3HT:PCBM solar cells — •Thomas J.K. Brenner, Yana Vaynzof, Zhe Li, Dinesh Kabra, Richard H. Friend, and Christopher R. McNeill — Cavendish Laboratory, Department of

Physics, University of Cambridge, JJ Thomson Ave., Cambridge CB3 0HE, United Kingdom

Inverted organic solar cells have attracted recent attention due to their enhanced environmental stability compared to the standard device architecture. However to date inverted cells have shown poorer efficiencies compared to the standard geometry. To clarify the origin of this behaviour, we have investigated inverted (ITO/ZnO/P3HT:PCBM/ WO3/Ag) and regular (ITO/PEDOT:PSS/P3HT:PCBM/Al) P3HT:PCBM solar cells with different active layer thickness. Using white light bias external quantum efficiency and photocurrent transient measurements, we propose an explanation for the reduced performance of inverted cells. Whereas for inverted devices high EQEs of up to 68% are measured under low light intensities (3 mW/cm^2), EQE drops with increasing white light bias (up to 140 mW/cm^2) down to 20%. This drop is accompanied by a severe distortion of the spectra. For increased thickness (from 90 nm to 550 nm), the drop and shape change can be seen at lower intensities. For regular devices we also observe a drop in EQE, however they still resemble the absorption spectrum showing minor distortion. Unbalanced charge transport and/or unfavourable vertical phase separation in inverted devices are presented as likely causes of the observed behaviour.

DS 53.5 Thu 17:15 GER 38

Organic Photovoltaic Cells with Pentacene Nanocolumn Arrays — •Shuwen Yu, Peter Schäfer, Jürgen P. Rabe, and Norbert Koch — Institut für Physik, Humboldt-Universität zu Berlin, Brook-Taylor-Str. 6, 12489 Berlin, Germany

Highly ordered pentacene nanocolumn arrays were fabricated by glancing angle deposition (GLAD) on indium tin oxide (ITO) substrates. The nanocolumn diameter was set to 100-150 nm as revealed by scanning electron microscopy and atomic force microscopy. Interdigitated bulk heterojunction photovoltaic cells (OPVCs) were formed by spin-coating [6,6]-phenyl-C61-butyric acid methyl ester (PCBM) as the acceptor material onto the pentacene nanocolumn film. Bathocuproine (BCP) was deposited on top of PCBM as exciton blocking layer. The conversion efficiency of nanocolumn-based OPVCs was significantly higher compared to planar heterojunction OPVCs of the same materials. Further device performance improvement was achieved through employing a thin pentacene seed layer before GLAD, which promoted PCBM solution infiltration between pentacene nanocolumns.

DS 53.6 Thu 17:30 GER 38

Performance and stability of P3HT/PCBM bulk heterojunction organic solar cells — •Nivedita Yumnam, Sidhant Bom, and Veit Wagner — School of Engineering and Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Organic photovoltaic cells are promising candidates for large-area, low-cost production of solar cells. However, the low stability in conjunction with their medium performance is one of the major drawbacks in comparison to their inorganic counterparts. In this investigation environmental conditions for degradation of bulk heterojunction P3HT/PCBM solar cells are systematically analyzed over a period of one week. Devices were prepared by spin coating from different compositions of P3HT and PCBM in Chlorobenzene (C_6H_5Cl). Performance parameters, efficiency and I-V characteristics were determined in a N_2 glove box showing optimized efficiency for a 1:1 ratio. Degradation behavior in N_2 atmosphere, vacuum and solvent-enriched atmosphere (Chlorobenzene) showed best results for vacuum stored solar cells while for solvent-enriched atmosphere rapid degradation was observed. Remarkable degradation (open-circuit voltage and short-circuit current reduced to 90% and 60% after one week) was also found for N_2 atmosphere of the glove box used for the solar cell production. Residual solvent vapor left dispersed in the atmosphere of the glovebox after the spin coating process is identified as an important parameter of this degradation.

DS 54: Nanoengineered Thin Films

Time: Thursday 18:00–19:30 Location: GER 38

DS 54.1 Thu 18:00 GER 38

Photothermal Laser Processing of thin silicon nanoparticle films: Prospects in photovoltaic applications — •Dennis Behrenberg[1,3], Hartmut Wiggers[2,3], Steffen Franzka[1,3], and Nils Hartmann[1,3] — [1]Fakultät für Chemie — [2]IVG — [3]CeNIDE, NETZ, Universität Duisburg-Essen, Universitätsstr. 5, 45141 Essen, Germany

Semiconductor nanoparticles (NPs) show great promise as building blocks in a variety of energy applications including thermoelectrics and photovoltaics [1]. A key step towards functional devices is the development of suitable techniques for the fabrication of NPs-based coatings. Here, photothermal laser processing of thin Si-NPs films on Si substrates is investigated. Si-NPs (d = 45 nm) dispersions are spin-coated on Si substrates yielding films with thicknesses < 0.5 microns. Subsequently, laser processing is carried out with a focused beam of an cw-DPSS-laser at a wavelength of 532 nm and a 1/e spot diameter of about 1.4 microns [2]. Using a focused laser beam allows one to conveniently investigate the dependence of the initiated processes on the laser parameters on a single sample. Generally, laser irradiation results in a local temperature rise. Depending on the ambient environment sintering, melting and oxidation of the NPs takes place. Prospects of photothermal laser procedures in photovoltaic applications are discussed, e.g. targeting back surface doping of solar cells.

[1] R. Lechner, H. Wiggers, A. Ebbers, J. Steiger, M. Brandt, M. Stutzmann, Phys. Stat. Sol. (RRL) 1, No. 6 (2007) 262.

[2] T. Balgar, S. Franzka, N. Hartmann, Appl. Phys. A82 (2006) 689.

DS 54.2 Thu 18:15 GER 38

Glancing angle deposited Ge nanorod arrays on Si patterns — •Chinmay Khare[1], Jens Bauer[1], Bodo Fuhrmann[2], Hartmut S Leipner[2], and Bernd Rauschenbach[1] — [1]Leibniz Institute of Surface Modification, Permoserstraße 15, 04318 Leipzig, Germany — [2]Interdisciplinary Centre of Materials Science, Martin-Luther-University Halle-Wittenberg, Heinrich-Damerow-Straße 4, 06120 Halle, Germany

A strong dominance of the shadowing mechanism facilitates growth of highly porous films by a physical vapour deposition technique, glancing angle deposition (GLAD). Under shadowing condition, an oblique particle flux incidence at the substrate with an angle β (usually β>80°, as measured to the substrate normal) enables realization of columnar thin films, which can be sculpted into manifold of structures. Here, ion beam sputter glancing angle deposition of Ge nanorod arrays on customized Si patterns fabricated with a combinational approach of nanospehere lithography and reactive ion etching are presented. The effective morphological variations in shape and dimension of GLAD-grown nanorods on hexagonal-closed-packed (hcp) arrays and honeycomb-like arrays are strongly influenced by Si seed heights and inter-seed distances. The nanorod growth optimization could be realized through alterations in the Si seed widths (ws) and inter-seed distances Rs, enabling growth of individual nanorods on each Si pattern seed. Furthermore, with this promising method Si/Ge heterojunction GLAD-nanostructures could be realized with alternating material supply for potential application in a thermoelectric module.

DS 54.3 Thu 18:30 GER 38

Novel Plasma Process for the Deposition of Nanocomposites for Plasmonic Applications — •Ralph Schmittgens[1], Marcus Wolf[1], Peter Frach[2], and Gerald Gerlach[1] — [1]Technische Universität Dresden, Dresden, Deutschland — [2]Fraunhofer Institut für Elektronenstrahl- und Plasmatechnik, Dresden, Deutschland

There is a growing interest in the application of plasmonic effects in metal nanostructures, e.g. surface plasmon resonances in metallic nanocrystals embedded in a dielectric matrix. Applications like photovoltaics, optics or sensors require a process to produce these structures efficiently on large area substrates using low-temperature processes. At TU Dresden a hybrid vacuum deposition process was developed,where nanoparticles are generated in a gas phase condensation and subsequently embedded in a plasma deposited thin film. The process operates at room temperature and is up-scalable. In this contribution, results on the deposition of Ag nanoparticles in a dielectric matrix are presented. The films exhibit plasmonic absorption/scattering due to the Ag nanoparticle's surface plasmon resonances. The fill factor of the Ag nanoparticles can be easily adjusted so that nanocomposites below and above the percolation threshold can be deposited. This performance is demonstrated by optical absorption and capacitance/resistance measurements.

DS 54.4 Thu 18:45 GER 38

Vertically contacting ultrathin semiconductor nanomembranes by rolled-up metallic contacts incorporating selective etching techniques. — •Dominic J. Thurmer[1], Carlos Cesar Bof Bufon[1], Christoph Deneke[1], and Oliver G. Schmidt[1,2] — [1]IFW Dresden, Dresden, Germany — [2]TU Chemnitz, Chemnitz, Germany

Merging modern self-assembly techniques with well established top-down processing methods is paving the way for more sophisticated device generations in the future. Nanomembranes, composed of many different material classes, have already been shown to provide the necessary framework for a diverse range of structures and devices incorporating wrinkling, buckling, folding and rolling of thin films. In the past decade, an elegant symbiosis of bottom-up and top-down methods has emerged to fabricate hybrid layer systems incorporating the controlled release and rearrangement of inherently strained layers. Using selective III-V etchants in combination with inherently strained layers we are able to fabricate structures which allow us to contact through single and multi-material semiconductor nanomembrane creating many devices in parallel and on the original semiconductor substrate. We demonstrate this technique by creating hybrid superconducting junctions created by sandwiching the semiconductor nanomembrane between two superconducting contacts. Using solely optical lithography techniques we are able to form junctions with lateral dimensions of a few micrometers and a semiconductor barrier thickness of down to 5 nm. D. J. Thurmer et al. Nano Lett. 10, 3704 (2010).

DS 54.5 Thu 19:00 GER 38

Sodium engineering in multifunctional Na_xCoO_2 thin films grown by pulsed laser deposition — •Sandra Hildebrandt[1], Ingo Fritsch[2], Dirk Becker[1], Philipp Komissinskiy[1], Hanns-Ulrich Habermeier[2], Wolfram Jaegermann[1], and Lambert Alff[1] — [1]Institut für Materialwissenschaft, TU Darmstadt, Petersenstr. 23, 64287 Darmstadt, Germany — [2]Max Planck Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart, Germany

We report on the growth of Na_xCoO_2 thin films by pulsed laser deposition. The sodium content in as grown films is always about $x = 0.6$. By annealing, x can be varied between 0.58 and 0.77. Further Na deintercalation down to $x = 0.35$ is achieved by chemical treatment of the film with a bromine solution. In the presence of water, a phase mixture of $Na_{0.35}CoO_2$ and $Na_{0.35}CoO_2{\cdot}0.9H_2O$ is obtained. This can be transformed into the superconducting compound $Na_{0.35}CoO_2{\cdot}1.3H_2O$ by subsequent water intercalation [1]. The Na_xCoO_2 films with higher sodium content ($0.6 < x < 1$) have typical resistivities of about 7 mΩcm at room temperature. This material already known for its large thermoelectric power, now comes in the focus as substitutional material for Li_xCoO_2 in solid state batteries. A high sodium ion conductance still has to be confirmed. We would like to acknowledge the financial support from DFG-Project AL560/6-1.

[1] Y. Krockenberger, I. Fritsch, G. Christiani, H.-U. Habermeier, Li Yu, C. Bernhard, B. Keimer, and L. Alff. Appl. Phys. Lett. 88, 162501 (2006).

DS 54.6 Thu 19:15 GER 38

Phase transitions in nano-grained close-packed Pd thin films — Erwin Hüger[1], •Tomas Kana[2,3], and Mojmír Šob[4,2] — [1]Institute of Metallurgy, Clausthal University of Technology, D-38678 Clausthal-Zellerfeld, Germany — [2]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, CZ-616 62 Brno, Czech Republic — [3]Faculty of Mechanical Engineering, Brno University of Technology, CZ-616 69 Brno, Czech Republic — [4]Department of Chemistry, Faculty of Science, Masaryk University, CZ-611 37 Brno, Czech Republic

Using ab initio density functional calculations, we analyze experimental data and corresponding energy barriers of phase transitions in the $(11\bar{2}0)$ oriented hcp Pd thin films grown on W(001) and Nb(001) substrates. We elucidate the feasibility of the experimentally observed phase transformation between the hcp and double hcp (dhcp) structures and absence of the hcp–fcc transformation in those films. The proposed model of the experimentally observed hcp–dhcp transformation preserves the existing domain topology of the Pd films and exhibits a sufficiently low energy barrier. On the other hand, the orthogonal pattern of rectangular domains induced by the four-fold symmetry of the substrate surface hinders the hcp Pd phase to convert back to the ground-state fcc phase, although there exists a transformation path exhibiting a very low energy barrier between the hcp and fcc structures. This path, however, would break the domain arrangement and, therefore, it cannot be accomplished. In this way, the hcp crystalline phase is locked inside of nanograins.

DS 55: Focused Session: Novel Green Laser Diodes (jointly with HL and O)

Time: Thursday 14:30–17:15 Location: POT 51

Invited Talk DS 55.1 Thu 14:30 POT 51

GaN-based green laser diodes grown on c-plane GaN substrate — •Shinichi Nagahama — Nitride Semiconductor Research Laboratory, Nichia Corporation, 491 Oka, Kaminakacho, Anan, Tokushima 774-8601, Japan

We have succeeded in developing the GaN-based green laser diodes (LDs) with an emission wavelength of 510-515 nm and output power of 50 mW for the green light source in the small laser projectors.The green LDs structures were grown on conventional c-plane GaN substrates by metal organic chemical vapour deposition. The operating current and threshold voltage with an output power of 50mW were 200 mA and 5.0 V, respectively. The lifetime test of these LDs was carried out under high driving temperature up to 60 °C in cw operation. Lifetime was estimated to be over 10,000 h with an optical output power of 50mW. These results ensure that GaN-based LDs is the best candidate for the green light source in the future small laser display applications.

Invited Talk DS 55.2 Thu 15:00 POT 51

Room-temperature CW operation of BeZnCdSe green laser diode — •shigehisa tanaka[1], jun-ichi kasai[2], sumiko fujisaki[1], ryouichi akimoto[2], takeshi kikawa[1], shinji tsuji[1], haruhiko kuwatsuka[2], toshifumi hasama[2], and hiroshi ishikawa[2] — [1]Hitachi Central Research Laboratory, Kokubunji-shi, Tokyo, Japan — [2]National Institute of Advanced Industrial Science and Technologies, Tsukuba-shi, Ibaraki, Japan

Recently, green laser diodes have been received much attention because they enable novel devices such as micro-projectors or vivid color displays when used in combination with red and blue laser diodes. Although several approaches using III-nitride-based semiconductors and their successful laser operations with wavelength of over 500 nm have already been reported, their threshold currents still increase as their lasing wavelengths approach to the pure green region. ZnSe based compound semiconductors are also promising materials for the green laser diodes. In particular, Be containing ZnSe based mixed crystals are expected to overcome the problem of limited lifetime of II-VI-based laser diodes.

In this study, a room temperature continuous-wave operation at 545 nm was demonstrated with a BeZnCdSe quantum-well laser diode. Its threshold current density was as low as 1.7 kA/cm2. This result indicates this material system is advantageous in realizing a green laser diode with low power consumption.

Invited Talk DS 55.3 Thu 15:30 POT 51

Growth and properties of semi-polar GaN on patterned silicon substrate — •Nobuhiko Sawaki — Aichi Institute of Technology, Yakusa, Toyota 470-0392, Japan

Growth and properties of semi-polar and non-polar GaN on Si substrate is reviewed. Particular attention is paid on selective MOVPE on patterned substrates. By tilting the c-axis of the GaN on the silicon surface, the thermal expansion coefficient mismatch and the threading dislocation density were much reduced to improve the crystalline quality. By the virtue of self-organized growth mode on a facet, we achieved excellent surface morphology. The incorporation of carbon and magnesium were investigated in (1-101)GaN which is terminated by nitrogen. We found that the sample doped with carbon shows p-type conduction. Optical spectra and Hall measurements suggested the formation of shallow acceptor levels in the sample.

Coffee Break

Invited Talk DS 55.4 Thu 16:15 POT 51

Advantages of Using Semipolar Orientation for Making Green InGaN QW Laser Diodes. — •Dmitry Sizov, Rajaram Bhat, Kechang Song, and Chung-en Zah — Corning Incorporated, One Science Center Dr., Corning, NY, 14831, USA

During recent years, several research groups demonstrated a steady progress in increasing InGaN quantum well (QW) laser diode lasing wavelength. Using c-plane substrates has been a preferred approach for it, thanks to established growth and fabrication techniques and available 2-inch substrates. More lately, semipolar substrates became available enabling faster progress in this field. Theoretical and experimental studies show that in green spectral range, because of lower built-in electric fields, the differential gain of semipolar QW is much higher than in c-plane if the stripe direction is properly chosen. For this, one needs to take into account that emission polarization depends not only on QW plane orientation, but also on pumping level. Another advantage of semipolar orientation is easier carrier transport in green semipolar multiple-QWs due to smoother band profile resulting from reduced pizeoelectrical effect, allowing uniform carrier injection among QWs when using more QWs to increase net optical gain. While having the improved optical gain, we found that the internal optical losses are not a strong function of substrate orientation, but rather depend on acceptor concentration in p-layers. Both quantum efficiency and optical gain can however be altered by strain relaxation, which is prone in the semipolar system, but can be avoided via proper strain management.

Invited Talk DS 55.5 Thu 16:45 POT 51

Optical gain of green (Al,In)GaN laser diodes — •Ulrich Schwarz — Fraunhofer IAF, Freiburg, Germany — IMTEK, University of Freiburg, Germany

To achieve lasing in the green spectral region with group III-nitrides, InGaN quantum wells with Indium content larger than 25% are necessary. It is extremely difficult to find growth conditions which are producing homogeneous InGaN quantum wells without dark spots at this high Indium content. Both, the density of nonradiative recombination centers and the width of inhomogeneously broadened photoluminescence spectra increase with Indium content. The consequences are broadened optical gain spectra and lower differential gain. For green laser diodes amplified spontaneous emission sets in far below lasing threshold due to the low differential gain. Going from c-plane to semi- and non-polar oriented quantum wells the differential gain as function of carrier density increases. However, the carrier liefetime decreases, lowering the differential gain as function of current density. The orientation of the quantum well has also an impact on the width of the gain spectra, both through intrinsic band structure effects and through dependency of the growth conditions and Indium fluctuations on the individual growth plane. For semipolar quantum wells also the effect of birefringence on the waveguide modes and optical gain has to be considered.

DS 56: Plasmonics and Nanophotonics O-VI (jointly with HL and O)

Time: Thursday 11:15–13:00 Location: WIL A317

DS 56.1 Thu 11:15 WIL A317

Nano-plasmonics with single epitaxial quantum dots — •Markus Pfeiffer[1,2], Klas Lindfors[1,2], Christian Wolpert[1,2], Paola Atkinson[3], Armando Rastelli[3], Oliver G. Schmidt[3], Harald Giessen[2], and Markus Lippitz[1,2] — [1]Max Planck Institute for Solid State Research — [2]4. Physikalisches Intitut, Universität Stuttgart — [3]Institute for Integrative Nanosciences Dresden

Plasmon resonant metal structures are a particularly interesting choice to alter the emission properties of single quantum emitters since the electromagnetic field can be significantly modified close to the metal surface. This offers exciting possibilities in both fundamental light-matter studies as well as in applications.

We have experimentally investigated the influence of gold nanostructures on the photoluminescence properties of individual semiconductor quantum dots (QDs). The quantum dots are epitaxially grown GaAs/AlGaAs QDs which are buried a few nanometers beneath the semiconductor surface. The position of these emitters can be determined with high precision from a characteristic feature in the surface topography above each dot.

We have studied the enhancement of the excitation rate of single quantum dots using spherical gold nanoparticles. We observe enhancement factors up to 8 on resonance. We furthermore demonstrate significant differences between the enhancement spectrum and the far-field scattering spectrum of the antennas. We have also taken first steps towards incorporating single QDs in integrated plasmonic circuits.

DS 56.2 Thu 11:30 WIL A317

Extraordinary Kerr effect in the transmission through ferromagnetic-plasmonic hybrid nanostructures — •M Pohl[1], V Belotelov[2], I Akimov[1,3], V Kotov[2,4], S Kasture[5], A Vengurlekar[5], A Gopal[5], D Yakovlev[3], A Zvezdin[2], and M Bayer[1] — [1]Experimentelle Physik E2, TU Dortmund, Germany — [2]A.M. Prokhorov General Physics Institute, Moscow, Russia — [3]A.F. Ioffe Physical-Technical Institute, St. Petersburg, Russia — [4]V.A. Kotelnikov Institute of Radio Engineering and Electronics, Moscow, Russia — [5]Tata Institute of Fundamental Research, Mumbai, India

The transverse magneto-optical Kerr effect (TMOKE) has been studied on a new magneto-optical heterostructure. The sample, consisting of a periodically nanostructured gold film on top of a ferromagnetic dielectric bismuth-iron-garnet film, allows the measurement of the TMOKE in transmission geometry via extraordinary optical transmission (EOT). It is shown that the effect is enhanced by up to three orders of magnitude exclusively near surface plasmon polariton resonances. The TMOKE signal is highly sensitive to the angle of light incidence, its polarization and the applied magnetic field strengths. Moreover, it changes sign for SPPs traveling in opposite directions. Thus, TMOKE can become an important tool for the complete characterization of plasmonic nanostructures. Additionally, the effect can be controlled by fields on the order of 100 Oe, which is very promising for ultra high sensitive devices and optical data processing.

DS 56.3 Thu 11:45 WIL A317

Distinguishing between ultrafast optical harmonic generation and multi-photon-induced luminescence from ZnO thin films by interferometric frequency-resolved autocorrelation microscopy — •Slawa Schmidt[1], Manfred Mascheck[1], Martin Silies[1], Takashi Yatsui[2], Kokoro Kitamura[2], Motoichi Ohtsu[2], and Christoph Lienau[2] — [1]Carl-von-Ossietzky-Universität, Oldenburg — [2]University of Tokyo

The nonlinear optical properties of a thin ZnO film are studied using interferometric frequency-resolved autocorrelation (IFRAC) microscopy. By exciting the film with 6-fs, below-bandgap laser pulses at 800nm focused to a spot size of 1 μm two emission bands in the blue and blue-green spectral region with distinctly different coherence properties can be detected. We show that an analysis of the wavelength-dependence of the interference fringes in the IFRAC signal allows for an unambiguous assignment of these bands as coherent second harmonic emission and incoherent, multiphoton-induced photoluminescence, respectively. More generally our analysis shows that IFRAC allows for a complete characterization of the coherence properties of the nonlinear optical emission from nanostructures in a single-beam experiment. Since this technique combines a very high temporal and spatial resolution we anticipate broad applications in nonlinear nano-optics.

DS 56.4 Thu 12:00 WIL A317

Nanooptical control of hot-spot field superenhancement and long-lived coherences on a corrugated silver surface — Martin Aeschlimann[1], Tobias Brixner[2], Stefan Cunovic[3], Alexander Fischer[1], Christian Kramer[2], Pascal Melchior[1], Walter Pfeiffer[3], Christian Schneider[1], •Christian Strüber[3], Philip Tuchscherer[2], and Dmitri V. Voronine[3,4] — [1]TU Kaiserslautern, Germany — [2]Universität Würzburg, Germany — [3]Universität Bielefeld, Germany — [4]Texas A&M University, College Station, USA

Hot-spots on deterministically or randomly structured metal surfaces enable ultra-sensitive optical spectroscopy by increasing the optical signals. For example, Raman signals from molecules placed on Ag surfaces may be enhanced dramatically and single molecule sensitivity is reached. Here we combine photoemission photoelectron microscopy (PEEM) and polarization pulse shaping to investigate the multiphoton photoemission from hot-spots on a corrugated silver surface. The hot-spot related multiphoton photoemission is enhanced and manipulated with high contrast. Adaptive optimization reproducibly yield long complex pulse shapes for various optimization goals. This and results from pre-determined few-parameter control scans indicate the presence of long-lived coherences. The existence of such resonances with coherence lifetimes in the order of 100fs is proven in time-resolved local coherent spectroscopy. The high resolution of PEEM allows spatial mapping of these resonances across the surface. Spectral correlations between neighboring hot-spots indicate that weakly localized plasmon polariton states are responsible for the hot-spot emission.

DS 56.5 Thu 12:15 WIL A317

Hotspot related plasmon assisted multiphoton photocurrents in metal-insulator-metal junctions — •Dominik Differt[1], Detlef Diesing[2], and Walter Pfeiffer[1] — [1]Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany — [2]Universität Duisburg-Essen, Universitätsstr. 5, 45117 Essen, Germany

Scanning photocurrent microscopy of metal-insulator-metal junctions (MIM) is used to investigate the mechanisms of femtosecond multiphoton photocurrent injection at liquid nitrogen temperature. The locally induced multiphoton photocurrent in a Ag-TaO-Ta MIM junction is measured in a scanning microscope cryostat under focused illumination (5μm focus diameter, 800nm, 30fs, 80MHz repetition rate). The intensity dependence reveals a mixture of two-photon and three-photon processes that are responsible for the photocurrent. Its lateral variation shows hotspot-like behaviour with significant magnitude variations on a 100 to 200nm length scale. Assuming an injection current duration of 40fs the peak injection current density of about 10^4 A cm^{-2} is estimated - 10^6 times higher than that for 400nm continuous wave illumination slightly below the damage threshold. The simultaneously measured extinction of the incident radiation reveals a 20 to 30% increased absorption at the hotspots. We attribute the local photocurrent enhancement to the defect-assisted excitation of surface plasmon polaritons at the silver electrode leading to an enhanced local excitation.

DS 56.6 Thu 12:30 WIL A317

Controlling two-photon excited luminescence in gold nanostructures with polarization pulse shaping — •Giovanni Piredda[1], Zhimin Shi[2], Caroline Gollub[3], Regina de Vivie-Riedle[1], and Achim Hartschuh[1] — [1]Physikalische Chemie, Department Chemie und Biochemie, Ludwig-Maximilians-Universität München — [2]The Institute of Optics, University of Rochester, Rochester, NY 14620, USA — [3]Institute for Materials Science, TU Dresden

Ultrafast nanooptics is an emerging field that combines the concepts and tools of ultrafast spectroscopy and coherent control with those of near-field optics [1]. A simple demonstration of coherent control is the ability to maximize the yield of nonlinear optical processes; we choose for our demonstration two-photon excited luminescence from gold nanostructures [2]. We compare optimization results in different nanostructures showing that the pulse characteristics that result in the highest luminescence yield depend on the single structure; control has therefore a local character. We also provide numerical simulations to support our experimental findings [3].

[1] M.I. Stockman, S.V. Faleev, and D.J. Bergman; Phys. Rev. Lett., 88, 067402 (2002).

[2] M.R. Beversluis, A. Bouhelier, and L. Novotny; Phys. Rev. B 68, 115433 (2003).

[3] G. Piredda, C. Gollub, R. de Vivie-Riedle, and A. Hartschuh; Appl. Phys. B-Lasers O., 100, 195 (2010).

DS 56.7 Thu 12:45 WIL A317

Investigation of polarization effects in reconstruction of highly focused vector beams using the knife-edge method — •Christian Huber[1,2], Pavel Marchenko[1,2], Sergejus Orlovas[1,2], Peter Banzer[1,2], Ulf Peschel[2], and Gerd Leuchs[1,2] — [1]Max Planck Institute for the Science of Light, Günther-Scharowsky-Str. 1, D-91058 Erlangen — [2]Institute of Optics, Information and Photonics, University Erlangen-Nuremberg, Staudtstr. 7/B2, D-91052 Erlangen

For experiments with highly focused vector beams the focal field distribution has to be known. The knife-edge method can be used to reconstruct the intensity distribution of the electric field in the focal plane of a high NA objective. For that purpose, a thin knife-edge fabricated on a photodiode is moved through the focal spot while the photocurrent is recorded. To calculate the beam profile by inverse Radon transform the measurements have to be performed for different angels from 0 to 180 degrees of the edge relative to the beam. As demonstrated previously [1] the focal spot can be experimentally characterized at a wavelength of 633 nm using a special mixture of Zink and Gold as knife-edge material. However for pure materials the reconstructed field distribution is modified by polarization dependent effects. To investigate these effects in detail we performed measurements for different edge materials, edge thicknesses and for different wavelengths. According to our experimental and theoretical results the observed polarization dependency for pure materials is caused by effects such as the excitation of plasmonic modes. [1] R. Dorn et al., Opt., 50 (12), 1917-1926 (2003)

DS 57: Plasmonics and Nanophotonics O-VII (jointly with HL and O)

Time: Thursday 15:00–16:15 Location: WIL A317

DS 57.1 Thu 15:00 WIL A317

Optical and electronic properties of Ag clusters on SiO_2 — •Sabrina Hoffmann[1], Kamil Latussek[1], Stefanie Duffe[1], Christian Sternemann[1], Ralph Wagner[2], and Heinz Hövel[1] — [1]TU Dortmund, Experimentelle Physik I, Otto-Hahn-Str. 4, 44221 Dortmund, Germany — [2]BU Wuppertal, Fachbereich C - Fachgruppe Physik - Materialwissenschaften, Gaußstraße 20, 42097 Wuppertal, Germany

Clusters assembled materials are of great impact for future applications in science and nanotechnology. In particular, advances in metal cluster-beam technology allow experiments on free and supported or embedded clusters resembling nanostructures in realistic, technical relevant environments. Optical properties of noble metal clusters and nanostructures such as their UV-VIS absorption band alter significantly with size, shape and interparticle spacing as well as with the properties of the local environment. The plasmon resonance of Ag clusters on SiO_2 before and after exposure to air is examined using optical spectroscopy [1]. Then the same clusters are examined with XANES at the Ag L_3 edge. With this method changes in the uDOS of clusters can be investigated which occur either due to the cluster size or a change in their chemical environment. After exposing the Ag clusters to H_2S the plasmon resonance disappears and the XANES spectra show that the clusters are transformed to silver sulfide.

[1] U. Kreibig et al., Optical Investigations of Surfaces and Interfaces of Metal Clusters, In: Advances in Metal and Semiconductor Clusters Vol. 4, (ed. M.A. Duncan), JAI press Inc., 345 (1998).

DS 57.2 Thu 15:15 WIL A317

Quantifying Chirality in 2D and 3D Metallic Metamaterials — •Martin Schäferling, Daniel Drégely, Thomas Weiss, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany

Chirality on the nanoscale is an emerging field for metamaterials. Circular dichroism in metallic spirals can exceed the best liquid crystals or helical molecules by many orders of magnitude. Broadband quarter-wave plates can be assembled by 3D spirals that are fabricated by direct laser writing [1]. Bichiral metallic photonic crystals exhibit phases and optical properties that are unattainable in nature [2,3].

In this contribution, we investigate numerically various planar and three-dimensional metallic metamaterials with respect to their degrees of circular dichroism and optical chirality. The latter is a measure for the local chirality of electromagnetic fields [4]. Chiral metamaterials can lead to local superchiral fields, which exhibit extremely high optical chirality. We discuss the structural, spectral and spatial dependence of these values. This provides a comparison of the chiroptical properties of different practical geometries.

[1] J. K. Gansel et al., Science **325**, 1513 (2009).
[2] M. Thiel et al., Adv. Mat. **21**, 4680 (2009).
[3] A. Radke, P. V. Braun, and H. Giessen, to be published.
[4] Y. Tang and A. E. Cohen, Phys. Rev. Lett. **104**, 163901 (2010).

DS 57.3 Thu 15:30 WIL A317

Weak localization of light in ZnO nanorods in space and time — •Manfred Mascheck[1], Slawa Schmidt[1], Martin Silies[1], David Leipold[2], Erich Runge[2], Takashi Yatsui[3], Kokoro Kitamura[3], Motoichi Ohtsu[3], and Christoph Lienau[1] — [1]Carl von Ossietzky Universität Oldenburg — [2]Technische Universität Ilmenau — [3]University of Tokyo

An array of ZnO nanorods is used to directly visualize the weak localization of light in both space and time. Ultrashort laser pulses from a Ti:Sapphire oscillator with a pulse duration of 6 fs are focused to their diffraction-limit of 1 μm^2 onto the ZnO nanorod array using an all-reflective Cassegrain objective. The generated SH emission is collected in reflection geometry and detected as a function of the lateral position of the laser focus. Pronounced intensity fluctuations on a sub-μm scale due to the multiple random scattering inside the nanoneedle array are taken as the spatial hallmark of weak the localization of light. By varying the delay between the phase-stabilized pair of laser pulses from a dispersion-balanced Michelson interferometer, interferometric frequency-resolved autocorrelation (IFRAC) traces are measured. By analyzing these traces in the frequency domain, the dephasing time and therewith the temporal evolution of the electric field within the ZnO array could be deduced.

DS 57.4 Thu 15:45 WIL A317

Octave-wide Photonic Band Gap in Three-Dimensional Plasmonic Bragg Structures — •Richard Taubert and Harald Giessen — University of Stuttgart, 4th Physics Institute and Research Center SCoPE, Pfaffenwaldring 57, 70550 Stuttgart

We investigate radiative coupling of particle plasmons in various three-dimensional, stacked geometries of plasmonic oscillators. The arrays of gold nanowires with fixed dimensions and lateral periodicity are stacked on top of each other, separated by a dielectric spacer layer. The vertical distance as well as the number of layers is varied.

The dependence of the optical spectra on spacing distance is investigated in a system consisting of two layers. We show that the coupled system exhibits a superradiant mode when the vertical distance of the oscillators matches half their emission wavelength. This means that the Bragg criterion for the particle plasmonic resonance wavelength is fulfilled.

Upon increase of the number of radiatively coupled oscillators, the spectral width of the superradiant mode increases alongside with a change of the spectral shape from Lorentzian to stop-gap like. Eventually the superradiant mode evolves into a very broad photonic band gap which spans almost over one octave.

By changing the dimensions of the gold nanowires, keeping their aspect ratio constant, the oscillator strength is modified, and therefore the radiative damping rate can be tuned. This allows for a convenient tailoring of very broad photonic band gaps.

DS 57.5 Thu 16:00 WIL A317

Palladium-based perfect plasmonic absorber in the visible and its application to hydrogen sensing — •Andreas Tittl[1], Patrick Mai[1], Richard Taubert[1], Thomas Weiss[1], Na Liu[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, 70569 Stuttgart, Germany — [2]Department of Chemistry, University of California, Berkeley, and Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California, 94720, USA

We report on the first experimental realization of a palladium-based perfect plasmonic absorber at visible wavelengths and its application to hydrogen sensing.

Our design utilizes palladium wires on top of a MgF_2 spacer layer on a 200 nm thick gold mirror and exhibits an absorbance $> 99\%$ at the given design wavelength in the red part of the visible spectrum.

Exposure to hydrogen causes a change in the complex refractive index of palladium, resulting in reduced absorption and hence enhanced reflection at the interrogation wavelength[1]. Our sensor has a very fast reaction time of less than 1 second, a recovery time of about 10 seconds, and a lower detection limit of less than 0.5% hydrogen in air.

This pronounced response and background-free operation should enable extremely sensitive optical gas detection schemes down to the ppm range in the future.

[1] N. Liu, et al., Nano Lett. **10**, 2342 (2010)

DS 58: Invited – Gelbstein

Time: Friday 10:15–11:00 Location: GER 37

Invited Talk DS 58.1 Fri 10:15 GER 37

Development of Highly Efficient IV-VI Thermoelectric Materials — •Yaniv Gelbstein — Ben-Gurion University of the Negev, Beer-Sheva, Israel

IV-VI based alloys, are known as superior candidates for thermoelectric applications. Improvement of the thermoelectric performance of IV-VI based alloys was recently obtained using several approaches based on optimal doping; nano-structuring for reduction of the lattice thermal conductivity; development of functionally graded materials with a desired dopant concentration profile; Fermi-level pinning effect, etc. Using these approaches both n- and p-type PbTe based alloys were prepared with maximal ZT values of about 1.7. However, although ZT values were dramatically increased over the last years, no correspondent increase in the efficiency of practical devices was observed. Possible reasons for that are deteriorating of nano-structures at the operating temperatures, poor mechanical properties and chemical instability. The present communication puts forward the overall factors affect the performance of alloys based on IV-VI compounds for thermoelectric power generation applications.

DS 59: Thermoelectric Materials, Thin Films, and Nanostructures I (Focused Session – Organisers: Nielsch, Rastelli, Balke)

Time: Friday 11:00–13:00 Location: GER 37

Topical Talk DS 59.1 Fri 11:00 GER 37

Nanocrystalline silicon for thermoelectricity — •Gabi Schierning — Center for NanoIntegration Duisburg-Essen (CeNIDE), University of Duisburg-Essen, 47057 Duisburg, Germany

A main focus in thermoelectricity is on the development and utilization of materials with high availability and sustainability. From this point of view, nanocrystalline silicon is a potential candidate for thermoelectric application, motivating the effort of optimizing its thermoelectric properties. In the first part of the talk, an overview over silicon-based thermoelectrics will be given.

In the second part of the talk, own work will be presented. Our bottom up approach starts with tailored silicon nanoparticles from a gas phase process. Compaction of the nanopowder is done by a dc-current sintering. In a combined experimental and theoretical work it is shown how the developing microstructure during sintering correlates to the percolation paths of the current through the powder. Observed density fluctuations on the micrometer scale are attributed to the specific heat profile of the simulated powder networks.

It is technologically highly demanding to exclude any contamination of the nanopowder with oxygen and moisture. As a result, a

Si/SiO_2 core/shell structure is always observed for nanocrystalline silicon powders having been in contact with air. In the sintered body, the initial core shell structure is dissolved. Instead, oxidic precipitates have formed during sintering. The role of these oxidic precipitates with respect to the sintering mechanism and the thermoelectric transport properties will be discussed.

Topical Talk DS 59.2 Fri 11:30 GER 37

Nanoscale Thermoelectrics — •Jan D. König — Fraunhofer IPM, Heidenhofstr. 8, 79110 Freiburg, Germany

The variety of TE materials extends from semiconductors via metalloids to ceramic oxides. Decisive factors for the efficiency of the material, in addition to the highest possible Seebeck coefficient, also known as the thermoelectric power, are a high electrical and at the same time a low thermal conductivity. Here physics has imposed laws; because these properties cannot easily be optimized independently of one another. Modern high ZT materials manage to trick nature to a certain degree: they have a fabricated atomic configuration in which the inner structure of the material restricts the mobility of the phonons, and hence its thermal conductivity, (phonon blocking) while not obstructing or even promoting that of the electrons (electron transmitting). Nanotechnologically produced materials are regarded as especially promising. They are manufactured on the basis of already familiar thermoelectric materials by, for example, embedding nanoparticles in a macroscopic matrix. Recent concepts for nanoscale thermoelectric materials will be discussed.

Topical Talk DS 59.3 Fri 12:00 GER 37

Thermal transport and thermoelectric effect in thin semiconductor membranes — •Matthias Schmidt, Thorben Bartsch, Christian Heyn, and Wolfgang Hansen — Institut für Angewandte Physik, Universität Hamburg, Germany

We study the heat conductance and the thermopower in single-crystalline semiconductor membranes which are fabricated by selective etching of AlGaAs-based heterostructures. The membranes have thicknesses up to a few 100 nm and are grown by molecular beam epitaxy. An airgap of thickness between 5 nm and 500 nm separates the membranes from the substrate and makes possible to establish large thermal gradients both to the substrate as well as within the membrane. In particular, the heat transport between a membrane that is held by few nanometer thin semiconductor columns and the substrate is studied. Furthermore, in thin semiconductor bridges containing a two-dimensional electron system the magneto-thermopower is investigated. The results demonstrate that we are able to establish strong thermal gradients even at very low temperature. With curved membranes in magnetic fields we can establish a system in which the spatial distribution of both the local density of states and the temperature can be controlled simultaneously.

Topical Talk DS 59.4 Fri 12:30 GER 37

Theoretical studies of electrical cross-plane transport in semiconductor multilayer heterostructures — •Peter Kratzer[1] and Vladimir M. Fomin[2] — [1]Faculty of Physics and CeNIDE, University Duisburg-Essen, 47048 Duisburg, Germany — [2]Institute for Integrative Nanosciences, IFW Dresden, 01069 Dresden, Germany

Using epitaxially grown multilayer heterostructures, it has been demonstrated experimentally that low lattice thermal conductivity κ_{ph} can be realized in crystalline samples made from standard semiconductors. In particular, built-in self-assembled quantum dot (QD) stacks offer the possibility to affect both the thermal and the electrical cross-plane transport in a way favorable for thermoelectrics. In this talk, we employ Boltzmann transport theory to explore the role of the electronic structure for further enhancement of the figure of merit Z by increasing its numerator σS^2. For a stack of quantum dots separated by nanometer-thin spacer layers, miniband transport may be used to realize an electronic transport regime with large σS^2 but still low κ_{el}. The geometry-dependent miniband dispersion is obtained from atomistic calculations of the electronic structure of QD arrays. Moreover, due to different quantum states available for scattering, the mean free path of carriers in low-dimensional transport differs strongly from bulk transport. Interesting effects are to be expected if the layer thickness in the structures is reduced below the mean free path. As one example, we predict values of $ZT > 2$ at room temperature for an array of InAs QDs in GaAs for suitably chosen geometry and doping level [Phys. Rev. B **82**, 045318 (2010)].

DS 60: Thermoelectric Materials, Thin Films, and Nanostructures II (Focused Session – Organisers: Nielsch, Rastelli, Balke)

Time: Friday 14:00–15:45 Location: GER 37

DS 60.1 Fri 14:00 GER 37

Harman measurements on laser-annealed thin films of Si and Ge nanoparticles — •Benedikt Stoib[1], Martin S. Brandt[1], Nils Petermann[2], Hartmut Wiggers[2], and Martin Stutzmann[1] — [1]Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, 85748 Garching — [2]Institut für Verbrennung und Gasdynamik, Universität Duisburg-Essen, Lotharstraße 1, 47048 Duisburg

We discuss Harman measurements of the thermoelectric figure of merit ZT for thin films made of nanoscale Si, Ge and SiGe particles. The particles are prepared by plasma decomposition of silane and/or germane in a microwave plasma reactor and have a size of around 25 nm in the case of SiGe particles. Thin films are prepared by a drop-casting process on quartz substrates, followed by an annealing step with a high intensity pulsed laser. Films with μm-range thicknesses are subjected to a specific current cycle at varying temperature. The Harman method is known to directly yield the thermoelectric figure of merit ZT under certain conditions. In this contribution, we show temperature-dependent measurements suggesting values of $ZT > 0.3$ at 650 K for SiGe. The presented data are discussed taking into account possible parasitic effects.

DS 60.2 Fri 14:15 GER 37

3ω measurements of half-Heusler thin films using a passive circuit — •Christian Mix, Tino Jäger, and Gerhard Jakob — Institut für Physik, Universität Mainz, Staudinger Weg 7, 55128 Mainz

One possibility to increase the thermoelectric Figure-of-Merit of thin films is to decrease the thermal conductivity, by replacing the thin film with a superlattice of the same thickness. This is one of the major challenges in ongoing research. For this purpose a 3ω-measurement system is built up to obtain the thermal conductivity of thin films. To nullify influences of active elements, a setup including a wheatstone bridge is used. Different aspects of the measurement system like the influence of thermal penetration depth and the energy losses by atmosphere are discussed. Additionally, first results on Half-Heusler thin films and superlattices are presented.

DS 60.3 Fri 14:30 GER 37

Cross-plane thermal conductivity of Ge/Si multilayers — •Peixuan Chen, Jianjun Zhang, Fabio Pezzoli, Mathieu Stoffel, Christoph Deneke, Armando Rastelli, and Oliver Schmidt — Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Germany

One of the approaches to increase the efficiency of a thermoelectric converter is the reduction of the lattice thermal conductivity k of the employed materials. By using multilayers of Ge nanodots separated by Si barriers we have shown that it is possible to precisely control the thermal conductivity of the resulting nanostructured material by simply varying the thickness of the Si spacer [1]. Here, we study the dependence of k of Ge/Si layers on the amount of deposited Ge. By gradual increasing the amount of deposited Ge, flat Ge/Si multilayers with different Ge thickness and nanodot Ge/Si multilayers with different dot density were obtained. We performed thermal conductivity measurements by using the 3-omega method and found that: (i) in the case of Ge/Si flat multilayers the total thermal resistance increases and k decreases with increasing Ge amount; (ii) in the case of Ge/Si nanodot multilayers, the change of total thermal resistance and thermal conductivity is smaller than the error bar. In order to study the effect of alloying and interface sharpness, we have performed postgrowth annealing on the nanodot multilayers. By gradual increase of the annealing temperature, the thermal conductivity of Ge/Si film increases and finally approaches the values of GeSi alloys.

[1] G. Pernot et al., Nature Materials 9, 491 (2010)

DS 60.4 Fri 14:45 GER 37

Half Heusler thin film superlattices — •Tino Jaeger[1], Christian Mix[1], Michael Schwall[2], Benjamin Balke[2], Sascha Populoh[3], Anke Weidenkaff[3], Claudia Felser[2], and Gerhard Jakob[1] — [1]Institut für Physik, Universität Mainz, Staudinger Weg 7, 55128 Mainz, Germany — [2]Institut für Anorganische Chemie und Analytische Chemie, Universität Mainz, Staudinger Weg 9, 55128 Mainz, Germany — [3]EMPA -Eidgenössische Materialprüfung und -forschungsanstalt, Festkörperchemie und Katalyse, Ueberlandstrasse 129, 8600 Duebendorf, Switzerland

Due to rising energy costs and carbon dioxide concentration in the atmosphere thermoelectric materials have moved into focus. Recently, the efficiency of thermoelectric materials is to be increased by nanostructuring. So, Seebeck coefficient and electrical conductivity are increased or/and thermal conductivity is reduced. Here, DC magnetron sputtering is used for epitaxial deposition of thin films containing Half-Heuslers. As bulk materials, TiNiSn and Zr$_{0.5}$Hf$_{0.5}$NiSn exhibit promising thermoelectric properties. It is shown that TiNiSn and Zr$_{0.5}$Hf$_{0.5}$NiSn are suitable to be epitaxially deposited on top of each other. Therefore, both Half-Heusler materials can be used for superlattice structures to decrease the thermal conductivity perpendicular to the surface. The relation between crystal quality and in-plane thermoelectric properties is been shown.

DS 60.5 Fri 15:00 GER 37

Investigations on the optimum Zr to Hf ratio in Zr$_{1-x}$Hf$_x$NiSn as n-type thermoelectric materials — •Michael Schwall and Benjamin Balke — Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, Mainz, Germany

Excellent XNiSn (X=Ti, Zr, Hf) n-type thermoelectric materials (ZTmax= 1.5) were reported from several groups in Asia and the USA. The best reported half-Heusler materials exhibit thereby always the same Zr to Hf ratio. Because of the demands on a thermoelectric converter (TEC) like environmental friendliness, low-cost and future availability of raw materials, we investigated the effect of varying the Zr to Hf ratio and the effect of Ti substitution on the X-position. The best Zr to Hf ratio was then substituted with the best Ti value. We will present the results of the thermal transport measurements, the structure analysis of the materials and outgoing from these results some ideas for further investigations to increase the ZT.

DS 60.6 Fri 15:15 GER 37

Electronic structure and thermoelectric properties of doped Heusler compounds CoTi$_{1-x}$M$_x$Sb$(M = \text{Sc,V})$ — •S. Ouardi[1], G. H. Fecher[1], B. Balke[1], X. Kozina[1], M. Schwall[1], G. Stryganyuk[1], S. Ueda[2], K. Kobayashi[2], and C. Felser[1] — [1]Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, Mainz, Germany — [2]NIMS Beamline Station at SPring-8, National Institute for Materials Science, Hyogo 679-5148, Japan.

Heusler compounds are considered to be promising thermoelectric materials because of their potential role in the realization of environmentally friendly technology. Complex $C1_b$ compounds such as CoTiSb are promising thermoelectrical materials. The substitutional series of Heusler compounds Co$Ti_{1-x}T'_x$Sn (T'= Sc, V) were synthesized and experimentally investigated with respect to their electronic structure and transport properties. The results show the possibility to create n-type and p-type thermoelectrics within one compound. The carrier concentration and temperature dependence of electrical conductivity, Seebeck coefficient, and thermal conductivity were investigated. Hard X-ray photoelectron spectroscopy was carried out to study the details of the electronic structure and relate it to the transport properties. Massive *"in gap"* states are found in pure CoTiSb that contain about 0.07 electrons per cell. This proves that the electronic states close to the Fermi energy play a key role on the behavior of the transport properties. *This work was financially supported by the Federal Ministry of Economics and Technology (0327876D thermoHEUSLER).*

DS 60.7 Fri 15:30 GER 37

Electronic structure and thermoelectric properties of doped Heusler compounds. — •G. H. Fecher, S. Ouardi, and C. Felser — Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, Mainz, Germany

Different substitutional series of Heusler compounds XTi$_{1-x}$Y$_x$Z (where X = Co, Ni, Y = Sc, V and $0 < x < 0.2$, and Z = Sn, Sb) were investigated by ab-initio calculations of their electronic structure, mechanical, optical, and transport properties. Different theoretical methods were applied. The results from the ground state electronic structure calculations were used together with Boltzmann transport theory to calculate the thermoelectric transport properties. The mixed compounds with random site occupancy were treated by the virtual crystal and coherent potential approximations. It is found that the in-gap states observed for the pure compound arise from anti-site disorder by partially filling the vacant site of the lattice by Ti through swap and contain about 0.1 electrons per cell. This "self-doping" results in the excellent thermoelectric properties of the pure material. The calculated carrier concentration and temperature dependence of electrical conductivity, Seebeck coefficient, and thermal conductivity were calculated in the range from 10 K to 300 K and agree very well with the experimental observation. The sign of the Seebeck coefficient changes from negative for V to positive for Sc substitution. The calculations reveal that the high n-type and low p-type power factors are explained by differences in the chemical disorder scattering induced electric resistivity.

DS 61: Thermoelectric Materials, Thin Films, and Nanostructures III (Focused Session – Organisers: Nielsch, Rastelli, Balke)

Time: Friday 16:00–17:30 Location: GER 37

DS 61.1 Fri 16:00 GER 37

Phonon transport calculations across interfaces 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

Modern electronic devices are rapidly approaching nanometer scales, and heat transport in these systems, particularly across embedded interfaces, is critical to their performance. In this work we present a phonon transport model that can calculate heat flow in layered structured systems. We perform ab initio calculations using the abinit package to obtain the interatomic force constants [1]. These force constants are plugged into a non equilibrium Green's function formalism to calculate the transmission function and the temperature dependence of thermal conductivity in the linear ballistic response regime [2, 3].

[1] http://www.abinit.org
[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 61.2 Fri 16:15 GER 37

Model calculations of the thermoelectric transport across a back to back Schottky barrier — •Michael Bachmann, Michael Czerner, and Christian Heiliger — Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany

We present results of electronic transport calculations across a back to back Schottky barrier [1]. The basic idea of the back to back Schottky barrier is the assumption of additional electronic states in the band gap at grain boundaries. For an n-type semiconductor these states can be filled by electrons from donor levels. This will lead to a negative space charge region directly at the grain boundary and to positive space charge regions on both sides of the grain boundary. We can change the potential profile by varying the total net charge trapped at the grain boundary. For a given total net charge the potential profile is a function of the donor concentrations. The potential profile is obtained by solving the Poisson equation with a finite difference method on a discrete net. From the potential profile we calculate the transmission function using non equilibrium Greens function formalism considering one parabolic band. For the temperature dependency of the chemical potential we consider one Gaussian shaped donor level and impose charge neutrality. The thermoelectric parameters are calculated using the momentum representation of the transmission function weighted with the energy derivative of the Fermi function [2].

[1] C R M Grovenor J.Phys. C: Solid State Phys. 184079 (1985)
[2] H. Fritzsche Solid State Com. Vol. 9 pp. 1813-1815 (1971)

DS 61.3 Fri 16:30 GER 37

Thermoelectric properties of low-dimensional clathrates from first principles — •Deepa Kasinathan and Helge Rosner — Max Planck Institute for Chemical Physics of Solids, Dresden

Type-I inorganic clathrates are host-guest structures with the guest atoms trapped in the framework of the host structure. From a thermoelectric point of view, they are interesting because they are semiconductors with adjustable bandgaps. Investigations in the past decade have shown that type-I clathrates $X_8\mathrm{Ga}_{16}\mathrm{Ge}_{30}(X = \mathrm{Ba, Sr, Eu})$ may have the unusual property of "phonon glass-electron crystal" for good thermoelectric materials. Among the known clathrates, $\mathrm{Ba}_8\mathrm{Ga}_{16}\mathrm{Ge}_{30}$ has the highest figure of merit (ZT 1). To enable a more widespread usage of thermoelectric technology power generation and heating/cooling applications, ZT of at least 2-3 is required. Two different research approaches have been proposed for developing next generation thermoelectric materials: one investigating new families of advanced bulk materials, and the other studying low-dimensional materials. In our work, we concentrate on understanding the thermoelectric properties of the nanostructured Ba-based clathrates. We use semi-classical Boltzmann transport equations to calculate the various thermoelectric properties as a function of reduced dimensions. We observe that there exists a delicate balance between the electrical conductivity and the electronic part of the thermal conductivity in reduced dimensions. Insights from these results can directly be used to control particle size in nanostructuring experiments.

DS 61.4 Fri 16:45 GER 37

Thermoelectric power of nanostructured thin Au films — •Sebastian Schnurr, Ulf Wiedwald, and Paul Ziemann — Institut für Festkörperphysik, Universität Ulm, Albert-Einstein-Allee 11, 89069 Ulm, Germany

The effect of ordered arrays of nanostructures like nanopillars (periodicities 50 - 100 nm) on the Seebeck coefficient S of thin polycrystalline Au films (thickness t = 10-100 nm) is investigated as function of temperature in the range 6-300 K. Nanostructures are prepared by combining a micellar approach [1] with reactive ion etching. Reference measurements of S were performed on thin continuous films. At low temperature a phonon drag peak is found, which is significantly reduced as compared to bulk Au for thicker films while it completely vanishes for film thicknesses below 20 nm. At ambient temperature, S follows a $[1 - \exp(-a \cdot t)]$-dependence similar to a recent report on thin Pt films [2].

For nanostructured Au films the ratio of the average grain size to the periodicity of nanostructures becomes important. For small grains (10-15 nm) electron scattering at grain boundaries dominates leading to a complete suppression of the influence of nanostructures. In the limit of large grains, however, scattering at nanostructures takes over decreasing S significantly below the reference level while its temperature dependence between 100 K and 300 K practically vanishes.

[1] U. Wiedwald et al., Beilstein J. Nanotechnol. 1, 24 (2010).
[2] M. C. Salvadori et al, Appl. Phys. Lett. 88, 133106 (2006).

DS 61.5 Fri 17:00 GER 37

Complex Chalcogenides for Thermoelectrics: Microstructure Analysis of $\mathbf{AgPb_{18}SbTe_{20}}$ — •Susanne Perlt[1], Thomas Höche[1], Jayaram Dadda[2], and Eckhard Müller[2] — [1]Leibniz Institute of Surface Modification, Leipzig — [2]German Aerospace Center, Institute of Materials Research, Köln

The thermoelectric (TE) bulk material $\mathrm{AgPb}_{18}\mathrm{SbTe}_{20}$ (LAST-18) is a highly promising candidate for application in the mid-temperature range. The manufacturing process needs to be controlled in such a way, that the figure of merit, ZT [1], gets maximized. In this respect, a high electronic conductivity σ, a high thermopower S, and a low thermal conductivity κ are crucial. The high TE performance of LAST is assumed to be caused by the nanoscale precipitates formed by nucleation and growth and/or spinodal decomposition [2].

The presented LAST samples are fabricated via different melting routes and annealing treatments in order to find favourable conditions, i.e. to get a homogeneous material on the microscale but introduce precipitates on the nm scale.

Based on properties monitored by a Seebeck scanning microprobe, structure-property relationships are studied by SEM and TEM analysis. Site-specific lift-out of TEM lamellae are made by focused ion beam (FIB) machining. High-resolution STEM is giving insight into the atomistic structure of the nanostructures.

[1] D. Bilc et al., Phys. Rev. Lett. **93**, 146403 (2004)
[2] J. Androulakis et al., J. Am. Chem. Soc. **129**, 9780 (2007)

DS 61.6 Fri 17:15 GER 37

First principle calculations of nanostructured LAST materials — Jadranka Dokic and •Beate Paulus — Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin

First principle calculations based on different density functionals are performed in order to explain the effects which occur in a solid environment on a microscopical level upon nanostructuring. We are especially interested in, so called LAST-m ($\mathrm{AgPb}_m\mathrm{SbTe}_{m+2}$) crystals which contain a small percentage of silver and antimony atoms incorporated in a lead telluride matrix. The enhancement of thermoelectric efficiency in doped-PbTe is stated to be a consequence of the local increase in the density of states (DOS) over a narrow energy range. Therefore we will analyze the influence of single atom impurities and AgSb pair impurities in various nanostructures within the parent material PbTe. The influence of different doping ratios, relative distances between the impurities, structural relaxations due to doping onto the DOS is determined and discussed. In addition formation energies of the nanostructured solids will be studied and relative stabilities evaluated.

DS 62: Organic Thin Films I

Time: Friday 10:15–11:45 Location: GER 38

DS 62.1 Fri 10:15 GER 38

AFM based density-of-states measurements on organic thin films — •Markus Kratzer[1], Igor Beinik[1], Astrid Wachauer[1], Mujeeb Ullah[2], Helmut Sitter[2], and Christian Teichert[1] — [1]Institute of Physics, University of Leoben, Franz Josef Straße 18, A8700 Leoben, Austria — [2]Institute of Semiconductor and Solid State Physics, Johannes Kepler University of Linz, A4040, Austria

The performance of electrical devices based on organic materials crucially depends on the charge transport properties. For the understanding of the charge carrier transport in organic molecular films knowledge on the density of states (DOS) is of fundamental importance. In this study, we present DOS measurements based on Kelvin Probe Force Microscopy (KPFM) [1, 2] of the organic n-type semiconductor C_{60} and the p-type semiconductor Para-hexaphenyl (6P). For the n-type conductor, the electron DOS and for the p-type conductor the hole density of states can be derived from the KPFM data. For this purpose, organic thin film transistor structures were prepared utilizing Hot Wall Epitaxy. The substrate temperature during deposition was varied between 273 K and 423 K resulting in films of different degrees of crystallinity. KPFM was then applied in inert atmosphere to prevent degradation of the films by oxidation. The results are discussed.

Supported by Austrian Science Fund (FWF) NFN projects S9706-N20, S9707-N20 and P19636.

[1] M. Nonnenmacher, et.al Appl. Phys. Lett. 58, 2921, (1991).
[2] O. Tal, et.al Phys. Rev. Lett. 95, 256405 (2005).

DS 62.2 Fri 10:30 GER 38

Structure formation during deposition of organic films on inorganic substrates - experiments 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

Organic-inorganic interfaces are of strongly increasing scientific interest, as they occur in a broad range of areas, including biomaterials and organic semiconductors. Detailed experimental and theoretical understanding - in particular of the inorganic/organic interaction and the resulting implications with respect to mechanical properties and structure - is still lacking. In the present study we investigate organic thin films which are grown from vapor on metal surfaces and focus on structure evolution during growth. Whereas poly(bisphenol A) carbonate - as a model system - is deposited via thermal evaporation. Characterization of structure formation is based primarily on atomic force microscopy measurements. Complementary, stochastic rate equations with surface free energy and interface potential driven surface diffusion as a central process are employed to model structure evolution. From an excellent agreement of experiments and simulations conclusions on the interface potential as well as underlying physics of structure formation can be drawn. This project is funded by the German BMBF, PTJ-BIO, Grant Number: 0313909
[1] C. Vree and S.G. Mayr, Applied Physics Letters 94 (2009) 093110

DS 62.3 Fri 10:45 GER 38

Templating effect for organic heterostructure film growth: Perfluoropentacene on Diindenoperylene — •Alexander Gerlach[1], Alexander Hinderhofer[1], Takuya Hosokai[1], Christian Frank[1], Jiří Novák[2], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen, Germany — [2]ESRF, BP 220, 38043 Grenoble Cedex 9, France

We present a systematic study of templating effects in organic heterostructure growth, i.e. the growth behavior of the top layer depends on the structural and morphological properties of the bottom layer [1,2]. We prepared thin films of the electron donor diindenoperylene (DIP) each with different crystal structure, grain size, and grain orientation. The electron acceptor perfluoropentacene (PFP) was evaporated on those template layers to form an organic heterostructure. Using x-ray reflectivity, grazing incidence x-ray diffraction, and atomic force microscopy we show that the structure and morphology of the PFP film varies with the properties of the DIP layer underneath. Two main structural effects are observed: PFP molecules in the top layer adopt partly the orientation of the DIP molecules in the bottom layer and the crystalline quality of the PFP layer correlates with the crystallinity of the DIP layer in terms of the coherent in-plane island size. Moreover, we find that the morphology and particularly the shape of the PFP domains depend strongly on DIP template layer.

[1] A. Hinderhofer et al., *Europhys. Lett.* **91** 56002 (2010).

[2] A. Hinderhofer et al., *submitted* (2010).

DS 62.4 Fri 11:00 GER 38

Structure solution of organic surface-induced polymorphs by x-ray diffraction reciprocal-space mapping — •Ingo Salzmann[1], Dmitrii Nabok[2], Martin Oehzelt[3], Steffen Duhm[4], Armin Moser[5], Georg Heimel[1], Peter Puschnig[2], Claudia Ambrosch-Draxl[2], Jürgen P. Rabe[1], and Norbert Koch[1] — [1]Humboldt-Universität zu Berlin, Germany — [2]Montanuniversity Leoben, Austria — [3]Johannes Kepler Universität Linz, Austria — [4]Chiba University, Japan — [5]Graz University of Technology, Austria

Thin films of pentacenequinone (PQ) and perfluoropentacene (PFP) on silicon oxide (SiO_x) and highly oriented pyrolytic graphite (HOPG) were investigated by x-ray diffraction reciprocal space mapping (RSM) providing the unit cell parameters of the respective substrate induced polymorphs (SIPs). In contrast to the monoclinic single-crystal phases (SCPs), RSM yields triclinic unit-cells for PQ and PFP on HOPG and for PQ on SiO_x, the latter with only one molecule per unit cell. Therefore, in contrast to its SCP, PQ does not exhibit a molecular herringbone arrangement in the SIP. It is shown that the same PFP SIP as found on HOPG grows on Au(111), Ag(111) and Cu(111), therefore demonstrating that, owing to the fiber texture of HOPG, growth investigations on HOPG can act as technique for SIP determination on metallic single crystalline substrates, where RSM cannot be applied. For both SIPs on SiO_x full structure solutions are derived via forcefield calculations and used for comparative electronic structure calculations of the two PQ polymorphs demonstrating significantly wider dispersion of the lowest unoccupied molecular orbital-derived band.

DS 62.5 Fri 11:15 GER 38

Reversible light-controlled capacity switching of chromophore based metal/polymer nanocomposites — •Christina Pakula[1], Sri Wahyuni Basuki[1], Vladimir Zaporojtchenko[1], Thomas Strunskus[1], Dordaneh Zargarani[2], Rainer Herges[2], and Franz Faupel[1] — [1]Institut für Materialwissenschaft - Materialverbunde, Technische Fakultät der Christian-Albrechts-Universität zu Kiel, Kaiserstr. 2, 24143 Kiel, Germany — [2]Institut für Organische Chemie, CAU Kiel, Otto-Hahn-Platz 4, 24098 Kiel, Germany

Electro-optical switching based on photochromism is under extensive research nowadays, due to applications in the new generation of organic electronics ranging from non-linear optical devices and optical switches to information storage. We report on photo-switchable AC conductance of nano sheet capacitors which are produced by sandwiching some hundred nm or μm thick polymer films containing dissolved chromophores between transparent percolated Pt nanoparticle electrodes. The photoactive thin polymer films show a complete and fully reversible switching of the capacitance with changes $> 50\%$ [1]. This change is correlated to the azo dye concentration. We observe an increase in the capacitance change with increasing temperature below and also in a small range above the glass transition temperature of the polymer blend. The dependence of the capacitance changes on the irradiation wavelength and on application of an electrical field under irradiation is discussed.

[1] Zaporojtchenko, V, Pakula, C, Basuki, SW, Strunskus, T, Zargarani, D, Herges, R, Faupel, F Applied Physics A, accepted.

DS 62.6 Fri 11:30 GER 38

Electronic structure of diindenoperylene-fullerene heterojunctions — •Andreas Wilke[1], Julia Wagner[2], Mark Gruber[2], Johannes Frisch[1], Patrick Amsalem[1], Antje Vollmer[3], Benjamin Bröker[1], Andreas Opitz[2], Wolfgang Brütting[2], and Norbert Koch[1] — [1]Humboldt-Universität zu Berlin, Brook-Taylor-Str. 6, 12489 Berlin — [2]Universität Augsburg, Universitätsstr. 1, 86135 Augsburg — [3]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Albert-Einstein-Straße 15,12489 Berlin

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 (BHJ), where charge separation occurs. We report on ultraviolet photoelectron spectroscopy (UPS) measurements on PHJ and BHJ of the donor diindenoperylene (DIP) and the acceptor C60. The results on energy level alignment at these heterojunctions are then discussed in comparison to the energy conversion efficiency achieved in corresponding OPVCs, which peaked at 4.1%. The offset between the highest occupied molecular orbital of DIP and the lowest unoccupied molecular orbital of C60, an estimate for the maximum achievable open circuit voltage, is 1.3 eV and 1.35 eV for the PHJ and BHJ, respectively. For comparison, OPVCs exhibited open circuit voltages up to 0.93 V. Our results demonstrate close agreement between the donor/acceptor energy level alignment and the open circuit voltage in devices and that induced carriers at contacts are beneficial for the energy conversion efficiency of OPVCs.

DS 63: Organic Thin Films II

Time: Friday 12:00–13:00 Location: GER 38

DS 63.1 Fri 12:00 GER 38

Investigation of contact resistance in organic thin film transistors by channel potential mapping — •Marko Marinkovic, Sidhant Bom, Dietmar Knipp, and Veit Wagner — School of Engineering and Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

One of the limiting factors for the commercial use of organic electronics is the limitation in high switching frequencies due to the contact resistance [1]. In this study, we investigate the contact resistance by measuring the potential distribution inside of the channel of transistors by additional buried sense electrodes. This allows the separate determination of the potential barriers at the source and drain electrode, that can be related directly to the injection and extraction of the majority carrier.

For this purpose, organic thin film transistors have been prepared on plastic (PET) substrates with P3HT as a p-type material and a similar n-type semiconductor in the top-gate bottom-contact configuration. The interface between the semiconductors and the metal electrode (Au) has been analyzed through current-voltage measurements, showing the contact resistance of less than 200 kΩcm and 300 kΩcm at source and drain electrical contacts, respectively. These results show good agreement with the transmission line method (TLM).

[1] V. Wagner et al. Appl. Phys. Lett. 89 (2006) 243515.

DS 63.2 Fri 12:15 GER 38

Trapping analysis of polythiophene based field-effect transistors with modified gate oxide — •Steve Pittner and Veit Wagner — School of Engineering, Jacobs University Bremen, Campus Ring 1, D-28759 Bremen, Germany

Organic semiconductors have proven to be suitable materials for electronic devices like organic field effect ransistors (OFET). But their charge mobility, an important parameter for technical applications, is very sensitive to the semiconductor-insulator interface, especially to unintended interface states.

We have investigated the influence of different interface state concentrations on the charge transport at the silicon oxide / poly(3-hexylthiophene) (P3HT) interface. Different surface treatments were applied to the silicon oxide layer covering a highly doped silicon wafer to modify the density of surface states. On this surface the P3HT was deposited. The carrier density in the P3HT was determined optically by charge modulation spectroscopy (CMS). This allows to map the carrier concentration spatially and energetically next to the electrodes. Parallel analysis by Impedance spectroscopy allowed to determine the doping profile of the whole semiconductor layer via analysis of the change of the depletion capacitance. This analysis allowed to correlate residual carrier density with high doping concentration close to the interface.

DS 63.3 Fri 12:30 GER 38

Electronic structure of thin spin-coated polyimide layers — •Daniel Friedrich[1], Yuri Koval[2], Paul Müller[2], and Dieter Schmeisser[1] — [1]Brandenburgische Technische Universität Cottbus, Angewandte Physik/Sensorik, K.- Wachsmann-Allee 1, 03046 Cottbus — [2]Universität Erlangen Nürnberg, Experimental Physik/Supraleitung, Erwin-Rommel-Str. 1, 91058 Erlangen

The conductivity of polyimide layers can be modified by several orders of magnitude by ion beam radiation. In order to understand the electronic structure of the pure polyimide before ion beam modification we focus in our preliminary experiments on spectroscopic investigations of thin as prepared polyimide films. The films were made by spin coating from a PMDA/ODA solution with subsequent vacuum annealing at 350°C. The layer thickness can be controlled by changing the concentration of PMDA/ODA in the solution realizing a thickness down to 3.5nm. For the characterization of the as prepared thin polyimide films the techniques NEXAFS, ResPES, XPS and CIS were applied at the U49/2-PGM2 beam line of Bessy II, Berlin. Our data including the valence band, core levels and absorption spectrum were compared with theoretical LCAO calculations. Based on these results we are able to attribute all spectral features to the specific atomic bonds in the molecule.

DS 63.4 Fri 12:45 GER 38

Locally Resolved Core-hole Screening, Molecular Orientation, and Morphology in Thin Films of Diindenoperylene Deposited on Au(111) Single Crystals — •Maria Benedetta Casu[1], Britt-Elfriede Schuster[1], Indro Biswas[1], Christoph Raisch[1], Helder Marchetto[2], Thomas Schmidt[2], and Thomas Chssé[1] — [1]IPTC, University of Tübingen, Tübingen, Germany — [2]Fritz-Haber-Institut, Berlin, Germany

By using a combination of microscopic imaging and diffraction techniques with structural and chemical sensitivity, we studied the growth of diindenoperylene (DIP) on Au(111) single crystals. Growth and structure of DIP films of different thickness were monitored in situ including real time PEEM and LEEM performed at the beamline UE49-PGM-b-SMART at BESSY. A layer-by-layer mechanism characterizes the initial growth followed by island nucleation, i.e., the growth follows the Stranki-Krastanov mode. Highly resolved spectromicroscopy reveals that electronic structure, core-hole screening, and molecular orientation depend on the local morphology of thin films. These phenomena, like different screening of the core hole, or different FWHM of the XPS lines, have been previously shown comparing different samples consisting of monolayers and multilayers. In our work we show their occurrence comparing islands versus monolayers in the same film.

DS 64: Organic Thin Films III

Time: Friday 14:00–15:45 Location: GER 38

DS 64.1 Fri 14:00 GER 38

Alkali metal-intercalated Picene thin films: Examination of the electronic structure by photoemission spectroscopy — •Andreas Ruff[1], Andreas Müller[1], Nis Hauke Hansen[2], Jens Pflaum[2], Michael Sing[1], and Ralph Claessen[1] — [1]Lehrstuhl für Experimentelle Physik 4, Physikalisches Institut, Universität Würzburg — [2]Lehrstuhl für Experimentelle Physik 6, Physikalisches Institut, Universität Würzburg

Recently, superconductivity was reported for potassium-doped picene single crystals (K_3Pic) from magnetization measurements [1]. We have investigated A_xPic thin films (A=K, Cs) on silicon oxide substrates by means of photoemission spectroscopy (PES) to follow the evolution of the spectral function with doping. The high quality of our Pic films is demonstrated by X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS). To clarify the growth mode of the films, surface images were taken with an atomic force microscope (AFM). In the PES spectra one can observe the gradual filling of the former lowest unoccupied molecular orbital (LUMO) with alkali metal evaporation time. As opposed to previous experiments on K-doped pentacene films, a two-peak structure, instead of one, appears in the former gap of the organic semiconductor. The origin of these features has not been unraveled as yet. We discuss these findings as well as the absence of a clear metallic Fermi cut-off against the background of experimental and theoretical work so far.

[1] R. Mitsuhashi et *al.*, Nature **464**, 76 (2010)

DS 64.2 Fri 14:15 GER 38

Interaction between Cobalt Phthalocyanine and Gold revealed by Photoexcited Electron Spectroscopies — •Fotini Petraki[1], Heiko Peisert[1], Indro Biswas[1], Umut Aygül[1], Florian Latteyer[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

Cobalt phthalocyanine (CoPc) monolayer films evaporated on Au(100) are studied by photoexcited electron spectroscopies (XPS, XAES, UPS, XAS, ResPES). A quite intense modification of the electronic structure of the CoPc molecule at the interface with Au, with respect to the molecule in the bulk phase, is observed by XPS, UPS and XAES (X-ray excited Auger electon spectroscopy). Local charge transfer towards the central metal atom of the phthalocyanine molecule from the gold substrate affects the charge state of the Co ion resulting in a different line shape of the Co related peaks and the presence of enhanced features in the energy region across the metal d-bands (UPS). This could be explained by a mixing of the transition metal 3d states with the underlying metallic states of gold. This suggestion is further supported by XAS data according to which, the Co 2p absorption spectra look different for monolayer and thicker organic films pointing to a possible interaction of the molecules with the substrate via the Co d-electrons. Co-related valence band states of CoPc were identified by Resonant Photoemission (ResPES).

DS 64.3 Fri 14:30 GER 38

Electronic structure and optical properties of P3HT - Evidence of 2D-polarons in P3HT — •Matthias Richter 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 investigations of the electronic structure and optical characteristics of poly(3-hexylthiophene) (P3HT) based films. Various techniques like NEXAFS, SRXPS, UPS, UV-VIS and FTIR were used. X-Ray based measurements were done at the U49/2-PGM2 beam line at BESSYII. The samples were produced by spin casting P3HT dissolved in chloroform and other suitable solvents on ITO (indium tin oxide) coated glass slides and silicon substrates. Regioregular-P3HT is known to form thin films with nanocrystalline lamellae. This 2D structure give rise to additional electronic excitations in photoinduced absorption measurements, which are attributed to 2D-polarons [1]. In the Total Electron Yield (surface sensitive) and Total Fluorescence Yield (bulk sensitive) NEXAFS spectra of regioregular-P3HT three additional features can be found prior to the first typical π^* excitation. The nature of these features was further investigated by means of SRXPS and UPS measurements. Energy differences relative to π^*-peak maximum (0.54eV, 0.87eV and 2.24eV) suggest that these features are due to 2D-polarons. This presence of polarons is further confirmed by our FTIR and UV-VIS results. [1] Osterbacka et al., Synth. Met. 116 (2001) 317

DS 64.4 Fri 14:45 GER 38

Correlation between the interface-energetics and thermal stability of SAMs on Gold — •Stefanie Winkler[1], Daniel Käfer[2], and Christof Wöll[3] — [1]Helmholtz Zentrum Berlin für Materialien und Energie GmbH Elektronenspeicherring, D-12489 Berlin, Germany — [2]Department of Chemical Engineering, Stanford University, CA 94305, USA — [3]Institute of Functional Interfaces, Karlsruhe Institute of Technology (KIT), 76012 Karlsruhe, Germany

Improved organic electronic device characteristics can be achieved via SAM-modification, which is attributed to enhanced crystal growth and a lowering of the injection barrier. A variety of thiol-based SAMs was used for an UPS-study to elucidate structure-related properties in such systems. We could generalize the dependency of the workfunction change on the alkanethiol-SAM dipoles to more complex systems based on functionalized aromatic backbones. By adjusting the size of a given SAM or substituting atoms the molecular dipole and subsequently the interface dipole can be tuned.

In addition we employed thermal desorption spectroscopy to correlate the magnitude of the covalent interactions between the SAM's sulfur groups and the gold to the interface energetics. We have indications that, for the investigated systems, varying the SAM functionalization does nof affect the sulfur-gold-bonding, which is in close agreement to the findings of Heimel et al. in 2008, reporting that the thiol- and the headgroup of a particular SAM are electronically decoupled.

DS 64.5 Fri 15:00 GER 38

Investigation of electronic properties and morphology of an n-channel perylene tetracarboxylic diimide thin film — •Franziska Lüttich[1], Harald Graaf[1], Christian von Borczyskowski[1], Antonio Facchetti[2], and Antoine Kahn[3] — [1]Chemntiz University of Technology, Chemnitz, Germany — [2]Polyera Corporation, Skokie IL, USA — [3]Princeton University, Princeton NJ, USA

We report on the influence of thickness and substrate on the electronic density of states and on the surface potential of an air-stable n-channel perylene tetracarboxylic diimide semiconductor thin film. Ultra-violet photoelectron spectroscopy (UPS) and Inverse photoelectron spectroscopy (IPES) show a variation of the band gap and of the electron affinity of the material as a function of substrate. The organic thin films were fabricated with Polyera ActivInk$^{\mathrm{TM}}$ N1200 (PDI8-CN$_2$) by molecular beam deposition on Gold or native Siliconoxide and then analyzed in an ultra-high vacuum chamber without exposure to ambient atmosphere.

The thin films were further investigated under ambient conditions using an atomic force microscope (AFM) to gain information of the topography. Additional Kelvin-Probe force microscopic (KPFM) measurements give insight into the local resolved surface potential.

DS 64.6 Fri 15:15 GER 38

UV-induced sample degradation can mimic band bending during photoemission of organic thin films — •Raphael Schlesinger[1], Johannes Frisch[1], Antje Vollmer[2], and Norbert Koch[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, 12489 Berlin, Germany — [2]HZB-BESSY II, Albert-Einstein-Str. 15, 12489 Berlin, Germany

Photoemission spectroscopy (PES) has evolved to a widely used method for characterizing conjugated organic materials' electronic structure at interfaces. Noteworthy, energy level shifts ascribed to band bending in thickness-dependent studies of organic thin films are often not unequivocally reproducible. We show for prototypical thiophene-based molecular and polymer materials that such energy shifts may in fact be induced by the PES measurement itself. The valence spectra of thin films on PEDT:PSS and Au exhibit irreversibly rigid shifts by up to 0.4 eV to higher binding energies, without notable changes of the spectral shape. This shift is a monotonous function of ultraviolet (UV) light irradiation time and photon flux. Photo-electron induced defects may be created in the sample that either lead to gap states, which shift the Fermi-level, or to the build-up of space charges. The degradation proceeds at a lower rate if a high-conductivity substrate is used for the organic materials, indicating that photo-electron induced degradation is enhanced by subtle sample charging.

DS 64.7 Fri 15:30 GER 38

Imaging ellipsometry of graphene — •Peter H. Thiesen[1], Christian Röling[1], and Ulrich Wurstbauer[2] — [1]Accurion GmbH, Stresemannstr. 30, 37079 Göttingen — [2]Physics Department, Columbia University, New York, NY 10027

A graphene monolayer flake on a SiO$_2$ (300 nm)|Si substrate was characterized. The sample was previously imaged by optical and atomic force microscopy and identified as a graphene monolayer by RAMAN spectroscopy. Ellipsometric contrast micrographs were recorded. Wavelength spectra of Delta and Psi at different angles of incidence were measured, as well as creation of Delta and Psi-maps. As described in literature, the determination of the dispersion function of graphene is done under the assumption of a layer thickness of 0.35 nm but using a Drude oscillator model. The spectra of Delta and Psi of the Graphene crystallites are significantly different from the substrate and the surrounding graphite flakes. The Dispersion function is in good agreement with literature values when using the same layer thicknesses.

Imaging ellipsometry offers the opportunity to measure the optical properties of graphene flakes at sizes typical for micro-mechanical cleavage. Ellipsometric contrast micrographs, in combination with Psi-maps, are promising tools for locating and identifing graphene crystallites. This was shown for the classic SiO$_2$|Si substrate as well as for GaAs.

DS 65: Organic Thin Films IV

Time: Friday 16:00–17:30 Location: GER 38

DS 65.1 Fri 16:00 GER 38

Changes in optical absorption during film growth — •Harald Graaf[1], Christopher Keil[2], and Derck Schlettwein[2] — [1]Center for nanostructured Materials (nanoMA), Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz — [2]Institut für Angewandte Physik, Justus-Liebig-Universität Gießen, 35392 Gießen

The optical properties of organic thin films are mainly dominated by the (ordered) arrangement of the molecules in the solid. Beside this also the interface to the substrate influences the optical characteristics. This can be seen in absorption measurements taken during the growth of such thin films. Here a clear blue shift of the lowest energy transition with decreasing film thickness can be obtained.

In the literature different explanations are given: decrease in dimension of coupled aggregates [1], quantum confinement of the layer [2], missing nearest neighbour approximation [3] and microscopic polarizability [4]. We will show recent results on different organic materials with comparable optical properties in solution but divers properties in the bulk. Also changes in the substrate will be presented and discussed with regard to the suggested models.

[1] Chau et al. J.Phys.Chem. 97 (1993) 2699

[2] Shen et al. Phys.Rev.B 55 (1997) 10578

[3] Heinemeyer et al. Phys.Rev.Lett. 104 (2010) 257401
[4] Beckers et al. J.Phys.:Condens.Matter 10 (1998) 1721

DS 65.2 Fri 16:15 GER 38

***In situ* studies of real-time changes in the optical spectrum of organic semiconducting thin films during growth** — •Katharina Broch[1], Ute Heinemeyer[1], Alexander Hinderhofer[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, 01062 Dresden

Fundamental issues related to organic semiconductors, such as interface effects and molecular coupling mechanisms, and in particular their influence on optical properties of the systems studied are still not thoroughly investigated. Real-time measurements are well suited for such studies since they enable the observation of possible transient structures and related features in the optical spectra of the films during growth. Using differential reflectance spectroscopy we performed real-time *in situ* studies of optical spectra during thin film growth of several prototype organic semiconductors (pentacene, perfluoropentacene, and diindenoperylene) on SiO_2. These data provide insight into surface and interface effects that are of fundamental importance and of relevance for applications in organic electronics [1]. We observe spectral changes - such as energy shifts and new transitions in specific systems - that decay inversely proportional to the film thickness in the simplest approximation, caused by the different molecular environment and structural changes within the first few monolayers with respect to the bulk.
[1] U. Heinemeyer et al., Phys. Rev. Lett. **104**, 257401 (2010)

DS 65.3 Fri 16:30 GER 38

Online monitoring of the adsorption and release of proteins on thin organic functional surfaces using infrared spectroscopic ellipsometry — •Dennis Aulich[1], Eva Bittrich[2], Klaus-Jochen Eichhorn[2], Petra Uhlmann[2], Manfred Stamm[2], Norbert Esser[1], and Karsten Hinrichs[1] — [1]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Albert-Einstein-Str.9, 12489 Berlin, Germany — [2]Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, 01069 Dresden, Germany

Infrared spectroscopic ellipsometry (IRSE) is a well established method for optical and structural analysis of ultra-thin organic films. However, in-situ measurements in the infrared range are limited in aqueous environments due to the low penetration depth of infrared radiation in water. An in-situ cell which was developed at ISAS in Berlin allows IRSE measurements of ultra-thin organic films in aqueous environments by probing the interface region through the back side of a silicon wedge. The adsorption and release of proteins such as human serum albumin (HSA) on functional surfaces was studied using in-situ IRSE. A polyelectrolyte brush prepared from poly(acrylic acid) was used for the controlled adsorption and release of the protein. The thickness of this functional surface was about 5 nm. Adsorption and release was controlled by adjusting the pH of an aqueous solution and monitored by measuring the amid I and II bands of the protein.

DS 65.4 Fri 16:45 GER 38

Electronic Coupling and Charge Transfer between Metals and Epitaxial Organic Layers — •Roman Forker and Torsten Fritz — Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Max-Wien-Platz 1, 07743 Jena, Germany

When molecules are adsorbed on metals, several processes may occur, such as the “push-back-effect”, chemical interaction, the formation of interface states or even charge transfer (CT) between substrate and adsorbate. The strength and in part also the direction of such effects strongly depend on the molecule–metal combination and, additionally, on the specific structure(s) formed [1].

Here we investigate epitaxial mono- and multilayers of 3,4,9,10-perylene tetracarboxylic dianhydride (PTCDA) *in situ* on various metal surfaces by a variant of optical absorption spectroscopy. During film growth we observe pronounced changes in the spectra from the first monolayer (ML) to 2 ML and higher film thicknesses. While our results suggest the formation of radical cations in the *second* ML of PTCDA on Au(111) and Au(100) [2], the situation on Ag(111) is somewhat different. There, no clear indications for charged molecules were observed. On aluminum surfaces we conclude that the direction of the charge transfer is reversed, i.e., the spectral signature of PTCDA anions becomes visible. This gives rise to the interpretation that the electronic properties of the metal substrate, in particular the work function, determine the occurrence of charge transfer.

[1] S. Braun *et al.*, Adv. Mater. **21** (2009), 1450.
[2] R. Forker *et al.*, Org. Electron. **10** (2009), 1448.

DS 65.5 Fri 17:00 GER 38

Coupling effects in mixed pentacene/perfluoropentacene thin films studied by Raman and photoluminescence spectroscopy — •Falk Anger[1,2], J. Oriol Ossó[2], Ute Heinemeyer[1], Katharina Broch[1], Reinhard Scholz[3], Alexander Gerlach[1], and Frank Schreiber[1] — [1]Institut fur Angewandte Physik, 72076 Tübingen — [2]Matgas 2000 AIE, Campus de la UAB, 08193 Bellaterra, Spain — [3]Walter Schottky Institut, TU München, 85748 Garching

One of the crucial issues in complex organic electronic device structures is the coupling between different organic components. Perfluoropentacene (PFP) and pentacene (PEN) form a donor-acceptor system and are expected to promote intermixing due to their structural similarity, which also raises the chance of spectral coupling [1, 2]. Blended PEN/PFP thin films (ratio 4:1, 1:1, and 1:2) are investigated by photoluminescence (PL) and resonant Raman spectroscopy using different wavelengths covering the main absorption features of pure and mixed films. The results point towards substantial coupling between the two components. Contrary to pure PEN and PFP, the mixtures reveal at low temperatures a pronounced PL-peak at around 1.4 eV. Raman spectroscopy shows a dependence of the strength of PEN and PFP peaks on the mixing ratio and the excitation wavelength. While both PEN and PFP peaks are observed for excitation at 488 nm and 514 nm, at 633 nm the strength of vibrational modes depends drastically on the mixing ratio.
[1] A. Hinderhofer et al., J. Chem. Phys. **127**, 194705 (2007)
[2] K. Broch et al. *submitted*

DS 65.6 Fri 17:15 GER 38

In Situ Surface Enhanced Raman Spectroscopy of Ultra-Thin CuPc Films — •Michael Ludemann, Ovidiu D. Gordan, and Dietrich R. T. Zahn — Semiconductor Physics, Chemnitz University of Technology

In order to characterize the vibrational properties of copper phthalocyanine (CuPc) films, specially designed substrates with metallic nanostructures are applied. Illuminating these substrates with a laser that meets the plasmonic resonance of the nanostructure gives rise to a dramatic enhancement of the Raman scattered intensity. This effect offers the possibility to detect ultra-thin films, even sub-monolayer coverage of CuPc molecules within short exposure times. For ultra-thin films strong enhancement is also found when the laser does not meet the designed resonance condition of the nanostructures.

The samples are prepared by nanosphere lithography and CuPc is deposited by organic molecular beam deposition (OMBD) afterwards. The measurements are performed *in situ* under ultra-high vacuum (UHV) conditions. The focus of this work lies on the Raman intensity dependence on the excitation wavelength and the influence of the CuPc layer thickness.

DS 66: Organic Electronics and Photovoltaics O-I (jointly with CPP, HL, and O)

Time: Friday 11:15–12:30 Location: WIL B122

DS 66.1 Fri 11:15 WIL B122

Spin-resolved photoemission study of the interface of transition metal phthalocyanines (CuPc, FePc, CoPc) on Co(100) — •Anna Altenhof, Felix Schmitt, Michael Vogel, Stefan Lach, and Christiane Ziegler — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany

Because of their unpaired electrons the three transition metal phthalocyanines (MePcs) CuPc, FePc and CoPc are promising candidates for the development of molecular spintronics devices based on organic-inorganic hybrid systems. For these future devices the injection of spin-polarized electrons is necessary. Therefore the interface between a ferromagnetic contact material and the organic layer plays a major role for the performance of the device.

In this study the electronic and magnetic properties of the interface between the ferromagnetic cobalt and the metal-organic molecules CuPc, FePc and CoPc were investigated by different means of ultraviolet photoelectron spectroscopy (UPS). Ultrathin MePc films were grown in situ on Co(100) under ultra high vacuum conditions. These were studied by spin-integrated and spin-resolved UPS. Linear dichroism with unpolarized light was used to examine the valence band structure. These studies show that all molecules interact with the cobalt substrate so that new states occur which are located at the interface. They also show that the interaction of FePc and CoPc with the Co substrate is similar to each other but differs from the interaction of CuPc with Co.

DS 66.2 Fri 11:30 WIL B122

Smooth growth of organic semiconductor films on graphene for high efficiency electronics — •Gregor Hlawacek[1,2], Fawad S. Khokhar[1], Raoul van Gastel[1], Bene Poelsema[1], and Christian Teichert[2] — [1]Physics of Interfaces and Nanomaterials, MESA+ Institute for Nanotechnology, University of Twente, P.O. Box 217, NL-7500AE, Enschede, The Netherlands — [2]Institute for Physics, University of Leoben, Franz Josef Str. 18, A-8700 Leoben, Austria

High quality thin films of conjugated molecules with smooth interfaces are important to assist the advent of organic electronics. Here, we report on the layer-by-layer growth of the organic semiconductor molecule para-sexiphenyl on the transparent electrode material graphene. State of the art Low Energy Electron Microscopy, micro Low Energy Electron Diffraction and spot profile analysis techniques revealed the morphological and structural evolution of the thin film. Subtle difference in the molecular arrangement in comparison to graphite are confirmed by molecular dynamics simulations. Initial islands are found to have a meta stable structure that is characterized by flat lying molecules. With increasing coverage this structure changes into a herringbone arrangement similar to the $\{1\bar{1}\bar{1}\}$ bulk layer. The layer-by-layer growth of 6P on graphene proceeds by subsequent adding of $\{1\bar{1}\bar{1}\}$ layers.

DS 66.3 Fri 11:45 WIL B122

Elucidation of Partial Charge Transfer from the Methoxy Groups of Substituted Pyrene as Donor in Complexes with Tetracyanoquinodimethane — •Katerina Medjanik[1], Sergej Nepijko[1], Hans-Joachim Elmers[1], Gerd Schönhense[1], Peter Nagel[2], Stefan Schuppler[2], Dennis Chercka[3], Martin Baumgarten[3], and Klaus Müllen[3] — [1]Ins. für Physik, Johannes Gutenberg-Universität,Mainz — [2]Karlsruhe Institute of Technology, ANKA — [3]Max-Planck Ins. for Polymer Research, Mainz

Novel charge transfer (CT) compounds can be synthesized on the basis of large polycyclic aromatic hydrocarbons [1]. Microcrystals of the CT-compounds tetra- and hexamethoxypyrene/tetracyanoquinodimethane (TMP_x/HMP_x-TCNQ_y) in different stoichiometries $x:y=1:1$, $1:2$ and 2:1 were grown from solution via vapour diffusion. These crystallite fractions were studied by NEXAFS with particular emphasis on direct fingerprints of a charge transfer. Oxygen and nitrogen K-edge NEXAFS gives direct access to the unoccupied orbitals in the donor and acceptor, respectively. With increasing HMP content, a strongly rising O $1s$ pre-edge signal comes along with a substantial drop of N $1s$ resonance intensity. Charge is transferred from the π^*-orbital of the methoxy-group to the σ^*-orbitals b_{1g} and b_{2u} and - to a weaker extent - to the π^*-orbitals b_{3g} and a_u of the cyano-group of TCNQ, particularly strong for the 2:1 compound. Funded by DFG/TR49, Graduate School of Excellence MAINZ, Centre of Complex Materials COMATT.

[1] K. Medjanik *et al.*, Phys. Chem. Chem. Phys. **12**, 7184 (2010)

DS 66.4 Fri 12:00 WIL B122

Tuning the hole-injection barrier at the organic-metal interface with a strong organic acceptor — •Jens Niederhausen[1], Patrick Amsalem[1], Johannes Frisch[1], Andreas Wilke[1], Benjamin Bröker[1], Antje Vollmer[2], Ralph Rieger[3], Klaus Müllen[3], Jürgen P. Rabe[1], and Norbert Koch[1] — [1]Humboldt-Universität, Institut für Physik, Berlin, Germany — [2]Helmholtz Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [3]Max Planck Institut für Polymerforschung, Mainz, Germany

Ultraviolet photoelectron spectroscopy was used to investigate how pre-adsorption of the strong electron acceptor hexaazatriphenylene-hexanitrile (HATCN) on Ag(111) affects the energy level alignment of two subsequent deposited conjugated organic materials (COM). The tuning of the sample work function (WF) by precovering Ag(111) with HATCN monolayers oriented either in a lying or in a standing fashion is found to induce important variations in the hole injection barrier (HIB) of the COM. An interface dipole of similar magnitude is observed upon adsorption of both COM overlayers on a lying HATCN monolayer with low WF. It is related to the push-back effect, which occurs at specific adsorption sites of the molecules at very low coverage. For COM adsorbed on Ag(111) precovered with a standing HATCN monolayer with high WF, Fermi level pinning is identified in both cases, and appears as a fundamental limit to further HIB lowering. The observed behavior is reminiscent of the adsorption characteristics of COM on high WF conducting polymers substrates. This leads to a situation where the HIB decreases by up to 1.1 eV.

DS 66.5 Fri 12:15 WIL B122

Experimental and theoretical spin-resolved investigations of the electronic structure of open shell metal-phthalocyanines. — •Michael Vogel, Anna Altenhof, Felix Schmitt, Jens Sauther, Benedikt Baumann, Stefan Lach und Christiane Ziegler — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin- Schroedinger-Strasse 56, D-67663 Kaiserslautern Tel.: +49-631-205- 2855 Fax: +49-631-205-2854 E-mail: cz@physik.uni-kl.de

The valence band structure of different metal-phthalocyanines (MePcs) was investigated by comparison of gas-phase ultraviolet photoelectron spectra (UPS) and spin-resolved thin film UPS spectra with simulated spectra calculated using density functional theory (DFT). High resolution gas phase UPS spectra of cobalt phthalocyanine (CoPc) and iron phthalocyanine (FePc) show states which were unresolved in earlier studies. They were compared to Kohn-Sham eigenvalue spectra, derived from unrestricted DFT calculations. The composition of the molecular orbitals (MOs) just below the highest occupied molecular orbital (HOMO) was studied using UPS thin film spectra recorded at different excitation energies and thus different cross sections for s-, p-, and d-orbitals. Further the spin polarization of these MOs was derived from the DFT calculations and compared to thin film spin-resolved UPS spectra. The combination of these methods leads to a detailed image of the ground state electron system configuration with new insights into the behavior of the spin system.