

## Thin Films Division Fachverband Dünne Schichten (DS)

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### Overview of Invited Talks and Sessions

(Lecture rooms: H 2032 and H 2032; Posters: A and F)

#### Invited Talks

DS 3.1	Mon	15:00–15:30	H 2032	<b>Thin film growth studies using time-resolved X-ray scattering</b> — •STEFAN KOWARIK
DS 9.1	Tue	9:30–10:00	H 2032	<b>Electronic doping of crystalline silicon nanoparticles</b> — •RUI N. PEREIRA
DS 9.3	Tue	10:15–10:45	H 2032	<b>Impurity doping of Si nanocrystals studied by single-quantum-dot spectroscopy</b> — •JAN VALENTA, ILYA SYCHUGOV, JAN LINNROS, MINORU FUJII
DS 9.4	Tue	10:45–11:15	H 2032	<b>Active Silicon Nanovolume Doping: Failure and Alternatives</b> — •DIRK KÖNIG
DS 9.5	Tue	11:30–12:00	H 2032	<b>Doping issues in semiconductor field-effect transistors</b> — •JOACHIM KNOCH
DS 9.6	Tue	12:00–12:30	H 2032	<b>Probing composition and conductivity in 3D-structures and confined volumes.</b> — •WILFRIED VANDERVORST
DS 9.7	Tue	12:30–13:00	H 2032	<b>Silicon Nanowire Devices and Applications</b> — •THOMAS MIKOLAJICK, WALTER WEBER
DS 19.1	Wed	9:30–10:00	H 2032	<b>Ferromagnetic shape memory alloys: From ion-beam assisted synthesis to plasma-aided functionalization for biomedical applications</b> — ARIYAN ARABI-HASHEMI, UTA ALLENSTEIN, FLORIAN SZILLAT, ASTRID WEIDT, MAREIKE ZINK, •STEFAN G. MAYR
DS 19.2	Wed	10:00–10:30	H 2032	<b>Writing magnetic patterns using ion-beams</b> — •RANTEJ BALI
DS 20.1	Wed	9:30–10:00	H 0111	<b>Differential Optical Spectroscopy for Surface Science</b> — •PETER ZEP-PENFELD
DS 20.2	Wed	10:00–10:30	H 0111	<b><i>In situ</i> Raman monitoring of Potassium intercalation in Manganese Phthalocyanine</b> — •OVIDIU D. GORDAN, MICHAEL LUDEMANN, FRANZISKA LÜTTICH, DMYTRO SOLONENKO, PHILIPP SCHÄFER, DIETRICH R.T. ZAHN
DS 20.3	Wed	10:30–11:00	H 0111	<b>Infrared surface and interface studies - vibrational analysis and beyond</b> — •ANNEMARIE PUCCI
DS 20.4	Wed	11:00–11:30	H 0111	<b>Correlation of IR spectra with thin film structure at solid-water interfaces</b> — •KARSTEN HINRICHS
DS 20.5	Wed	11:30–12:00	H 0111	<b>In-situ characterization of electronic materials by optical second-harmonic generation</b> — •MICHAEL DOWNER
DS 34.1	Thu	9:30–10:00	H 2032	<b>Growth, properties and devices of gallium-oxide-based widegap semiconductors</b> — •SHIZUO FUJUTA
DS 34.6	Thu	11:30–12:00	H 2032	<b>BaSnO<sub>3</sub>; The next generation of transparent conducting oxide?</b> — •DAVID SCANLON
DS 37.1	Thu	15:00–15:30	H 2032	<b>Optical properties and band structure of transparent semiconducting oxides</b> — •RÜDIGER GOLDHAHN

DS 37.6	Thu	16:45–17:15	H 2032	<b>Thermodynamic stability and electronic structure of TCO surfaces: A computational approach</b> — •KARSTEN ALBE, PETER AGOSTON, MANUEL DIEHM, ARNO FEY
DS 37.10	Thu	18:00–18:30	H 2032	<b>Synthesis and Stability of Indium (III) Oxide Polymorphs</b> — •ALEKSANDER GURLO, MAGED BEKHEET
DS 40.1	Fri	9:30–10:00	H 2032	<b>From 2D to 1D: Honeycomb crystals and their nanoribbons</b> — •FRIEDHELM BECHSTEDT

### Invited talks of the joint symposium SYDW

See SYDW for the full program of the symposium.

SYDW 1.1	Mon	9:30–10:00	H 0105	<b>Domain walls: from conductive paths to technology roadmaps</b> — •GUSTAU CATALAN
SYDW 1.2	Mon	10:00–10:30	H 0105	<b>Domain walls and oxygen vacancies - towards reversible control of domain wall conductance</b> — •PATRYCJA PARUCH
SYDW 1.3	Mon	10:30–11:00	H 0105	<b>Novel mechanisms of domain-wall formation</b> — •ANDRES CANO
SYDW 1.4	Mon	11:30–12:00	H 0105	<b>Novel materials at domain walls</b> — •BEATRIZ NOHEDA
SYDW 1.5	Mon	12:00–12:30	H 0105	<b>Controlling and mapping domain wall behaviour in ferroelectrics</b> — •JOHN MARTIN GREGG, JONATHAN WHYTE, RAYMOND MCQUAID, MICHAEL CAMPBELL, AMIT KUMAR, ROGER WHATMORE

### Invited talks of the joint symposium SYMM

See SYMM for the full program of the symposium.

SYMM 1.1	Thu	9:30–10:15	H 0105	<b>From MAX to MXene - From 3D to 2D</b> — •MICHEL BARSOUM
SYMM 1.2	Thu	10:15–10:45	H 0105	<b>Structure evolution during low temperature growth of nanolaminate thin films</b> — •J.M. SCHNEIDER, L. SHANG, H. BOLVARDI, Y. JIANG, A. AL GABAN, D. MUSIC, M. TO BABEN
SYMM 1.3	Thu	11:00–11:30	H 0105	<b>Autonomous healing of crack damage in MAX phase ceramics</b> — •WILLEM G. SLOOF
SYMM 1.4	Thu	11:30–12:00	H 0105	<b>Magnetic MAX phases from first principles and thin film synthesis</b> — •JOHANNA ROSEN
SYMM 1.5	Thu	12:00–12:30	H 0105	<b>Weak Field Magneto-Transport Properties of Mn+1AXn Phases</b> — •THIERRY OUISSE, LU SHI, BENOIT HACKENS, BENJAMIN PIOT, DIDIER CHAUSSENDE

### Sessions

DS 1.1–1.14	Mon	9:30–13:00	H 2032	<b>Organic Electronics and Photovoltaics</b>
DS 2.1–2.13	Mon	9:30–13:00	H 0111	<b>Thin Film Characterisation I: Structure Analysis and Composition</b>
DS 3.1–3.15	Mon	15:00–19:30	H 2032	<b>Organic Thin Films</b>
DS 4.1–4.13	Mon	15:00–18:30	H 0111	<b>Thin Film Characterisation II: Structure Analysis and Composition</b>
DS 5.1–5.9	Mon	15:00–17:45	A 053	<b>Transport: Topological Insulators 1 (joint session with DS, HL, MA, O)</b>
DS 6.1–6.7	Mon	15:00–16:45	EW 202	<b>Organic photovoltaics and electronics - mostly cell design (jointly with CPP,DS)</b>
DS 7.1–7.8	Mon	17:00–19:00	EW 202	<b>Organic photovoltaics and electronics - mostly properties of the absorber (jointly with CPP,DS)</b>
DS 8.1–8.5	Mon	18:45–20:00	H 0111	<b>Application of Thin Films</b>
DS 9.1–9.7	Tue	9:30–13:00	H 2032	<b>Focused Session: Doped Si nanostructures (joint session with HL)</b>
DS 10.1–10.6	Tue	9:30–11:00	H 0111	<b>Thermoelectric materials</b>
DS 11.1–11.12	Tue	9:30–13:00	H 3005	<b>Transport: Topological Insulators 2 (joint session with DS, HL, MA, O)</b>
DS 12.1–12.10	Tue	9:30–12:15	A 053	<b>Transport: Graphene (joint session with DS, DY, HL, MA, O)</b>

DS 13.1–13.9	Tue	10:00–12:30	C 243	<b>Interfaces and Thin Films I (joint session with CPP)</b>
DS 14.1–14.11	Tue	10:30–13:15	MA 043	<b>Plasmonics and nanooptics: Structure, fabrication and characterization (joint session with O)</b>
DS 15.1–15.4	Tue	11:15–12:15	H 0111	<b>High-k and Low-k Dielectrics (joint session with DF)</b>
DS 16.1–16.3	Tue	12:15–13:00	H 0111	<b>Atomic Layer Deposition</b>
DS 17.1–17.8	Tue	14:00–16:00	H 0110	<b>Transport: Topological Insulators 3 (joint session with DS, HL, MA, O)</b>
DS 18.1–18.7	Tue	14:00–16:00	C 243	<b>Interfaces and Thin Films II (joint session with CPP)</b>
DS 19.1–19.9	Wed	9:30–12:15	H 2032	<b>Ion and electron beam induced processes</b>
DS 20.1–20.9	Wed	9:30–13:00	H 0111	<b>Focussed Session: In-situ optical spectroscopy</b>
DS 21.1–21.13	Wed	9:30–13:00	EB 107	<b>Multiferroics I (joint session with DF)</b>
DS 22.1–22.13	Wed	9:30–13:00	C 243	<b>Interfaces and Thin Films III (joint session with CPP)</b>
DS 23.1–23.8	Wed	9:30–11:30	ER 270	<b>Topological insulators: Theory (HL with DS/MA/O/TT)</b>
DS 24.1–24.9	Wed	10:30–12:45	MA 042	<b>Metal substrates: Structure, epitaxy and growth (joint session with O)</b>
DS 25.1–25.1	Wed	13:15–13:45	HE 101	<b>GAEDE-PREIS 2015</b>
DS 26.1–26.15	Wed	15:00–19:00	H 2032	<b>Layer Properties: Electrical, Optical, and Mechanical Properties</b>
DS 27.1–27.5	Wed	15:00–16:15	H 0111	<b>Micro- and Nanopatterning</b>
DS 28.1–28.13	Wed	15:00–18:50	EB 107	<b>Multiferroics II (joint session with DF)</b>
DS 29.1–29.13	Wed	15:00–18:15	MA 042	<b>Oxide and insulator surface: Structure, epitaxy and growth (joint session with O)</b>
DS 30.1–30.6	Wed	15:00–16:30	ER 270	<b>Topological insulators: Structure and electronic structure (HL with DS/MA/O/TT)</b>
DS 31.1–31.5	Wed	11:45–13:00	ER 270	<b>Topological insulators: Transport (HL with DS/MA/O/TT)</b>
DS 32.1–32.9	Wed	16:30–18:45	H 0111	<b>Spins in organics</b>
DS 33	Wed	19:00–20:00	H 0111	<b>Mitgliederversammlung</b>
DS 34.1–34.9	Thu	9:30–12:45	H 2032	<b>Focussed Session: Oxide semiconductors I (joint session with HL)</b>
DS 35.1–35.13	Thu	9:30–13:00	H 0111	<b>Graphen</b>
DS 36.1–36.110	Thu	9:30–12:00	Poster A	<b>Poster Session I</b>
DS 37.1–37.12	Thu	15:00–19:00	H 2032	<b>Focussed Session: Oxide semiconductors II (joint session with HL)</b>
DS 38.1–38.14	Thu	15:00–18:45	H 0111	<b>Phase change/ resistive switching</b>
DS 39.1–39.35	Thu	16:00–18:30	Poster F	<b>Poster Session II</b>
DS 40.1–40.13	Fri	9:30–13:15	H 2032	<b>Metallic nanowires on the atomic scale (joint session with O)</b>
DS 41.1–41.9	Fri	10:30–12:45	MA 042	<b>Semiconductor substrates: structure, epitaxy and growth (joint session with O)</b>

## Annual General Meeting of the Thin Films Division

Wednesday 19:00–20:00 H 0111

- Bericht
- Wahl
- Verschiedenes

## DS 1: Organic Electronics and Photovoltaics

Time: Monday 9:30–13:00

Location: H 2032

DS 1.1 Mon 9:30 H 2032

**Metal-organic interfaces: from molecular self-assembly to electronic transport through ultrathin functional monolayers** — ●FLORIAN VON WROCHEM — Sony Deutschland GmbH, Stuttgart

The continuous development of organic electronic devices, combined with the advances in spectroscopy and electrical characterization, dramatically extended our understanding of the physical and chemical processes occurring at metal/organic interfaces. Here, an overview of experimental and theoretical efforts aiming towards the selective modification of interfaces is given. Various anchor groups designed to connect organic materials to metal electrodes are presented (e.g. thiolates, dithiocarbamates, mercuryls and stannyls) and their potential for optimizing the charge injection as well as the morphological, chemical, and electronic nature at the contact is illustrated. On this basis, functional molecular building blocks are grafted to the surface by self-assembly, providing rectification, switching, or chemical selectivity. Once the key parameters for interface formation and fabrication are under control, a huge number of potential applications emerge, ranging from optoelectronics to organic printed circuits. As one example, electrostatic dipole layers for tuning the injection barrier between metals and organic semiconductors are presented, which may find applications in organic light emitting diodes, field effect transistors, and solar cells. When further reducing device dimensions towards the nanoscale, organic monolayers might foster the development of molecular electronics, as illustrated here by highly robust metal-molecule-metal junctions based on FeII-terpyridine molecular wires or by optically switchable protein layers.

DS 1.2 Mon 9:45 H 2032

**Grain boundaries in CuInSe<sub>2</sub> and CuGaSe<sub>2</sub> solar cell materials: New insights from hybrid functional calculations** — HOSSEIN MIRHOSSEINI, ●JANOS KISS, and CLAUDIA FELSER — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany.

Polycrystalline thin-film solar cells based on CuIn<sub>1-x</sub>Ga<sub>x</sub>Se (CIGSe) are an economically viable alternative to the Si based technology. During the deposition of the polycrystalline light absorber layer grain boundaries (GBs) are formed in the CIGSe material, and the effect of these GBs upon the structural and electronic properties of the thin-film solar cells are not yet fully understood. Different atomic structures of the GBs in CIGSe have been reported experimentally. The outcomes of the theoretical calculations, however, are diverse and sometimes inconsistent due to the limitation of the functionals, which fail to properly describe the band gap of thin film solar cell materials. Employing a state of the art method using the HSE hybrid functional, which is known to predict the atomic and electronic structure of solar cell materials rather well, we have looked at the behavior and properties of GBs in CuInSe<sub>2</sub> and CuGaSe<sub>2</sub>. In the framework of our investigation, we have studied the atomic relaxation and electronic structure of various GBs and also considered the effect of the impurity segregation close to the GBs.

DS 1.3 Mon 10:00 H 2032

**Relationship between the chemical structure of low band gap polymers and self-organization properties** — ●MILUTIN IVANOVIC<sup>1</sup>, U MUT AYGÜL<sup>1</sup>, ULF DETTINGER<sup>1</sup>, AURELIEN TOURNEBIZE<sup>1</sup>, DAVID BATCHELOR<sup>2</sup>, STEFAN MANGOLD<sup>2</sup>, HEIKO PEISERT<sup>1</sup>, and THOMAS CHASSÉ<sup>1</sup> — <sup>1</sup>) University of Tuebingen, Institute of Physical and Theoretical Chemistry, 72076 Tuebingen, Germany — <sup>2</sup>Karlsruhe Institute of Technology (KIT), ANKA Synchrotron Radiation Facility, 76344 Eggenstein-Leopoldshafen, Germany

A possible approach to improve the efficiency of donor-acceptor based bulk heterojunction (BHJ) of OPV cells is the use of low band gap (LBG) polymers as donor materials. Basic electronic processes in OPV cells are however strongly influenced by the morphology and the ability for self-organization of the polymers in the thin-films. We utilize NEXAFS spectroscopy to study the molecular orientation of novel LBG polymers (PCPDTTBTT, PCPDTTBT and PCPDTzTBT) for OPVs in thin films. The influence of post-processing annealing as well as of blending with Phenyl-C61-butyrac acid methyl ester (PCBM) on the orientation is investigated. The studied LBG polymers are characterized by a variation of (hexyl-) thiophene groups compared to related LBG polymers recently studied.[1,2]. Acknowledgments: This

research is funded by the European Union Seventh Framework Programme (FP7/2011 under grant agreement ESTABLIS n° 290022). References: 1.\*Aygül, U. et al. J. Phys. Chem. C 2012, 116, 4870-4874. 2.\*Aygül, U. et al. Sol. Energ. Mat. Sol. Cells 2014, 128, 119-125.

DS 1.4 Mon 10:15 H 2032

**Organic ambipolar field-effect transistors: *In situ* electrical investigation of MnPC-OFETs** — ●FRANZISKA LÜTTICH, OVIDIU D. GORDAN, and DIETRICH R. T. ZAHN — Semiconductor Physics, Technische Universität Chemnitz, Chemnitz, Germany

On the way to low-cost and flexible applications organic semiconducting materials are promising. Devices like organic light-emitting diodes, organic solar cells, and organic field-effect transistors (OFETs) can be produced e.g. on flexible and elastic substrates and with chemical variation of side groups or substitution of metal centers their properties like optical absorption and charge carrier mobilities can be influenced.

Here we present a temperature dependent study on Manganese Phthalocyanine (MnPc)-OFETs, which reveal an ambipolar behaviour. In order to investigate the electrical properties of MnPc we used OFET "end-of-line" substrates from Fraunhofer IPMS with a 100 nm thick thermal silicon dioxide layer as dielectric. The investigated bottom-contact OFETs were fabricated under high vacuum conditions ( $p < 4 \cdot 10^{-7}$  mbar) by evaporating MnPc on top of the pre-structured substrates. The electrical DC characteristics were measured *in situ* as a function of temperature. This procedure enables us to determine the activation energies for the hole and electron transport. The influence of ambient atmosphere was also investigated and revealed strong impact on the electrical performance. The topography was determined using an Atomic Force Microscope (AFM).

DS 1.5 Mon 10:30 H 2032

**Photoelectron spectroscopy studies on efficient air-stable molecular n-dopants** — ●MARTIN SCHWARZE<sup>1</sup>, MAX L. TIETZE<sup>1</sup>, PAUL PAHNER<sup>1</sup>, BEN NAAB<sup>2</sup>, ZHENAN BAO<sup>2</sup>, BJÖRN LÜSSEM<sup>1</sup>, DANIEL KASEMANN<sup>1</sup>, and KARL LEO<sup>1</sup> — <sup>1</sup>Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany — <sup>2</sup>Department of Chemical Engineering, Stanford University, Stanford, California 94305, United States

Understanding the working mechanism of electrical doping in organic semiconductors is essential for the optimization of organic semiconductor devices such as organic light emitting diodes or organic solar cells. A defined doping concentration allows for the control of the Fermi-level position as well as the adjustment of the conductivity of transport layers. In comparison to molecular p-doping of organic semiconductors, n-doping creates the additional problem of air instability. To successfully transfer an electron to the lowest unoccupied molecular orbital (LUMO) of the matrix material, dopants exhibiting shallow highest molecular orbitals (HOMO) are necessary, rendering them prone to reactions with e.g. oxygen. In this study, three different types of n-dopants are compared: air stable cationic DMBI dopants, halogen-free DMBI dimers, and the established but air sensitive Cr<sub>2</sub>(hpp)<sub>4</sub>. Fermi-level shift and conductivity of co-evaporated Bis-Hf1-NTCDI layers at different doping concentrations as well as stability during air exposure are investigated by UPS and electrical measurements.

DS 1.6 Mon 10:45 H 2032

**Mode-selective vibrational manipulation of charge transport in  $\pi$ -conjugated molecular materials** — ●ROBERT LOVRINCIC<sup>1,2</sup>, ARTEM A. BAKULIN<sup>3,4</sup>, YU XI<sup>1</sup>, OLEG SELIG<sup>3</sup>, HUIB J. BAKKER<sup>3</sup>, YVES L. A. REZUS<sup>3</sup>, PABITRA K. NAYAK<sup>1</sup>, ALEXANDR FONARI<sup>5</sup>, VEACESLAV COROPCEANU<sup>5</sup>, JEAN-LUC BREDAS<sup>5,6</sup>, and DAVID CAHEN<sup>1</sup> — <sup>1</sup>Department of Materials & Interfaces, Weizmann Institute of Science, Israel — <sup>2</sup>IHF, TU Braunschweig & Innovationlab, Germany — <sup>3</sup>FOM Institute AMOLF, The Netherlands — <sup>4</sup>Cavendish Laboratory, University of Cambridge, UK — <sup>5</sup>School of Chemistry and Biochemistry, Georgia Institute of Technology, USA — <sup>6</sup>Solar & Photovoltaics Center, King Abdullah University, Saudi Arabia

The soft character of organic materials leads to strong coupling between molecular nuclear and electronic dynamics. This coupling opens the way to control charge transport in organic electronic devices by directing molecular vibrational motions. However, despite encouraging

theoretical predictions, experimental realization of such control has remained elusive. Here we demonstrate experimentally that photoconductivity in a model organic optoelectronic device can be controlled by the selective excitation of molecular vibrations. Using an ultrafast infrared laser source to create a coherent superposition of vibrational motions in a pentacene/C<sub>60</sub> photoresistor, we observe that excitation of certain modes in the 1500–1700 cm<sup>-1</sup> region leads to photocurrent enhancement. The effect depends on the nature of the vibration and its mode-specific character can be well described by the vibrational modulation of intermolecular electronic couplings.

DS 1.7 Mon 11:00 H 2032

**Investigation of charge transfer in organic semiconductors using infrared spectroscopy** — ●TOBIAS GLASER<sup>1,2</sup>, SEBASTIAN BECK<sup>1,2</sup>, and ANNEMARIE PUCCI<sup>1,2,3</sup> — <sup>1</sup>Universität Heidelberg, Kirchhoff-Institut für Physik — <sup>2</sup>InnovationLab GmbH, 69115 Heidelberg — <sup>3</sup>Universität Heidelberg, Centre for Advanced Materials

Charge transfer in organic semiconductors is used in various ways to increase the performance of organic electronic devices. For example electrochemical doping is used to increase the conductivity in charge transport layers. Additionally, charge injection layers are used to decrease injection barriers between electrodes and organic transport layers. In both cases molecular charge transfer plays an important role, but the basic mechanisms are still subject of heated debate. Due to strong relaxation effects upon molecular charging, infrared (IR) spectroscopy is very well suited to investigate charge transfer in organic semiconductors. Neutral and charged molecules can be distinguished by their different specific vibrational features in spectra of doped layers as well as for interfaces. In this study we investigated charge transfer in thin layers of commonly known transport materials such as 4,4'-bis(N-carbazolyl)-1,1'-biphenyl (CBP) doped with inorganic and organic dopants such as MoO<sub>3</sub> or F4TCNQ and at interfaces of organic semiconductors. By quantitative analysis of the experimental spectra the doping efficiency and the degree of charge transfer can be determined for the doped layers. Whereas, for interfacial charge transfer, the formation of a space charge region can be mapped. Financial support by BMBF (project MESOMERIE) is gratefully acknowledged.

DS 1.8 Mon 11:15 H 2032

**Structure and Photovoltaic Performance of Chiral Anilino Squaraines** — ●MANUELA SCHIEK<sup>1</sup>, MATTHIAS SCHULZ<sup>2</sup>, STEFANIE BRÜCK<sup>1</sup>, MARTIN SILIES<sup>3</sup>, HEIKO KOLLMANN<sup>3</sup>, CHRISTOPH LIENAU<sup>3</sup>, ARNE LÜTZEN<sup>2</sup>, and JÜRGEN PARISI<sup>1</sup> — <sup>1</sup>Energy and Semiconductor Research Laboratory, University of Oldenburg, Germany — <sup>2</sup>Kekule-Institute for Organic Chemistry and Biochemistry, University of Bonn, Germany — <sup>3</sup>Ultrafast Nano-Optics, University of Oldenburg, Germany

Small molecular semiconductors such as squaraines are advantageous compared to polymeric materials because they allow a more direct control of the structure on the molecular level and consequently solid state properties. Especially the implementation of chiral side chains introduces new functionalities such as circular dichroism. Different 1,3-bis(N,N-substituted-2,6-dihydroxy-anilino)squaraines with varying terminal N-substitution, in some cases including a stereogenic center, are investigated as single crystals, in thin films and blended with a fullerene acceptor as active layer in bulk heterojunction organic solar cells.

DS 1.9 Mon 11:30 H 2032

**Charge separation and C<sub>60</sub> crystallinity in bulk heterojunction solar cells: the decisive role of device architecture** — ●FELIX SCHELL<sup>1,2</sup>, MICHAEL SCHERER<sup>1,3</sup>, DIANA NANOVA<sup>1,2,3</sup>, ANNE KATRIN KAST<sup>2,4</sup>, WOLFGANG KOWALSKY<sup>1,2,3</sup>, RASMUS R. SCHRÖDER<sup>1,4,5</sup>, and ROBERT LOVRINCIC<sup>1,3</sup> — <sup>1</sup>InnovationLab GmbH, Heidelberg — <sup>2</sup>Kirchhoff-Institute for Physics, Heidelberg University — <sup>3</sup>Institute for High-Frequency Technology, TU Braunschweig — <sup>4</sup>CellNetworks, BioQuant, Heidelberg University — <sup>5</sup>Center for Advanced Materials, Heidelberg University

The crucial influence of C<sub>60</sub> crystallinity on the charge separation in organic solar cells (OSC) has been realized very recently. Here, we show the importance of the device architecture on C<sub>60</sub> crystallisation in the bulk-heterojunction (BHJ). Active layer morphology of small molecule BHJ OSC and its influence on device performance are studied by means of energy-filtered transmission electron microscopy (EFTEM) and electrical characterization. The influence of substrate temperature during deposition and of pure sublayers is assessed. BHJs fabricated at room temperature are found to be finely mixed and amorphous, whereas the

corresponding films deposited onto heated substrates show pronounced phase separation. Despite these clear morphological changes, substrate heating does not increase efficiency of OSCs in a non-inverted device architecture. Improvements found in literature for inverted cells can be attributed to stronger acceptor crystallization, present, if deposited onto a pure C<sub>60</sub> layer but not with an F<sub>4</sub>ZnPc substrate, leading to more efficient exciton dissociation.

DS 1.10 Mon 11:45 H 2032

**Influence of DMSO-treatment on morphology, composition and performance of PEDOT:PSS layers in organic photovoltaic cells** — SIDHANT BOM, ●TORSTEN BALSTER, MARLIS ORTEL, and VEIT WAGNER — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

PEDOT:PSS layers in organic solar cells are used as hole transport (HTL) and electron blocking layers. Therefore the morphology and composition of the layer and the interface have a great influence on the performance of organic photovoltaic devices.

Additional post-deposition treatment of the PEDOT:PSS layers (HTL) in P3HT/PCBM solar cells were studied in this work. For this purpose, pristine PEDOT:PSS layers were spin coated with dimethyl sulfoxide (DMSO) after annealing. Pristine and treated layers were characterized by means of electrical characterization, atomic force microscopy (AFM) and x-ray photoelectron spectroscopy (XPS).

The additional post-deposition DMSO treatment induces an increase in power conversion efficiency by more than 50%. In addition, the open circuit voltage and the short-circuit current were enhanced, whereas the fill factor remained constant. This behavior is explained by modification of the PEDOT:PSS-semiconductor interface. On the one hand smoothening of the interface by reduction of large PSS particles visible in AFM occurs. On the other hand XPS data show a reduction of PSS-sulphur species. Less PSS at the interface should improve the charge carrier injection properties, as observed experimentally.

DS 1.11 Mon 12:00 H 2032

**Charge transfer, optical and transport properties in pure organic heterostructures** — ●LIEBING SIMON, HAHN TORSTEN, and KORTUS JENS — Institute of Theoretical Physics, TU Bergakademie Freiberg, Leipziger Strasse 23, 09599 Freiberg

We will present theoretical investigation on pure charge transfer materials within the density functional theory framework (DFT). Starting from the recently fabricated picene-F<sub>4</sub>TCNQ [1] we explore the electronic and optical properties of novel representatives of this new class of materials. These representatives are formed of polycyclic hydrocarbons and TCNQ derivatives and we compare our results with experimental spectroscopic data.

The picene-F<sub>4</sub>TCNQ system shown pronounced diode transistor behavior [2]. By means of DFT/NEGF (non equilibrium green function formalism) [3,4] we obtain the IV-characteristics of selected model devices for these systems. The formation of hybrid orbitals together with intrinsic charge transfer seems to be the origin of the novel electronic and transport properties [5].

[1] Mahns, B. et. al. *Crystal Growth & Design* (2014). [2] Hahn T., Liebing S., and Kortus J., *Nanoscale* 6, 14508 (2014). [3] Pederson, M. et. al. *Phys. Status Solidi b* 217, 197. (2000) [4] Enkovaara, J. et al. *Journal of Physics: Condensed Matter* 22, 253202 (2010). [5] Lindner S. et. al. *Phys. Rev. Lett.* 109, 027601 (2012).

DS 1.12 Mon 12:15 H 2032

**Single molecule circuits with N-heterocyclic carbene linkers** — ●HECTOR VAZQUEZ — Inst. of Physics, Academy of Sciences of the Czech Rep., CZ

In single molecule circuits, where an electrical current flows through a molecule, conducting molecules often have terminal linker groups which bind to the metallic electrodes [1]. These chemical link groups strongly influence the conducting properties, often acting as bottlenecks for electron transmission and result in low-transmission resonances localized at the interface. Therefore, identifying adequate chemical linker groups is essential for achieving ideal mechanical and conducting properties in molecular circuits.

Recently, SAMs of N-heterocyclic carbenes on gold were shown to have very high thermal and oxidative stability [2], making N-heterocyclic carbenes potentially very useful linkers for single molecule transport. In this talk, I will present results from first-principles simulations based on DFT-NEGF for the electronic and conducting properties of carbene-terminated molecules. I will show results for the adsorption properties of N-heterocyclic carbenes on gold. I will also

present transmission calculations of carbene-terminated molecules and discuss these results in the context of other metal-molecule links with Au-C bonds [3].

[1] F. Schwarz and E. Loertscher, *J. Phys. Condens. Matter* 26 474201 (2014).

[2] C.M. Crudden et al., *Nature Chemistry* 6 409 (2014).

[3] W. Chen et al., *J. Am. Chem. Soc.* 133 17160 (2011).

DS 1.13 Mon 12:30 H 2032

**Charge and spin transfer materials for molecular electronic and spintronic applications** — ●TORSTEN HAHN, SIMON LIEBING, and JENS KORTUS — TU Freiberg, Institut für Theoretische Physik, Leipziger Str. 23, 09599 Freiberg

The combination of different functionalized metal phthalocyanines was found to lead to novel charge- and spin transfer compounds [1,2]. The recently synthesized picene / F4TCNQ charge transfer salt [3] also shows promising physical properties and the theoretical modeling predicts the material to act as a molecular diode with high rectification ratio [4]. Based on density-functional theory calculations we show that in case of the metal phthalocyanines as well as for the picene / F4TCNQ system hybrid states formed by the donor / acceptor system are playing the key role to determine the spectroscopic and quantum transport properties. We further conclude that the tuning of quantum transport properties through hybrid states is a general concept which opens a new route towards functional materials for molecular electronics.

[1] R. Friedrich et al., *Phys. Rev. B* 87, 115423 (2013).

[2] R. Friedrich, B. Kersting, and J. Kortus, *Phys. Rev. B* 88, 155327 (2013).

[3] Mahns, B. et. al., *Cryst. Growth and Design* 14, 1338-1346 (2014).

[4] T. Hahn, S. Liebing, and J. Kortus, *Nanoscale* 6, 14508 (2014).

DS 1.14 Mon 12:45 H 2032

**Device-like calcium corrosion test for ultra-barrier materials** — ●FREDERIK NEHM<sup>1</sup>, HANNES KLUMBIES<sup>1</sup>, JOHN FAHLTEICH<sup>2</sup>, FELIX DOLLINGER<sup>1</sup>, KARL LEO<sup>1</sup>, and LARS MÜLLER-MESKAMP<sup>1</sup> — <sup>1</sup>Institut für Angewandte Photophysik, TU Dresden, Dresden, Deutschland — <sup>2</sup>Fraunhofer FEP, Dresden, Deutschland

The continuous progress of organic electronics demands for flexible moisture barriers with water vapor transmission rates (WVTRs) below  $10^{-4} \frac{g(H_2O)}{m^2d}$  and quick, reliable measurement techniques for such WVTRs. The electrical calcium corrosion test is an extremely sensitive technique used widely in research groups. However, setups differ strongly as do their accuracy and background rates. We report on common issues and show how we manage them in our setup. Barrier corrosion because of direct water condensation on its surface is prevented by a glued-on PET film and Ca-induced stress is mitigated by organic decoupling layers. We demonstrate the effectiveness of our approach with studies on sputtered Zinc-Tin-Oxide and atomic layer deposited (ALD) alumina moisture barriers in different aging climates. Single barriers show a linear WVTR increase with rising absolute humidity at given temperature. Below 40°C, this is even valid independent of temperature. A divergence at higher temperatures probably originates from the actual barrier layer, since this effect cannot be observed for the pure substrate. Also, nanolaminates using ALD alumina, titania and alkoxide, and multilayer barriers with polymer interlayers with WVTRs down to at least  $2 \cdot 10^{-5} \frac{g(H_2O)}{m^2d}$  in 38°C, 90% relative humidity environments are investigated.

## DS 2: Thin Film Characterisation I: Structure Analysis and Composition

Time: Monday 9:30–13:00

Location: H 0111

DS 2.1 Mon 9:30 H 0111

**Probing the oxygen deficit in YBCO thin films with a positron beam** — ●MARKUS REINER<sup>1</sup>, THOMAS GIGL<sup>1</sup>, RAINER JANY<sup>2</sup>, GERMAN HAMMERL<sup>2</sup>, and CHRISTOPH HUGENSCHMIDT<sup>1</sup> — <sup>1</sup>Heinz Maier-Leibnitz Zentrum (MLZ) and Physik Department E21, Technische Universität München, Lichtenbergstraße 1, 85748 Garching, Germany — <sup>2</sup>Experimentalphysik VI, Elektronische Korrelationen und Magnetismus, Institut für Physik, Universität Augsburg, D-86135 Augsburg, Germany

High quality single-crystalline  $YBa_2Cu_3O_{7-\delta}$  (YBCO) thin films were grown epitaxially by pulsed laser deposition. After tempering under different conditions they were characterized by various techniques such as electrical conductivity measurements, X-ray diffraction and electron microscopy. The highly intense reactor based positron beam NEPOMUC was applied for Doppler Broadening Spectroscopy (DBS). A strong correlation between the Doppler broadening of the positron annihilation line and the oxygen deficit was found and its origin was examined by ab-initio calculations. This correlation enabled the study of the kinetics of oxygen out diffusion from the YBCO thin film during in-situ measurements at temperatures up to 673 K. Furthermore, the high spatial resolution of the positron beam (up to around 0.3 mm) was used for mapping the oxygen deficit and hence, to probe the spatial homogeneity of the oxygen distribution in the examined YBCO films. Financial support within the Project No. 05KIOWOB by the BMBF is gratefully acknowledged.

DS 2.2 Mon 9:45 H 0111

**Reference-free, depth dependent characterization of nanoscale materials by combined X-ray reflectivity and grazing incidence X-ray fluorescence analysis** — ●PHILIPP HÖNICKE<sup>1</sup>, MATTHIAS MÜLLER<sup>1</sup>, BLANKA DETLEFS<sup>2</sup>, CLAUDIA FLEISCHMANN<sup>3</sup>, and BURKHARD BECKHOFF<sup>1</sup> — <sup>1</sup>Physikalisch-Technische Bundesanstalt (PTB), Abbestr. 2-12, 10587 Berlin, Germany — <sup>2</sup>CEA-LETI, 17 rue des Martyrs, 38054 Grenoble, France — <sup>3</sup>imec, Kapeldreef 75, BE-3001 Leuven, Belgium

The accurate in-depth characterization of nanoscaled systems is an essential topic for todays developments in many fields of materials research, especially in the semiconductor related ones.

Synchrotron-based Grazing Incidence X-ray Fluorescence (GIXRF) analysis in combination with X-Ray Reflectometry (XRR) provides ad-

ditional access to the optical properties of the sample allowing for an improved characterization reliability of GIXRF [1].

Employing the radiometrically calibrated instrumentation at the laboratory of the Physikalisch-Technische Bundesanstalt at the BESSY II synchrotron radiation facility, the combination of XRR and GIXRF allows for a more reliable reference-free quantitative in-depth analysis [1,2,3].

[1] P. Hönicke et al., *JAAS* 27, (2012), 1432.

[2] M. Müller et al., *Materials* 7(4), (2014), 3147.

[3] P. Hönicke et al., *Solid State Phenomena* 195, (2013), 274.

DS 2.3 Mon 10:00 H 0111

**Model-based thin film characterization by confocal and total interference contrast microscopy** — ●MATTHIAS VAUPEL — Carl Zeiss Microscopy GmbH, 37081 Göttingen, Germany

It is investigated how optical models improve the accuracy of thickness measurements of a layer stack. Starting with an optical model for ellipsometry on thin films, we derive optical models for total interference contrast (TIC) and confocal microscopy. The confocal model of incoherent superposition of reflections is tested in case of one thin transparent passivation layer on an electronic chip. The model parameters are obtained by a cross-section with FIB-SEM. Thickness and refractive index of the layer are obtained from the confocal measurement by means of the optical model. TIC measures the phase difference of two adjacent spots on a sample. Consequently the phase difference is independent of vertical sample vibration. This allows for pm-vertical resolution of film thickness. As an example the TIC-optical model is applied to obtain the thickness profile of mono- and bilayers of graphene[1] out of the phase profile measured by means of a micrograph recorded in less than 100 ms. The advantages and restrictions of TIC in comparison to AFM, imaging ellipsometry, Mirau-type white light interferometry are discussed.

[1] M. Vaupel et al., Topography, complex refractive index, and conductivity of graphene layers measured by correlation of optical interference contrast, atomic force, and back scattered electron microscopy, *J.Appl.Phys.* 114, 183107 (2013)

DS 2.4 Mon 10:15 H 0111

**Atom probe tomography study of the p-n junction in CIGS thin-film solar cells** — ●ANNA KOPREK<sup>1</sup>, OANA COJOCARU-MIRÉDIN<sup>1</sup>, CHRISTOPH FREYSOLDT<sup>1</sup>, ROLAND WUERZ<sup>2</sup>, and DIERK

RAABE<sup>1</sup> — <sup>1</sup>Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, 40237 Düsseldorf, Germany. — <sup>2</sup>Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg, Industriestrasse 6, 70565 Stuttgart, Germany.

Solar cells based on Cu(In,Ga)Se<sub>2</sub> (CIGS) are one of the most promising among thin film technology. Despite high efficiency over 20%, the cells are still far below the theoretical limit of ~ 30%. Recent studies indicate that the Cd, S, and Cu that interdiffuse across the p-n junction strongly affect the electrical properties of the device.

In this work atomic scale investigation combined with electrical measurements is presented for CdS/CIGS interfaces of CIGS solar cells annealed at different temperatures. The electrical characterization shows decrease of efficiency of the cells with increasing temperature of annealing. By means of atom probe tomography Cd and S diffusion is traced. Indeed, after annealing, besides the Cu-depleted and Cd-enriched CIGS surface, Cd had diffused over a long distance into the absorber. This is contrasted with an as-grown sample for which Cd-enriched and Cu,Ga-depleted zones were observed only at the CIGS surface. The Cd<sup>2+</sup> ions are expected to occupy Cu rather than Ga sites as Cd<sup>2+</sup> and Cu<sup>+</sup> have similar ionic radii. Such Cd<sub>Cu</sub><sup>+</sup> donors could change the p-n junction properties as it was suggested by “Buried homojunction” and “Type inversion of the CIGS surface region” models.

DS 2.5 Mon 10:30 H 0111

**Crystallization of Ge nanoparticles in ZrO<sub>2</sub>-based dielectrics for electrical applications.** — ●DAVID LEHNINGER<sup>1</sup>, LARYSA KHOMENKOVA<sup>2</sup>, FRANK SCHNEIDER<sup>1</sup>, CAMELIU HIMCINSCHI<sup>3</sup>, VOLKER KLEMM<sup>4</sup>, DAVID RAFAJA<sup>4</sup>, and JOHANNES HEITMANN<sup>1</sup> — <sup>1</sup>Institut für Angewandte Physik, TU Bergakademie Freiberg, D-09596 Freiberg — <sup>2</sup>Lashkaryov Institute of Semiconductor Physics, National Academy of Sciences of Ukraine, 03028 Kiev, Ukraine — <sup>3</sup>Institut für Theoretische Physik, TU Bergakademie Freiberg, D-09596 Freiberg — <sup>4</sup>Institut für Werkstoffwissenschaft, TU Bergakademie Freiberg, D-09596 Freiberg

Crystallization of Ge was studied in high-k ZrO<sub>2</sub> and TaZrOx host materials using Ge<sub>3.6</sub>ZrO<sub>2</sub>/ZrO<sub>2</sub> or GeTaZrOx/TaZrOx superlattices, sputtered on Si wafers which were either covered by a SiO<sub>2</sub> or Si<sub>3</sub>N<sub>4</sub> starting layer. In order to achieve a better understanding of the Ge-NCs-high-k interface, the formation of Ge-NCs was analyzed by different analytical methods for different annealing temperature. In pure ZrO<sub>2</sub>, elongated non-spherical Ge-NCs with insufficient control of shape, size, and spatial distribution were observed on wafers covered by SiO<sub>2</sub>. A Si<sub>3</sub>N<sub>4</sub> starting layer led to formation of multilayer structures with thin Ge films within the ZrO<sub>2</sub> matrix. Using TaZrOx as matrix, Ge-NCs with spherical shape and well-defined size were formed in amorphous TaZrOx. In this system, charge trapping phenomena were investigated using MIS structures with single and double layer storage nodes. A memory window of up to 5 V together with a programming-to-flatband-voltage slope of near 1 could be observed.

DS 2.6 Mon 10:45 H 0111

**First Synthesis Approach of Layered ZrSe<sub>2</sub> and New Misfit Layer Compounds (PbSe)<sub>1+δ</sub>(ZrSe<sub>2</sub>)<sub>n</sub> Using Modulated Elemental Reactants** — ●BENJAMIN EICKMEIER<sup>1</sup>, MATTI ALEMAYEHU<sup>2</sup>, ROBERT ZIEROLD<sup>1</sup>, MATTHIAS FALMBIGL<sup>2</sup>, SAGE BAUERS<sup>2</sup>, JOHANNES GOOTH<sup>1</sup>, TORBEN DANKWORT<sup>3</sup>, JULIE CHOUNARD<sup>2</sup>, CARMEN VOIGT<sup>4</sup>, CARSTEN RONNING<sup>4</sup>, DAVID C JOHNSON<sup>2</sup>, and KORNELIUS NIELSCH<sup>1</sup> — <sup>1</sup>Universität Hamburg, Hamburg, Germany — <sup>2</sup>University of Oregon, Eugene, USA — <sup>3</sup>Christian-Albrechts-Universität zu Kiel, Kiel, Germany — <sup>4</sup>Universität Jena, Jena, Germany

A first synthesis approach of the layered dichalcogenide ZrSe<sub>2</sub> and a new family of misfit layer compounds (PbSe)<sub>1+δ</sub>(ZrSe<sub>2</sub>)<sub>n</sub> (n = 1, 2, 3) using the physical vapor deposition technique of modulated elemental reactants is reported. Thin films of about 30 nm were deposited onto Si and SiO<sub>2</sub> and characterized with XRD, XRR, and TEM. Composition data was acquired with electron probe microanalysis. These misfit layer compounds are metastable systems and consist of an intergrowth structure between one rock salt sublattice PbSe and n dichalcogenide sublattices ZrSe<sub>2</sub>, which are alternately stacked upon each other. In the temperature range of 120–200 K hopping transport was observed on the presumable (PbSe)<sub>1+δ</sub>(ZrSe<sub>2</sub>)<sub>1</sub>, due to crystalline grains embedded in an amorphous matrix. Previous studies of misfit layer compounds report an unusual decrease up to six times of the in-plane thermal conductivity compared to single dichalcogenides. This trend makes those systems promising alternatives for e.g. thermoelectric applications.

15 min. break.

DS 2.7 Mon 11:15 H 0111

**Growth and Properties of Crystalline Silicon deposited on Glass by Steady-State Solution Growth** — ●CHRISTIAN EHLERS, ROMAN BANSEN, JAN SCHMIDTBAUER, FRANZISKA RINGLEB, THOMAS TEUBNER, and TORSTEN BOECK — Leibniz Institute for Crystal Growth, Berlin, Germany

For a thin-film silicon solar cell, only several tens of micrometer of crystalline silicon are needed for sufficient light absorption. Therefore we have developed a two-step process for depositing thin silicon layers on inexpensive glass substrates below the softening point of glass.

In the first step a seed layer of nanocrystalline silicon is formed on the heated glass substrates by two different approaches. Either only silicon is evaporated by physical vapor deposition which subsequently forms a thick nanocrystalline layer, or a metal is co-evaporated which leads to the metal-induced crystallization of nanocrystalline silicon. In the second growth step, a subsequent silicon layer is grown on the initial seed layer by steady-state solution growth from a tin or indium solution.

In comparison to traditional liquid phase epitaxy where the supersaturation of the solution is driven by cooling of the metallic solvent, we employ a steady temperature gradient between the silicon source material and substrate. Therefore, growth conditions are similar to a commercial float glass production-process, which potentially allows for the deposition of silicon in a continuous fashion. The electrical and structural properties of the grown silicon layers are analyzed with regard to their suitability for solar cell device production.

DS 2.8 Mon 11:30 H 0111

**Comparative Studies in the Physical and Optical Properties of Indium Tin Oxide Films by Various Fabrication Processes** — ●AKEMI TAMANAI and ANNEMARIE PUCCI — Kirchoff-Institut für Physik der Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg

Tin-doped indium oxide (ITO) is a highly transparent n-type semiconductor material in VIS\UV region caused by its wide band gap. For improving the resistivity and high optical transmittance performances of ITO films, various ITO fabrication processes have been introduced so far. Since their physical and optical properties are strongly influenced by fabrication processes such as sputtering, electron beam evaporation, and pulsed-laser deposition, changes in, for instance, the annealing temperature and environment, the surface resistance, and its morphology directly affect both properties. Hence, in order to enhance and deepen the understanding for the dielectric properties of various ITO films, spectroscopic IR ellipsometry (Woollam IR-VASE) measurements have been carried out for determining the dielectric constants ( $\epsilon_1$  and  $\epsilon_2$ ), the degree of electric scattering time ( $\tau$ ), the plasma frequency ( $\omega_p$ ), and the damping constant ( $\gamma$ ) defined in the Drude model which describes free-carrier contribution to dielectric properties.

DS 2.9 Mon 11:45 H 0111

**Microstructure and mechanical properties of Pd-Si amorphous thin films** — ●SREE HARSHA NANDAM<sup>1</sup>, DI WANG<sup>1</sup>, RUTH SCHWAIGER<sup>2</sup>, ZBIGNIEW SNIADOCKI<sup>1</sup>, YULIA IVANISENKO<sup>1</sup>, HERBERT GLEITER<sup>1</sup>, and HORST HAHN<sup>1</sup> — <sup>1</sup>Institute for Nanotechnology, Karlsruhe Institute of Technology, D-76344 Eggenstein-Leopoldshafen, Germany. — <sup>2</sup>Institute for Applied Materials, Karlsruhe Institute of Technology, D-76344, Eggenstein-Leopoldshafen, Germany.

Amorphous thin films of Pd<sub>80</sub>Si<sub>20</sub> were co-sputtered using Pd and Si targets in a direct current sputtering system. X-ray diffraction of the thin films clearly revealed the amorphous nature and the microstructure of the films showed a morphology consisting of nanograins. Such amorphous nanograined thin films are termed as “nanoglasses” in the present day literature. Transmission electron microscopic studies on these films confirmed the amorphous nature of the films with little variation of the composition (segregation) on the scale of the nanograined substructure. Annealing of the thin films below 200°C (for 24h) caused no big change of the nanostructure, at temperatures around 250°C (for 24h) crystallization of the films was observed. Nanoindentation of the films showed a slightly higher Young’s modulus compared to the melt-spun counterparts reported in the literature. Possible reasons for the appearance of a “nanoglass” structure and for the increased Young’s modulus of the Pd-Si amorphous thin films are discussed.

DS 2.10 Mon 12:00 H 0111

**Cu-poor/Cu-rich transition of co-evaporated CuInSe<sub>2</sub>: Na**

**prevents annihilation of planar defects** — ●HELENA STANGE<sup>1,2</sup>, STEPHAN BRUNKEN<sup>2</sup>, HUMBERTO RODRIGUEZ-ALVAREZ<sup>2</sup>, DIETER GREINER<sup>2</sup>, CHRISTIAN ALEXANDER KAUFMANN<sup>2</sup>, ANJA SCHEU<sup>2</sup>, JAKOB LAUCHE<sup>2</sup>, NORBERT SCHÄFER<sup>2</sup>, DANIEL ABOU-RAS<sup>2</sup>, and ROLAND MAINZ<sup>2</sup> — <sup>1</sup>TU Berlin, Institut für Werkstoffwissenschaften — <sup>2</sup>Helmholtz-Zentrum-Berlin für Energie und Materialien

Highest efficiencies of Cu(In,Ga)Se<sub>2</sub> solar cells have been achieved with absorbers deposited by a 3-stage-based co-evaporation. The Cu-poor/Cu-rich transition during the growth process and the presence of small amounts of Na and K are known to be favorable for solar cell performance. We investigate the influence of Na on the structural evolution of CuInSe<sub>2</sub> by interrupting the growth process at overall Cu-poor and Cu-rich film compositions. CuInSe<sub>2</sub> layers without and with NaF precursor are prepared at growth temperatures below 400°C and analyzed by XRD, XRF, EDX and GDOES. For the samples without NaF a XRD signal characteristic for planar defects are observed only for the Cu-poor samples, while for the Cu-rich samples the signal vanishes. In contrast, for the Na-containing absorbers the characteristic signal are present also for the Cu-rich samples. For Cu(In,Ga)Se<sub>2</sub> layers without NaF precursor, real-time XRD shows annihilation of planar defects coinciding with the Cu-poor/Cu-rich transition. We conclude that the presence of Na during growth impedes annihilation of planar defects during the Cu-poor/Cu-rich transition in CuInSe<sub>2</sub> at low growth temperatures.

DS 2.11 Mon 12:15 H 0111

**In situ X- Rays measurements of lattice expansion on metallic superlattices.** — ●SOTIRIOS A. DROULIAS, LENNARD MOOLJ, GUNNAR K. PALSSON, XIN XIAO, VASSILIOS KAPAKLIS, BJORGVIN HJORGVARSON, and MAX WOLFF — Materials Physics, Division of Physics and Astronomy, Uppsala University, Sweden

Transition metals are exceptional candidates for hydrogen storage applications since large H quantities can be effectively absorbed. By growing superlattices of such materials, finite size and proximity effects can be investigated. In our work, we present expansion measurements of Cr-V and Fe-V superlattices by using in situ X-Ray diffraction. From the expansion measurements the elastic constants of the material can be extracted and related to the hydrogen interaction which is mediated by elastic forces. A complete and accurate description of the host lattice under various H pressures (concentrations) and different temperatures provide us with a unique tool for understanding the system's thermodynamics. From the volume expansion one can derive the site occupancy of H in the host material and if combined with other techniques, such as optical transmission, and curvature measurements a complete image of the system can be drawn. The different techniques can be correlated directly through resistivity measurements. This forms the basis for understanding the observed phase transitions in such systems and the influence of finite size and proximity. Furthermore, characterization of the host lattice under various conditions is a detailed quality description after repeated loading and unloading of

the hydrogen containing material.

DS 2.12 Mon 12:30 H 0111

**GISAXS investigation of growth of Ag nanoparticles from atomic deposition: experiment and simulation** — CELINE DURNIK, ●MARINA GANEVA, GENNADY POSPELOV, WALTER VAN HERCK, and JOACHIM WUTTKE — Jülich Centre for Neutron Science, Forschungszentrum Jülich, Outstation at MLZ, Garching, Germany

Grazing-Incidence Small-Angle X-ray Scattering (GISAXS) is a powerful tool for the investigation of the growth of noble metal particles on various substrates. Understanding of the underlying growth mechanisms allows for a control of the properties of the nanocoatings. Due to the complexity of the GISAXS data analysis, appropriate software is required to deduce the structural information from the measured GISAXS pattern. Here we present our software BornAgain [1]. BornAgain is a multi-platform open-source project that aims at supporting scientists in the analysis and fitting of their GISAXS data, both for synchrotron (GISAXS) and neutron (GISANS) facilities. As a case study, the growth of Ag nanoparticles on Si and PTFE substrates during DC magnetron sputtering of Ag is taken. The GISAXS investigation of structural properties was performed at the high-resolution diffractometer GALAXI (Jülich).

[1] <http://bornagainproject.org>

DS 2.13 Mon 12:45 H 0111

**In-situ GIXD/GISAXS investigation of intercalation processes in bulk-heterojunction organic solar cells** — ●MARVIN BERLINGHOF<sup>1</sup>, THAER KASSAR<sup>1</sup>, NUSRET SENA GÜLDAL<sup>2</sup>, CHRISTOPH BRABEC<sup>2</sup>, and TOBIAS UNRUH<sup>1</sup> — <sup>1</sup>Chair for Crystallography and Structural Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg — <sup>2</sup>Chair for Materials for Electronics and Energy Technology, Friedrich-Alexander-Universität Erlangen-Nürnberg

Organic solar cells are a promising technology for cost efficient energy production, because – compared to traditional inorganic solar cells – they only need low temperatures during production, are cheaper to produce in industrial-scales and are flexible. Doctor-bladed thin film solar cells were investigated in-situ during drying by GIXD and GISAXS using our in-house X-ray source and synchrotron radiation. Using different polymers (pBTTT, P3HT, PQT) as organic semiconductors and a wide variety of fullerenes, we observed a change in a different behavior of the d-spacing of pure polymers and polymer-fullerene-mixtures during drying. While the pure polymers showed a decreasing of the d-spacing of the (100)-polymer-peaks during drying, caused of the evaporation of solvent. In the mixtures this d-spacing stayed constant during drying, which is a indicator for intercalation of fullerenes in-between the polymer sheets, which directly influences the efficiency of the organic solar cells. Furthermore the fullerenes hinder the presence of higher diffraction orders and with that decreases the crystallinity of the films. In addition the results of our GISAXS investigation and depth-dependent measurements will be presented.

## DS 3: Organic Thin Films

Time: Monday 15:00–19:30

Location: H 2032

### Invited Talk

DS 3.1 Mon 15:00 H 2032

**Thin film growth studies using time-resolved X-ray scattering** — ●STEFAN KOWARIK — Institut für Physik, Newtonstr. 15, 12489 Berlin

Thin film growth inherently is a non-equilibrium process. This means that the route to the final film structure is determined not simply by a minimization of the free energy, but by a non-trivial competition between thermodynamics and kinetics. For a quantitative understanding one therefore needs information on the nanoscopic surface processes such as molecular binding as well as surface diffusion and step-edge crossing. In situ X-ray scattering is ideally suited for such measurements as it can be used to monitor temporal changes on the atomic scale. We show how real-time in situ Grazing Incidence Small Angle Scattering (GISAXS) can be combined with simultaneous X-ray reflectivity measurements to characterize both in-plane and out-of-plane film structure as a function of time. While GISAXS gives information on nucleation densities and island sizes, reflectivity measurements make it possible to extract the out-of-plane density profile so that both measurements together give a rather complete morphological charac-

terization. We give examples for growth of small-molecule organic semiconductors such as C60, where we determine diffusion barrier, step edge barrier and binding energy, but the techniques are equally applicable to growth of atomic systems. S. Bommel, N. Kleppmann, C. Weber, H. Spranger, P. Schäfer, J. Novak, S.V. Roth, F. Schreiber, S.H.L. Klapp, S. Kowarik, "Unravelling the multilayer growth of the fullerene C60 in real-time", Nature Communications 5, 5388 (2014).

DS 3.2 Mon 15:30 H 2032

**Epitaxial Growth of a Methoxy-Functionalized Quaterphenylene** — ●FRANK BALZER<sup>1</sup>, ROLAND RESEL<sup>2</sup>, ARNE LÜTZEN<sup>3</sup>, HORST-GÜNTER RUBAHN<sup>1</sup>, and MANUELA SCHIEK<sup>4</sup> — <sup>1</sup>MCI, NanoSyd, University of Southern Denmark, Alision 2, DK-6400 Sønderborg, Denmark — <sup>2</sup>Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria — <sup>3</sup>University of Bonn, Kekulé Institute for Organic Chemistry and Biochemistry, Gerhard-Domagk-Str. 1, D-53121 Bonn, Germany — <sup>4</sup>University of Oldenburg, Energy and Semiconductor Research Laboratory, Institute of Physics, Carl-von-Ossietzky-Str. 9-11, D-26111 Oldenburg, Germany

Thin films from conjugated small molecule semiconductors are important building blocks for organic electronics. Functionalization can control their electrical and optical properties, but also change thin film morphology. Here the epitaxial growth of a methoxy functionalized *para*-quaterphenylene (MOP4) on alkali halides as well as on mica is investigated by a combination of low energy electron diffraction (LEED), polarized (confocal) light microscopy (PLM), atomic force microscopy (AFM), and X-ray diffraction (XRD). On both substrates a thin film phase is present, resulting however in different morphologies: On the alkali halides mainly islands from upright molecules form, whereas on mica clusters and nanofibers from lying molecules grow. LEED even detects an initial wetting layer on mica with a different structure. Especially the fibers show a specific polarization pattern of the emitted blue fluorescence. Clusters and fibers age via Ostwald ripening due to water vapor, resulting in a strong change of morphology.

DS 3.3 Mon 15:45 H 2032

**Influencing the growth of *para*-sexiphenyl through chemical tuning** — ●ANTON ZYKOV<sup>1</sup>, MINO SPARENBERG<sup>1</sup>, PAUL BEYER<sup>1</sup>, LINUS PITHAN<sup>1</sup>, CHRISTOPHER WEBER<sup>1</sup>, YVES GARMSHAUSEN<sup>2</sup>, FRANCESCO CARLÀ<sup>3</sup>, STEFAN HECHT<sup>2</sup>, SYLKE BLUMSTENGEL<sup>1</sup>, FRITZ HENNEBERGER<sup>1</sup>, and STEFAN KOWARIK<sup>1</sup> — <sup>1</sup>Inst. f. Physik, Humboldt-Universität zu Berlin — <sup>2</sup>Inst. f. Chemie, Humboldt-Universität zu Berlin — <sup>3</sup>ESRF, Grenoble

We investigate the molecular growth of hybrid organic-inorganic semiconductor systems (HIOS) and show that chemical tuning can be used to optimize the growth mode [1]. We employ fluorination of *para*-sexiphenyl (6P) to drastically alter the growth mode from a rough three-dimensional towards a smooth, crystalline layer-by-layer growth as demanded for efficient opto-electronic devices with advanced properties. Our study combines *in situ* atomic force microscopy and *in situ* real-time X-ray scattering performed at the ID03 beamline at ESRF to monitor the evolution of the molecular thin film structure and morphology on non-polar ZnO (1010) substrates. In contrast to the parent molecule 6P, we observe for the fluorinated 6P a suppression of the growth of a second crystal phase and an increased molecular diffusivity together with a lower Ehrlich-Schwoebel barrier. As a consequence the interlayer mass transport is increased, which leads to the observed improvement in growth-mode.

[1] M. Sparenberg\*, A. Zykov\*, P. Beyer, L. Pithan, C. Weber, Y. Garmshausen, F. Carlà, S. Hecht, S. Blumstengel, F. Henneberger and S. Kowarik. *Phys. Chem. Chem. Phys.*, 2014, **16**, 26084-26093.

DS 3.4 Mon 16:00 H 2032

**Negative thermal expansion based on collective rotational motions of PTCDI-C8 in a crystalline organic thin film** — ●SEBASTIAN BOMMEL<sup>1,2</sup>, LINUS PITHAN<sup>2</sup>, CHRISTOPHER WEBER<sup>2</sup>, GONZALO SANTORO<sup>1</sup>, STEPHAN V. ROTH<sup>1</sup>, EDGAR WECKERT<sup>1</sup>, and STEFAN KOWARIK<sup>2</sup> — <sup>1</sup>Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — <sup>2</sup>Institut für Physik, Humboldt-Universität zu Berlin, Germany

The understanding of the structure-function relationship in molecular thin films for the fabrication of advanced functional nano-materials is still challenging because molecules possess many conformational and rotational degrees of freedom. Here we report on temperature-dependent rotation of the organic semiconductor PTCDI-C8. Highly crystalline organic thin films have been investigated using Grazing Incidence X-ray Diffraction (GIXD), which enables us to determine the temperature-dependent unit cell and the arrangement of molecules within the unit cell. From fitting the intensities of the Bragg reflections at different temperatures we find that the tilt angle of the molecules changes continuously with temperature and does not exhibit hysteresis. A change in molecular tilt of 4° is observed for a 200 K temperature difference. This collective mechanical response of a molecular rotation is connected with a large negative thermal expansion coefficient of the *a*-axis within the thin film unit cell of -135 ppm/K. Such negative thermal expansion offers highly desirable properties for the design of thermo-mechanical devices such as actuators.

DS 3.5 Mon 16:15 H 2032

**Shape anisotropy of organic thin films induced by ion-beam irradiated rippled substrates** — ●MARKUS KRATZER<sup>1</sup>, DOMINIK WRANA<sup>2</sup>, KONRAD SZAJNA<sup>2</sup>, FRANCISZEK KROK<sup>2</sup>, and CHRISTIAN TEICHERT<sup>1</sup> — <sup>1</sup>Institute of Physics, Montanuniversität Leoben, Franz Josef Straße 18, 8700 Leoben, AUSTRIA — <sup>2</sup>Institute of Physics, Jagiellonian University, Lojasiewicza 11, 30-348 Krakow, POLAND

Control over thin film growth morphologies of conjugated molecules is

a key issue in organic electronics. Here, we investigated the growth of the organic semiconductor *para*-hexaphenyl (6P) on ion bombarded, rippled TiO<sub>2</sub>(110) surfaces. Such substrates are highly anisotropic, representing one-dimensionally patterned templates with alternating ascending and descending step trains exhibiting typical step distances smaller 1 nm. 6P islands have been observed featuring clear shape anisotropy and discrete island widths according to the ripple wavelength. These observations are addressed to anisotropic detachment of molecules differently bound to the island rim at ascending and descending steps. A change of the average ripple length from ~11 nm to ~60 nm, resulted in a change of the average islands' length-to-width ratio from ~1.5:1 and ~4.5:1. In addition, strong diffusion anisotropy along and perpendicular to the ripples was found to be responsible for an increasing island density with decreasing ripple length.

15 min. break.

DS 3.6 Mon 16:45 H 2032

**Thin film growth analysis of quinacridone on SiO<sub>2</sub>** — ●BORIS SCHERWITZL and ADOLF WINKLER — Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria

Quinacridone (C<sub>20</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub>) is part of the group of H-bonded organic dyes with remarkable air stability and attractive semiconducting properties. The combination of inter- as well as intramolecular H-bonding with pi-pi stacking leads to highly crystalline film formations with unique charge transport behaviors. Understanding the initial growth, namely from the sub-monolayer regime up to a few layers, is a key factor in evaluating possible applications in future microelectronic devices. In this contribution, we report our recent efforts and studies on the initial growth behavior of thin quinacridone films on a silicon dioxide substrate under UHV conditions with respect to sample treatment. After preparing and analyzing the substrate surface with Auger Electron Spectroscopy, thin films were created via physical vapor deposition from a Knudsen cell and subsequently analyzed with Thermal Desorption Spectroscopy, Atomic Force Microscopy and Raman Spectroscopy. Both sputter cleaned samples and samples with a carbon layer on top were investigated and yielded similar results. It could be shown, that quinacridone films tend to form bulk-like structures bound by strong hydrogen bonds, even at sub-monolayer coverages. Furthermore, a comparison between metal Knudsen cell and glass evaporation source deposition was made.

DS 3.7 Mon 17:00 H 2032

**Interface dipole and growth mode of partially and fully fluorinated rubrene on Au(111) and Ag(111)** — FALK ANGER<sup>1</sup>, HENDRIK GLOWATZKI<sup>2</sup>, ANTONI FRANCO-CAÑELLAS<sup>1</sup>, CHRISTOPH BÜRKER<sup>1</sup>, ●ALEXANDER GERLACH<sup>1</sup>, REINHARD SCHOLZ<sup>3</sup>, YUICHI SAKAMOTO<sup>4</sup>, TOSHIYASU SUZUKI<sup>4</sup>, NORBERT KOCH<sup>2</sup>, and FRANK SCHREIBER<sup>1</sup> — <sup>1</sup>Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen, Germany — <sup>2</sup>Helmholtz-Zentrum für Materialien und Energie GmbH, Berlin, Germany — <sup>3</sup>Institut für Angewandte Photophysik, TU Dresden, 01069 Dresden, Germany — <sup>4</sup>Institute for Molecular Science, Myodaiji, Okazaki 444-8787, Japan

Thin films of fully and partially fluorinated rubrene deposited on Au(111) and Ag(111) were investigated using ultraviolet and X-ray photoelectron spectroscopy [1]. We demonstrate that fluorination of the molecules is an efficient way for tuning the metal-organic interface dipole and the hole injection barrier [2,3].

Moreover, the results indicate that the pronounced electrostatic dipole moment of partially fluorinated rubrene (F<sub>14</sub>-Rub) has a strong impact on the growth mode of these molecules. Most notably, we infer that the first layer of F<sub>14</sub>-Rub on Au(111) and Ag(111) is formed by molecules with alternating orientation of their dipole moments, whereas the second layer shows a nearly uniform orientation.

[1] F. Anger et al., submitted

[2] F. Anger et al., *Appl. Phys. Lett.* **102** (2013) 13308

[3] M. Kytka et al., *J. Chem. Phys.* **130** (2009) 214507

DS 3.8 Mon 17:15 H 2032

**Small organic molecules for strongly coupled microcavities** — ●FELIX LEMKE, VADIM LYSSENKO, and KARL LEO — Institut für Angewandte Photophysik, TU Dresden, Deutschland

Strongly coupled organic microcavities are a promising system to investigate exciton-polaritons. Due to their non-crystalline structure, the phonon-assisted relaxation to the  $k = 0$  state is more probable than in inorganic microcavity systems. Even if organic materials are

quite promising, small organic molecules showing strong coupling are very rare. The advantages are easier production procedures and long lifetimes.

An estimation of the usability for the investigated materials will be presented. Using absorption spectra and the Kramers-Kronig-Relation, the complex refractive index is calculated. By comparing these results with the cavity mode, already a first statement can be given. Further insight is gained with transfer matrix calculations. These calculations can also be used to optimise the coupling strength and therefore the splitting. The results are then compared to the measured data.

DS 3.9 Mon 17:30 H 2032

**Magnetic transition metal phthalocyanine thin films: morphology, ordering, electronic structure and tuning of electronic properties via alkali metal doping** — ●OLGA MOLODTSOVA<sup>1</sup>, SERGEY BABENKOV<sup>1</sup>, KARINA SCHULTE<sup>2</sup>, VOLODYMYR MASLYUK<sup>3</sup>, INGRID MERTIG<sup>3</sup>, THOMAS BREDOW<sup>4</sup>, and VICTOR ARISTOV<sup>1,5,6</sup> — <sup>1</sup>DESY Hamburg, Germany — <sup>2</sup>MAX-lab Lund, Sweden — <sup>3</sup>Uni Halle, Germany — <sup>4</sup>Uni Bonn, Germany — <sup>5</sup>Uni Hamburg, Germany — <sup>6</sup>ISSP RAS, Russia

Magnetic transition metal phthalocyanines (MTM-Pc\*s) are considered as materials for development of low dimensional molecular magnets, quantum computers and hybrid systems for memory devices. To make further progress in development such devices both the understanding and the tailoring of the physical, chemical and transport properties of the organic semiconductor components are required. The evolution of electronic structure of the MTM-Pc\*s intrinsic and with potassium doping has been studied by means of photoemission spectroscopy, near-edge X-ray absorption fine structure and DFT calculations. The DFT calculations and detailed analysis of the core-level spectra permit us to suggest possible lattice sites for the potassium ions. The data disclosed filling of the lowest unoccupied molecular orbital upon doping and associated changes of the core level absorption spectra. None of the films prepared in our studies showed a finite electronic density of states at the Fermi level. Acknowledgements: This work was supported by the RFBR Grant No. 13 -02-00818 and the BMBF-Project No. 05K12GU2, PSP-Element No. U4606BMB1211

DS 3.10 Mon 17:45 H 2032

**Cross-linking-induced disappearance of surface-enhanced Raman scattering in aromatic self-assembled monolayers** — ●ANDRÉ BEYER<sup>1</sup>, MARCEL MAINKA<sup>1</sup>, XIANGHUI ZHANG<sup>1</sup>, THOMAS HUSER<sup>2</sup>, and ARMIN GÖLZHÄUSER<sup>1</sup> — <sup>1</sup>Physics of Supramolecular Systems, University of Bielefeld, 33615 Bielefeld, Germany — <sup>2</sup>Biomolecular Photonics, University of Bielefeld, 33615 Bielefeld, Germany

Surface-enhanced Raman scattering (SERS) spectra from aromatic self-assembled monolayers (SAMs) were recorded with the assistance of gold nanoparticles in different geometries. SAMs on planar gold surfaces with gold nanoparticles on top as well as SAMs on gold nanoparticles yielded comparable spectra with high signal-to-noise ratios. The cross-linking of aromatic SAMs by electron exposure results in the formation of carbon nanomembranes (CNMs). We demonstrate the formation of CNM-shells due to electron exposure of SAM-covered gold nanoparticles. Surprisingly, no Raman scattering in the range between 200 – 3100 cm<sup>-1</sup> was detectable from any aromatic SAM after cross-linking in the different SERS detection geometries. This finding was supported by performing SERS measurements on CNM/SAM samples which yielded no signal from the CNM but an intense signal from the SAM. Implications, possible mechanisms, and potential applications of this effect will be discussed.

15 min. break.

DS 3.11 Mon 18:15 H 2032

**High-speed confocal Raman imaging of carbon nanotubes** — ●MICHAEL LUDEMANN, SUSANNE HARTMANN, ANNE-D. MÜLLER, and FALK MÜLLER — Anfatec Instruments AG, Melanchthonstr. 28, D-08606 Oelsnitz (V)

Raman spectroscopy is a powerful tool in terms of chemical analysis and determination of physical properties. The ability of scanning the sample during a measurement provides an insight into these properties in a spatially resolved way by converting spectral features into color code images.

Due to a huge number of image points, Raman mapping is seriously

affected by long acquisition times. A new Raman spectrometer is designed for excellent coupling to an atomic force microscope (AFM) with the focus of maximized light throughput. Here, the optimum compromise for a sufficiently high signal-to-noise ratio is achieved at 8 ms exposure time per pixel resulting in an image acquisition time of less than 3 minutes, even with a non-cooled CCD. Based on this development, high-speed Raman mapping measurements on carbon nanotube (CNT) bundles on a silver/glass substrate are presented.

Raman mapping of single CNTs enables to distinguish between different types of CNTs. The spatial distribution of the CNT bundles and hot spot induced surface enhanced Raman spectroscopy (SERS) will be presented, as well.

DS 3.12 Mon 18:30 H 2032

**Fast IR laser mapping ellipsometry for the study of functional organic thin films** — ●ANDREAS FURCHNER<sup>1</sup>, GUO GUANG SUN<sup>1</sup>, HELGE KETELSEN<sup>2</sup>, JÖRG RAPPICH<sup>3</sup>, and KARSTEN HINRICHS<sup>1</sup> — <sup>1</sup>Leibniz-Institut für Analytische Wissenschaften – ISAS – e. V., Schwarzschildstraße 8, 12489 Berlin, Germany — <sup>2</sup>SENTECH Instruments GmbH, Schwarzschildstraße 2, 12489 Berlin, Germany — <sup>3</sup>Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium-Photovoltaik, Kekuléstraße 5, 12489 Berlin, Germany

The infrared spectral range provides information about the structural and chemical properties of functional organic thin films. The need to characterize these properties with high lateral resolution in short measurements times requires a new generation of infrared ellipsometer. A novel laboratory-based infrared laser mapping ellipsometer is presented that allows for measurements with lateral resolutions of 0.12 mm and time resolutions down to 80 ms per spot. The ellipsometer is applied for the optical characterization of inhomogeneous poly(3-hexylthiophene) and poly(*N*-isopropylacrylamide) organic thin films used for opto-electronics and bioapplications.

DS 3.13 Mon 18:45 H 2032

**Characterization of advanced biomaterials for the medical device industry using Synchrotron Radiation-based FTIR microspectroscopy and X-Ray spectroscopic techniques** — ●ANDREA HORNEMANN<sup>1</sup>, BEATRIX POLLAKOWSKI<sup>1</sup>, BONNIE TYLER<sup>2</sup>, GERALD HOLZLECHNER<sup>3</sup>, ANNA BELU<sup>4</sup>, ARNE HOEHL<sup>1</sup>, and BURKHARD BECKHOFF<sup>1</sup> — <sup>1</sup>Physikalisch-Technische Bundesanstalt, Berlin, Germany — <sup>2</sup>National Physics Laboratory, London, United Kingdom — <sup>3</sup>BAM Federal Institute of Materials Research and -Testing, Berlin, Germany — <sup>4</sup>Medtronic, Minneapolis, U.S.A.

Since its early development implantable medical devices had tremendous impact on the quality of life. But still today many implants cause inflammations due to incompatibility with human tissues or due to device related infections. Hence, there is a need for exploring new advanced biomaterials that comprise thin film coatings, surface grafted biomolecules, nanoparticle coatings, drug-eluting films, and especially bioresorbable components. Reliable metrological tools for the rapid characterization of medical devices are essential to probe their physicochemical properties. Both vacuum-based and ambient techniques, represented here by X-ray and FTIR spectroscopic techniques, allow for a characterization of surface layers, contaminants on the surface of medical devices in the manufacturing environment, and enable the detection of defects and chemical constituents in the near-surface region. The measurement sequences exhibit the potential of the use of orthogonal methods as FTIR and X-ray spectrometry to significantly contribute to the traceable and reliable characterization of medical devices.

DS 3.14 Mon 19:00 H 2032

**Molecular Orientations in Photochromic Layers on Silicon(111) Investigated by X-ray Absorption Spectroscopy** — ●DANIEL PRZYREMBEL<sup>1</sup>, MICHAEL AXMAN PETERSEN<sup>2,3</sup>, ANDREAS HEBERT<sup>2</sup>, KAROLA RÜCK-BRAUN<sup>2</sup>, CORNELIUS GAHL<sup>1</sup>, and MARTIN WEINELT<sup>1</sup> — <sup>1</sup>Department of Physics, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — <sup>2</sup>Department of Organic Chemistry, Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany — <sup>3</sup>Department of Chemistry, Danmarks Tekniske Universitet, Anker Engelds Vej 1, 2800 Kongens Lyngby, Denmark

Fulgimides are a class of photochromic molecular switches that undergo ring closing and opening upon illumination with UV and visible light, respectively.[1] When coupled to self-assembled monolayers (SAMs) of suitable anchoring molecules they retain the ability to reversibly isomerize and show photostationary states dominated by either a ring-

opened  $E/Z$  mixture or the ring-closed form.[2] We have investigated individual preparation steps towards as well as the resulting densely packed SAMs of a fulgimide on Si(111) single crystal surfaces by X-ray absorption spectroscopy. From the polarization-dependent contrast of the near edge X-ray absorption fine structure (NEXAFS) we deduced mean molecular orientations with respect to the sample surface and we evaluated the changes induced by UV illumination.

[1] Y. Yokoyama *Chem. Rev.* **2000**, *100*, 1717-1739.

[2] K. Rück-Braun, M. Å. Petersen, F. Michalik *et al. Langmuir* **2013**, *29*, 11758-11769.

DS 3.15 Mon 19:15 H 2032

**Nucleation of Vaterite-Phase Calcium Carbonate by Poly Glutamic Acid Peptides on Gold** — •HAO LU, MATTHEW A. HOOD, RAFAEL MUÑOZ-ESPÍ, MISCHA BONN, and TOBIAS WEIDNER — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Nature uses proteins and peptides containing acidic residues to control the crystal structure of polymorph materials such as calcium carbonate. Among the three most typical anhydrous polymorphs - calcite, aragonite and vaterite - the latter is the most thermodynamically unstable phase, and occurs rarely as biomineral. However, the vaterite structure can be stabilized in vitro by the presence of soluble biomolecules. Previous studies have focused on nucleation in the solution phase. Here we demonstrate interfacial nucleation: vaterite can be stabilized by specifically designed peptides bound to inorganic substrates. As a model system, we used a thiol-terminated poly glutamic acid sequences attached to a gold surface. The data show that the adsorbed peptides act as effective templates for the crystallization of a vaterite film. Using several complementary surface analytical techniques we follow structural changes of the peptide structure induced by the crystallization, which provides molecular-level insights into the biomineralization process of calcium carbonate.

## DS 4: Thin Film Characterisation II: Structure Analysis and Composition

Time: Monday 15:00–18:30

Location: H 0111

DS 4.1 Mon 15:00 H 0111

**Ferromagnetic InMnAs with perpendicular magnetic anisotropy synthesized by ion implantation** — •YE YUAN<sup>1,3</sup>, MUHAMMAD KHALID<sup>1</sup>, YUTIAN WANG<sup>1,3</sup>, EUGEN WESCHKE<sup>2</sup>, CARSTEN BAEHTZ<sup>1</sup>, WOLFGANG SKORUPA<sup>1</sup>, MANFRED HELM<sup>1,3</sup>, and SHENGQIANG ZHOU<sup>1</sup> — <sup>1</sup>Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — <sup>2</sup>Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — <sup>3</sup>Technische Universität Dresden, Dresden, Germany

Dilute magnetic semiconductors (DMS) have attracted much attention both from the application and fundamental physics points of view due to potential materials for spintronic device [1]. From application view, the perpendicular magnetic anisotropy (PMA) meets the need, of which the current-induced magnetization reversal originating from a spin transfer torque (STT). For InMnAs, which could only be obtained by low temperature molecule beam epitaxy (LT-MBE) before, achieving high Curie temperature (TC) layer with PMA is relatively difficult. The reason is that, although much lattice mismatch between the DMS layer and the substrate brings inner strain and further PMA, the dislocations also come and suppress TC. However, low inner strain from mismatch make layer lose PMA.

We prepare high TC InMnAs layers with strong PMA by ion implantation and pulsed layer melting. The TC appears the highest one of InMnAs with PMA up to 77 K so far.

[1]. T. Dietl, *et al.*, *Rev. Mod. Phys.* **86**, 187-251 (2014)

DS 4.2 Mon 15:15 H 0111

**Crystallinity of the Fe/GaAs interface for spintronics** — •RAJKIRAN THOLAPI, LENNART LIEFEITH, MICHAEL WACHTEL, GERDA EKINDORF, TARAS SLOBODSKYY, and WOLFGANG HANSEN — Institute of Nanostructure and Solid State Physics, Jungiusstr. 11, D-20355 Hamburg, Germany.

Epitaxial Fe thin film on GaAs metal-semiconductor heterojunction system is a prospective hybrid structure for spin injection. The presence of either tunneling or Schottky barrier, crystalline quality, interface states and intermixing at the interface influence the overall efficiency of the spin injection process [1]. We will discuss results of X-ray and electron diffraction studies performed on epitaxial Fe films deposited with and without MgO tunneling barriers on GaAs (001) substrate. Moreover, the morphological, crystalline and electrical properties of the Fe films will be presented. We will also discuss the in situ strain evolution of the Fe films during deposition. We observed a high degree of crystallinity in epitaxial thin Fe films which is considered to be favorable for electrical spin injection.

[1] L. R. Fleet *et al.*, \*Correlating the interface structure to spin injection in abrupt Fe/GaAs (001) films\*, *Phys. Rev. B* **87**, 024401 (2013)

DS 4.3 Mon 15:30 H 0111

**Twisted twin domains in epitaxial thin MnSi layers on Si(111)** — •MIRKO TRABEL, BENEDIKT HALBIG, NADEZDA V. TARAKINA, CHRISTOPH POHL, UTZ BASS, CHARLES GOULD, JEAN GEURTS, KARL BRUNNER, and LAURENS W. MOLENKAMP — Experimentelle Physik 3,

Physikalisches Institut, Universität Würzburg, Am Hubland, D-97074, Würzburg, Germany

Thin layers of MnSi are grown by molecular beam epitaxy on Si(111) substrates and their crystal properties are investigated by X-ray diffraction (XRD), Raman spectroscopy and transmission electron microscopy (TEM) measurements. Both XRD analysis and the observed Raman phonon modes prove that the layers of 5 - 32 nm thickness are single phase MnSi. The B20 crystal structure of MnSi lacks inversion symmetry and allows right- and left-handed crystals. We demonstrate by azimuthal  $\phi$ -scans of several asymmetric X-ray reflections that certain reflections reveal the formation of twin domains in the layer as well as their corresponding azimuthal twists of  $\Delta\phi = \pm 30^\circ$  with respect to the Si substrate. The observed intensities of corresponding reflexes are equal, indicating the same volume fractions for both domains. Cross-sectional TEM confirms the formation of the twisted twin domains and reveals a typical domain size of about 200 nm. The sheet resistivity shows the same temperature dependence as bulk MnSi with helical magnetic order, but the critical temperature is increased from the bulk value of 29.5 K to about 40 - 45 K.

DS 4.4 Mon 15:45 H 0111

**Diffusion controlled solid state reactions in Fe/Pt thin-film systems with additional Ag layer** — •NATALIYA SAFONOVA<sup>1</sup>, GABOR KATONA<sup>2</sup>, FABIAN GANSS<sup>3</sup>, DMITRIY MITIN<sup>1</sup>, IURIY MAKOGON<sup>4</sup>, GUNTER BEDDIES<sup>1,3</sup>, DEZSO BEKE<sup>2</sup>, and MANFRED ALBRECHT<sup>1</sup> — <sup>1</sup>Institute of Physics, University of Augsburg, Germany — <sup>2</sup>University of Debrecen, Hungary — <sup>3</sup>Chemnitz University of Technology, Germany — <sup>4</sup>National Technical University of Ukraine "KPI", Kyiv, Ukraine

Fe(15 nm)/Ag(10 nm)/Pt(15 nm)/Si<sub>2</sub>(100 nm)/Si(100) and FePt(15 nm)/Ag(7.5 nm)/SiO<sub>2</sub>(100 nm)/Si(100) thin film systems were prepared by magnetron deposition at room temperature. Rapid thermal annealing (RTA) for 30s was performed between 600°C and 900°C. In addition samples also were isothermally annealed between 245°C and 390°C (from 0.5 to 52 hours). Composition profiles of trilayer samples (obtained by secondary neutral mass spectrometry) after the low and high temperature heat treatments show a strong intermixing between Ag and Pt, resulting in the formation of Ag<sub>x</sub>Pt<sub>1-x</sub>. Afterwards Pt diffuses through the remaining Ag layer and penetrates into the Fe grain boundaries (GBs) reducing the amount of Pt in the Ag<sub>x</sub>Pt<sub>1-x</sub> layer. This process leads to the formation of a FePt reaction product and Ag appears to "move" towards the substrate. High temperature RTA on the same samples give similar composition distributions and eventually the formation of a homogeneous L1<sub>0</sub> ordered FePt alloy (observed by X-ray diffraction). Furthermore, corresponding magnetic properties will be discussed.

DS 4.5 Mon 16:00 H 0111

**Observing the Morphology of Single Layered Embedded Silicon Nanocrystals by Using Temperature-stable TEM Membranes** — •SEBASTIAN GUTSCH<sup>1</sup>, JAN LAUBE<sup>1</sup>, DANIEL HILLER<sup>1</sup>, MARGIT ZACHARIAS<sup>1</sup>, and CHRISTIAN KÜBEL<sup>2</sup> — <sup>1</sup>Laboratory for Nanotechnology, University of Freiburg, Freiburg, Germany —

<sup>2</sup>Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany

Standard structural analysis of Si nanocrystal/SiO<sub>2</sub> superlattices is carried in TEM by using cross-sectional sample preparation revealing clearly the presence of the multilayer stack [1]. In this work, we use TEM compatible high temperature stable SiN membranes to investigate single layers of Si nanocrystal ensembles prepared from precipitation of a silicon-rich oxide layer sandwiched between two SiO<sub>2</sub> diffusion barriers [2]. In this way size distribution, shape and areal density of the Si nanocrystals can be easily accessed by energy-filtered TEM without the need of further specimen preparation. Using this unique approach, we demonstrate, how the nanocrystal size distribution develops from a broad to a narrow log-normal distribution, when the precipitation layer thickness and stoichiometry are below a critical value. The results are crucial to understand doping [3] and transport properties [4] of Si nanocrystals embedded in dielectrics.

- [1] Hartel et al., *Thin Solid Films*, 520, 121-125 (2011)
- [2] Gutsch et al., Beilstein J. Nanotechnology, submitted
- [3] Gnaser et al., *J. Appl. Phys.* 115, 034304 (2014)
- [4] Gutsch et al., *J. Appl. Phys.* 113, 133703 (2013)

DS 4.6 Mon 16:15 H 0111

**Silicon nanocrystals in silicon nitride: the absence of quantum-confinement photoluminescence** — ●ANASTASIYA ZELENINA<sup>1</sup>, SERGEY DYAKOV<sup>2</sup>, DANIEL HILLER<sup>1</sup>, and MARGIT ZACHARIAS<sup>1</sup> — <sup>1</sup>IMTEK University of Freiburg, Freiburg, Germany — <sup>2</sup>Royal Institute of Technology (KTH), Kista, Sweden

Amorphous superlattices containing SiN<sub>x</sub> sublayers of different thicknesses altered with Si<sub>3</sub>N<sub>4</sub> barriers were deposited by PECVD and further annealed at high temperatures in order to form silicon nanocrystals (Si NCs). TEM images combined with XRD spectra confirmed the formation of well separated Si NCs of controllable sizes in the range of 2 - 5 nm. The expected photoluminescence (PL) peak shift is observed at 550 - 600 nm for the films with Si NCs of 3, 4 and 5 nm in size. However, the origin of the PL peak shift induced some doubts. Firstly, the PL peaks have a very low intensity and rather broad FWHM in comparison to literature results. Secondly, the sample with Si NCs of 2 nm in size did not follow the trend and had a peak position at 580 nm. Finally, spectral position of all peaks was similar to the PL of reference Si<sub>3</sub>N<sub>4</sub> bulk film. Our research also revealed that PL decay time is in the range of nanoseconds for all the samples, which confirm a defect-related luminescence. Thereby, we concluded that all the samples demonstrate Si<sub>3</sub>N<sub>4</sub> defect-related PL, which originates from Si<sub>3</sub>N<sub>4</sub> barriers. We assumed that the PL peak shift is an optical artifact. Our well-developed simulations based on the use of the method of transfer matrix confirmed the presence of optical interference in the films, which caused the PL peak shift.

DS 4.7 Mon 16:30 H 0111

**k-resolved electronic structure by soft-X-ray ARPES: From 3D systems to heterostructures and impurities** — ●V.N. STROCOV, M. KOBAYASHI, L.L. LEV, J. KREMPASKY, V.A. ROGALOV, U. STAUB, H. VOLFOVÁ, J. MINÁR, X. WANG, T. SCHMITT, and C. CANCELLIERI — Swiss Light Source, Paul Scherrer Institute, Switzerland

The spectroscopic power of soft-X-ray ARPES in the energy range around 1 keV arises from enhanced photoelectron escape depth, sharp definition of 3D electron momentum **k**, and resonant photoexcitation delivering elemental and chemical state specificity. We demonstrate that the advanced instrumentation at the Swiss Light Source has enabled stretching this technique from 3D materials to the most photon-hungry cases of buried heterostructures and impurities [1].

One of the applications to 3D materials is the magnetoresistive 3D perovskite La<sub>1-x</sub>Sr<sub>x</sub>MnO<sub>3</sub>. Its experimental Fermi surface shows shadow contours manifesting the rhombohedral lattice distortion affecting the CMR. The heterostructures are illustrated with the LaAlO<sub>3</sub>/SrTiO<sub>3</sub> buried interface. Exploiting resonant photoexcitation of the interface Ti<sup>3+</sup> ions, we resolve different subbands of the interface quantum well states. Their spectral function reveals prominent polaronic coupling which reduces the electron mobility. An example of the impurity systems is the diluted magnetic semiconductor GaMnAs. Resonant photoexcitation at the Mn 2*p* edge enables identification of the ferromagnetic Mn impurity band as well as its energy alignment and mechanism of hybridization with the host GaAs bands.

- [1] V.N. Strocov *et al.*, *Synchr. Rad. News* **27**, N2 (2014) 31

DS 4.8 Mon 16:45 H 0111

**Modification of energy band alignment and electric prop-**

**erties of Pt/Ba<sub>0.6</sub>Sr<sub>0.4</sub>TiO<sub>3</sub>/Pt thin-film ferroelectric varactors by Ag impurities at interfaces** — STEFAN HIRSCH, ●PHILIPP KOMISSINSKIY, STEFAN FLEGE, SHUNYI LI, KARSTEN RACHUT, ANDREAS KLEIN, and LAMBERT ALFF — Institute for Materials Science, Technische Universität Darmstadt, Alarich-Weiss-Straße 2, 64287 Darmstadt, Germany

We report on the effects of Ag impurities at interfaces of parallel-plate Pt/Ba<sub>0.6</sub>Sr<sub>0.4</sub>TiO<sub>3</sub>/Pt thin film ferroelectric varactors. Ag impurities occur at the interfaces due to diffusion of Ag from colloidal silver paint used to attach the varactor samples with their back side to the plate heated at 600-750 °C during deposition of Ba<sub>0.6</sub>Sr<sub>0.4</sub>TiO<sub>3</sub>. X-ray photoelectron spectroscopy and secondary ion mass spectrometry suggest that amount and distribution of Ag adsorbed at the interfaces depend strongly on the adsorbent surface layer. In particular, Ag preferentially accumulates on top of the Pt bottom electrode. The presence of Ag significantly reduces the barrier height between Pt and Ba<sub>0.6</sub>Sr<sub>0.4</sub>TiO<sub>3</sub> leading to an increased leakage current density and, thus, to a severe degradation of the varactor performance.

- [1] S. Hirsch, P. Komissinskiy, S. Flege, S. Li, K. Rachut, A. Klein, and L. Alff, *J. Appl. Phys.* **115**, 243704 (2014).

15 min. break.

DS 4.9 Mon 17:15 H 0111

**Morphology and Optoelectronics at Metal-Polymer-Interfaces during Sputter Deposition** — ●MATTHIAS SCHWARTZKOPF<sup>1</sup>, GONZALO SANTORO<sup>1</sup>, OLEKSANDR POLONSKIY<sup>2</sup>, ALEXANDER HINZ<sup>2</sup>, EZZELDIN METWALLI<sup>3</sup>, YUAN YAO<sup>3</sup>, THOMAS STRUNSKUS<sup>2</sup>, FRANZ FAUPEL<sup>2</sup>, PETER MÜLLER-BUSCHBAUM<sup>3</sup>, and STEPHAN V. ROTH<sup>1</sup> — <sup>1</sup>DESY, Notkestr. 85, 22607 Hamburg — <sup>2</sup>CAU zu Kiel, Kaiserstr. 2, 24143 Kiel — <sup>3</sup>TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

The reproducible low-cost fabrication of functional polymer-metal nanocomposites with tailored optoelectronic properties remains a major issue in applied nanotechnology. In order to obtain full control over the nanostructural evolution at the metal-polymer interface and its impact on optoelectronic properties, we employed the combination of in-situ time-resolved GISAXS [1] with in-situ surface differential reflectivity spectrometry during sputter deposition of gold on thin polystyrene films. We correlate the evolution of the metallic layer morphology with changes in the key scattering. This enabled us to identify the different growth regimes with their specific thresholds and permits a better understanding of the growth kinetics of gold clusters on polymer substrates. Our study opens up the opportunity to improve nanofabrication of tailored metal-polymer nanostructures for organic electronics like photovoltaic applications and plasmonic-based technologies. [1] Schwartzkopf et al., *Nanoscale* **5**, 5053-62 (2013).

DS 4.10 Mon 17:30 H 0111

**Metallic nanoparticles (Au, Al and Ag) blended into n-type organic semiconducting matrix of F4CuPc: morphology and electronic properties** — ●SERGEY BABENKOV<sup>1</sup>, OLGA MOLODTSOVA<sup>1</sup>, IRINA ARISTOVA<sup>2</sup>, OLEG VILKOV<sup>3</sup>, MAXIM TCHAPLYGUINE<sup>4</sup>, and VICTOR ARISTOV<sup>1,2,5</sup> — <sup>1</sup>DESY Hamburg, Germany — <sup>2</sup>ISSP RAS, Russia — <sup>3</sup>BESSY Berlin, Germany — <sup>4</sup>MAX-lab Lund, Sweden — <sup>5</sup>Uni Hamburg, Germany

Nowadays there is huge demand for more capacious, compact and faster memory storages. In this regard the resistive random-access memory (RRAM) with 3D cross point architecture filled out by organic based nano-composite film could become the new technological breakthrough. Such systems have two programmable high and low resistance states which can be controlled and probed by applying a voltage. Taking it into account, the morphology and electronic properties of nano-composite films based on blended aluminum, gold and silver nanoparticles into n-type organic semiconductor of fluorinated copper phthalocyanine (CuPcF4) have been investigated by means of TEM and SR-PES measurements as function of nominal amount of metal deposition. TEM measurements reveal organic film with self-assembled nanoparticles, whose size and distribution are strongly correlated with nominal amount of deposited metal. Moreover, comparative study of electronic properties self-assembled nanoparticles detects strong interaction of metal atoms with organic substrate. Acknowledgments: This work was supported by the RFBR Grant No. 13-02-00818 and the BMBF-Project No. 05K12GU2, PSP-Element No. U4606BMB1211.

DS 4.11 Mon 17:45 H 0111

**Structure and morphology of organic semiconductor-nanoparticle hybrids prepared by soft deposition** — ●RUPAK BANERJEE<sup>1</sup>, JIŘÍ NOVÁK<sup>1</sup>, CHRISTIAN FRANK<sup>1</sup>, MARIA GIRLEANU<sup>2</sup>, MARTIN BRINKMANN<sup>2</sup>, FALK ANGER<sup>1</sup>, CHRISTOPHER LORCH<sup>1</sup>, JOHANNES DIETERLE<sup>1</sup>, ALEXANDER GERLACH<sup>1</sup>, and FRANK SCHREIBER<sup>1</sup> — <sup>1</sup>Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany — <sup>2</sup>Institut Charles Sadron CNRS, 23 rue du loess, 67034 Strasbourg, France

We present an extensive structural evaluation of hybrid architectures prepared by the “non-invasive” incorporation of gold nanoparticles (AuNPs) within an organic semiconductor matrix of diindenoperylene (DIP). The hybrid structures were characterized by advanced X-ray scattering techniques including grazing incidence small angle scattering (GISAXS), grazing incidence X-ray diffraction (GID), X-ray reflectivity (XRR) and complemented by atomic force microscopy (AFM) and transmission electron microscopy (TEM) measurements. We show that different strategies of incorporating the nanoparticles in the host matrix lead to drastically different structure and morphology. Particularly remarkable is the morphological change observed in the matrix of DIP as well as the AuNPs due to the influence of organic solvents. It is also demonstrated that AuNPs can be successfully used as tunable templates for the growth of the organic semiconductors with desired island sizes and distances.

DS 4.12 Mon 18:00 H 0111

**Metal/biopolymer interface for packing application** — ●SHUN YU<sup>1,2</sup>, GONZALO SANTORO<sup>2</sup>, PENG ZHANG<sup>2</sup>, HESHMAT NOEI<sup>3</sup>, MIKAEL HEDENQVIST<sup>1</sup>, and STEPHAN ROTH<sup>2</sup> — <sup>1</sup>Fibre and Polymer Technology, Royal Institute of Technology, Stockholm, Sweden — <sup>2</sup>Photon Science, Deutsches Elektron-Synchrotron (DESY), Hamburg, Germany — <sup>3</sup>Nanolab, Deutsches Elektron-Synchrotron (DESY), Hamburg, Germany

Wheat gluten (WG), one of key biopolymers, has shown great potential to substitute some of the synthetic counterparts in terms of excellent foaming ability, oxygen barrier and mechanical properties. Their availability from renewable resources, biodegradable, and less energy consumption during the manufacture are suitable for packing

applications. Modern packaging industry, especially the food packaging, gradually turns to a complicated material design with a multilayer structure and nanocomposite components. In this study, we investigate the interfacial structures between chemical treated WG and noble metal thin films (i.e. Au and Ag) prepared by radio frequency sputter deposition. The WG chemical structure was investigated via IR spectroscopy. Grazing incidence small angle scattering technique was used to follow the entire thin film development of Au and Ag on top of WG in real-time. Acid and base treatment renders different WG film structure. It further causes the different growth mode of noble metals on top of both. Doping effects of acid and basic additives may play as a role of the driving forces behind.

DS 4.13 Mon 18:15 H 0111

**Dynamic glass transition of ultrathin poly(2-vinyl pyridine) films** — ●SHERIF MADKOUR<sup>1</sup>, HUAJIE YIN<sup>1</sup>, MARIEKE FUELLBRANDT<sup>1,2</sup>, and ANDREAS SCHOENHALS<sup>1</sup> — <sup>1</sup>BAM Bundesanstalt für Materialforschung und -prüfung, Berlin, Germany — <sup>2</sup>Stranski-Laboratorium für Physikalische und Theoretische Chemie/ Institut für Chemie, Technische Universität Berlin, Berlin, Germany

Specific heat spectroscopy utilizing differential AC-chip calorimetry in the frequency range from 1 Hz to 2 kHz with a sensitivity of pJ/K was employed to study the dynamic glass transition behavior of ultrathin poly(2-vinyl pyridine) (P2VP) films with thicknesses from 400 down to 10 nm. The amplitude and the phase angle of the complex differential voltage as a measure of the complex heat capacity were obtained as a function of temperature at given frequencies simultaneously. Both spectra were used to determine the dynamic glass transition temperature as a function of the film thickness. As a main result, no thickness dependence of the dynamic glass transition temperature or its width was observed for P2VP thin films down to a film thickness of 10 nm, within the experimental uncertainty of \*3 K. This also indicates that the extent of the cooperativity is essentially smaller than the lowest thickness. Further, contact angle measurement was employed to measure the polymer/substrate interfacial interaction, which was found to be strong (4.09mJ/m<sup>2</sup>). Consequently, an absorbed layer at the interface and an increase in T<sub>g</sub> should be detected. Therefore, further analyses are in progress as an endeavor to quantify the contributions of the interfacial and the free surface layers.

## DS 5: Transport: Topological Insulators 1 (joint session with DS, HL, MA, O)

Time: Monday 15:00–17:45

Location: A 053

### Invited Talk

DS 5.1 Mon 15:00 A 053

**The Wires’ Approach to Topological Insulators** — ●YUVAL OREG — Weizmann Institute of Science, Rehovot, Israel

We suggest a construction of a large class of topological states using an array of quantum wires. We will show how to construct a Chern insulator using an array of alternating wires that contain electrons and holes, correlated with an alternating magnetic field. A generalization to wires, with alternating spin-orbit couplings which give rise to integer and fractional (Abelian and non-Abelian) topological insulators, is then straightforward.

Following this construction we will discuss suggestions for two possible experiments which give rise to a fractional Josephson-effect and in addition a novel spin-resolved current correlation effect.

DS 5.2 Mon 15:30 A 053

**Helical Majorana surface states of strongly disordered topological superconductors with time-reversal symmetry** — ●RAQUEL QUEIROZ and ANDREAS SCHNYDER — Max Planck Institute for Solid State Research, Stuttgart, Germany

Noncentrosymmetric superconductors with strong spin-orbit coupling and the B phase of <sup>3</sup>He are possible realizations of topological superconductors with time-reversal symmetry. The nontrivial topology manifests itself at the material’s surface in terms of linearly dispersive helical Majorana modes protected by symmetry from disorder weaker than the superconducting gap. Using extensive numerical simulations, we investigate the stability and properties of these Majorana states under strong surface disorder, which influences both bulk and surface states. A critical crossover from weak to strong disorder is observed in both two and three dimensions, through which an extended state exactly at zero energy always persists. The localization properties of the

ingap states are studied through the distribution of the local density of states and level repulsion statistics.

DS 5.3 Mon 15:45 A 053

**Intrinsic conduction through topological surface states of insulating Bi<sub>2</sub>Te<sub>3</sub> epitaxial thin films** — ●KATHARINA HOEFER<sup>1</sup>, CHRISTOPH BECKER<sup>1</sup>, DIANA RATA<sup>1</sup>, JESSE SWANSON<sup>1,2</sup>, PETER THALMEIER<sup>1</sup>, and LIU HAO TJENG<sup>1</sup> — <sup>1</sup>Max Planck Institute for Chemical Physics of Solids, Dresden — <sup>2</sup>University of British Columbia, Vancouver

Topological insulators represent a new state of matter that open up new opportunities to create unique quantum particles. Many exciting experiments have been proposed by theory, yet, the main obstacle for their execution is material quality and cleanliness of the experimental conditions. The presence of tiny amounts of defects in the bulk or contaminants at the surface already mask these phenomena.

We present the preparation, structural and spectroscopic characterisation of MBE-grown Bi<sub>2</sub>Te<sub>3</sub> thin films that are insulating in the bulk. Moreover, temperature dependent four-point-probe resistivity measurements of the Dirac states on surfaces that are intrinsically clean were conducted. The total amount of surface charge carriers is in the order of 10<sup>12</sup> cm<sup>-2</sup> and mobilities up to 4600 cm<sup>2</sup>/Vs are observed.

Importantly, these results are achieved by carrying out the preparation and characterisation all in-situ under ultra-high-vacuum conditions [1].

[1] K. Hofer et al. PNAS, 2014, 111(42), 14979-14984.

DS 5.4 Mon 16:00 A 053

**Quantum interference of edge supercurrents in a two-dimensional topological insulator** — ●GRIGORY TKACHOV,

PABLO BURSET, BJÖRN TRAUZETTEL, and EWELINA HANKIEWICZ — Würzburg University

Josephson weak links made of two-dimensional topological insulators (TIs) exhibit magnetic oscillations of the supercurrent that are reminiscent of those in superconducting quantum interference devices (SQUIDS). We propose a microscopic theory of such a TI SQUID effect [1]. The key ingredient of our model is the exact treatment of the influence of an external magnetic field on the edge supercurrents. We show that this influence has the form of a 1D Doppler effect that describes the flux-controlled interference of the edge currents with superimposed suppression of Andreev reflection. Both long and short junctions are discussed. In particular, for long junctions the theory shows a temperature-driven crossover from the normal  $\Phi_0$ -periodic SQUID pattern to a  $2\Phi_0$ -quasiperiodic pattern consisting of a series of alternating even and odd peaks (where  $\Phi_0 = ch/2e$  is the magnetic flux quantum). The predicted even-odd effect is the signature of gapless (protected) Andreev bound states with a sawtooth dependence on the magnetic flux. Our findings may shed some light on the recently observed even-odd interference pattern in InAs/GaSb-based TI Josephson junctions, suggesting new operation regimes for nano-SQUIDS.

[1] G. Tkachov, P. Buset, B. Trauzettel, and E. M. Hankiewicz, arXiv:1409.7301.

DS 5.5 Mon 16:15 A 053

**Rashba spin-orbit coupling at the quantum spin Hall edge** — ●FLORIAN GEISSLER, FRANCOIS CREPIN, and BJÖRN TRAUZETTEL — Universität Würzburg, Institut für Theoretische Physik und Astrophysik, Germany

Not only since the discovery of the quantum spin Hall effect, and up to most recent questions in the context of topological insulating materials, transport through one-dimensional systems is a problem of great importance and interest. In a quantum spin Hall system, electron transport occurs in conducting edge channels, that are spin-filtered with respect to their direction of motion, and was shown to be topologically protected by time-reversal symmetry. We use the helical Luttinger liquid model to study transport in such systems, when the perfect conductance is perturbed. Particularly, we show that a potential source of backscattering is provided by the combination of a Rashba spin-orbit coupling (SOC) impurity and electron-electron interactions, even though time-reversal symmetry remains preserved. Based on both renormalization group and Keldysh calculations, the scaling of the conductance with the external bias is derived at zero temperature. Moreover, we illustrate, that such SOC-impurities may give rise to interesting effects when being present in an interface of a Luttinger liquid connected to a superconductor.

15 min. break.

DS 5.6 Mon 16:45 A 053

**Coexisting edge states and gapless bulk in topological states of matter** — YUVAL BAUM<sup>1</sup>, ●THORE POSSKE<sup>2</sup>, ION COSMA FULGA<sup>1</sup>, BJÖRN TRAUZETTEL<sup>2</sup>, and ADY STERN<sup>1</sup> — <sup>1</sup>Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot 76100, Israel — <sup>2</sup>Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany

We consider two dimensional systems in which edge states coexist with a gapless bulk. Such systems may be constructed, for example, by coupling a gapped two dimensional state of matter that carries edge states to a gapless two dimensional system in which the spectrum is composed of a number of Dirac cones. We find that in the absence of disorder the edge states could be protected even when the two systems are coupled, due to momentum and energy conservation. We distinguish between weak and strong edge states by the level of their mixing with the bulk. In the presence of disorder, the edge states may be stabilized when the bulk is localized or destabilized when the bulk is metallic. We analyze the conditions under which these two cases occur. Finally, we propose

a concrete physical realization for one of our models on the basis of bilayer Hg(Cd)Te quantum wells.

DS 5.7 Mon 17:00 A 053

**Spin texture of generic helical edge states** — ●ALEXIA ROD<sup>1</sup>, THOMAS L. SCHMIDT<sup>2</sup>, and STEPHAN RACHEL<sup>1</sup> — <sup>1</sup>Institut für Theoretische Physik, TU Dresden, Germany — <sup>2</sup>Department of Physics, University of Basel, Switzerland

Edge states of time-reversal topological insulators can be described as helical Luttinger liquids. The generic helical liquid is the most general model of a time-reversal invariant helical liquid without axial spin symmetry. This symmetry is usually broken in experimental realizations, and it has been shown that its absence changes the transport properties significantly [1]. For a translation invariant system, the breaking of axial spin symmetry manifests itself in a momentum-dependent rotation of the spin quantization axis. Its manifestation in real space has remained, however, elusive so far.

Here we show that one can extract the rotation of spin quantization axis also in real space, e.g. for topological insulator disks with broken spin symmetry but also other geometries which are not rotationally invariant [2]. This suggests that the concept of a generic helical liquid is independent of the microscopic model and the considered geometry.

[1] T.L. Schmidt, S. Rachel, F. von Oppen, L. Glazman, Phys. Rev. Lett. 108, (2012).

[2] A. Rod, T.L. Schmidt, S. Rachel, manuscript in preparation.

DS 5.8 Mon 17:15 A 053

**Manipulation of helical edge state transport by a quantum magnet** — ●PETER SILVESTROV<sup>1</sup>, PATRIK RECHER<sup>1</sup>, and PIET BROUWER<sup>2</sup> — <sup>1</sup>Institute for Mathematical Physics, TU Braunschweig — <sup>2</sup>Dahlem Center for Complex Quantum Systems, FU Berlin

Application of a magnetic field is usually considered as a way to open the gap in the spectrum of helical edge states, leading to a blocking of the edge current. Nevertheless, it was shown recently that the current is fully transmitted through the gapped region in case of interaction with a quantum magnet[1]. Here we consider other interesting features of the helical edge state current interacting with the magnet. First, we notice that although the current is transmitted, all electrons with energies close to the Fermi energy are fully reflected. The actual current is carried by the electrons with energies below the gap and well below the Fermi energy. This suggests that the magnet while allowing passing the current, fully blocks the thermal transport thereby acting as a cooler for the injected electron beam. Our second setup consists of two helical edges covered by the same magnet. The current injected into one edge creates a non-equilibrium magnetization driving a current in the second edge. The current in the first edge is now half-reflected and half-transmitted by the magnet. However, the partial reflection of the current does not cause any shot noise.

[1] Q.Meng, S.Vishveshwara, T.L.Hughes, arXiv:1312.7303.

DS 5.9 Mon 17:30 A 053

**Probing spin-polarized edge state superconductivity by Andreev reflection in in-plane magnetic fields** — ●ROLF W. REINTHALER, GRIGORY TKACHOV, and EWELINA M. HANKIEWICZ — Faculty of Physics and Astrophysics, University of Würzburg, Würzburg, Germany

Finding signatures of unconventional superconductivity in Quantum Spin Hall systems is one of the challenges of solid state physics. Here we induce superconductivity in a 3D topological insulator thin film to cause the formation of helical edge states, which are protected against backscattering even in finite magnetic fields. Above a critical in-plane magnetic field, which is much smaller than the critical field of typical superconductors, the quasi-particle gap closes, giving rise to energy-dependent spin polarization. In this regime the spin-polarized edge state superconductivity can be detected by Andreev reflection. We propose measurement setups to experimentally observe the spin-dependent excess current and  $dI/dV$  characteristics.

## DS 6: Organic photovoltaics and electronics - mostly cell design (jointly with CPP,DS)

Time: Monday 15:00–16:45

Location: EW 202

DS 6.1 Mon 15:00 EW 202

**Polymer/cathode interface barrier limiting the open circuit voltage in polymer:fullerene organic bulk heterojunction solar cells** — ●JAIRO CESAR NOLASCO — Energy and Semiconductor Research Laboratory, Department of Physics, Carl von Ossietzky University of Oldenburg, D-26111, Germany

Factors which limit the open circuit voltage  $V_{oc}$  in polymer bulk heterojunction solar cells is still a topic of controversy. Fundamentally, the  $V_{oc}$  is determined by the balance of photogeneration and recombination, with recombination occurring either at the internal donor/acceptor interface or at the contacts. In case of ohmic contacts the losses have been mainly attributed to the donor/acceptor interface, whereas for the case of non-ohmic contacts, the dominant losses have been discussed in terms of minority carrier surface recombination occurring at the acceptor/cathode interface. In this contribution it is demonstrated the existence of a majoritary free carrier recombination occurring at the polymer/cathode barrier interface [1].

[1] J. C. Nolasco, G. Ramos-Ortiz, J.L. Maldonado, O. Barbosa-Garcia, B. Ecker, E. Von Hauff, Appl. Phys. Lett., 104, 043308 (2014).

DS 6.2 Mon 15:15 EW 202

**Accurate Characterization of Serial Tandem Organic Solar Cells** — ●TONI MEYER, RONNY TIMMRECK, CHRISTIAN KÖRNER, KOEN VANDEWAL, and KARL LEO — Institut für Angewandte Photophysik, TU Dresden, Germany

A well known concept for further improvement of the efficiency of solar cells are tandem solar cells. The most common representative of this concept are the serial tandem solar cells (sTSC) where the subcells are connected electrically in series. Due to Kirchhoff's law this leads to a current limitation of the whole device by the subcell generating less current under a specific spectrum. For scientific comparison and practical application it is inevitable to determine the exact performance of such a device under different illumination conditions. However, the current limitation of a sTSC represents a major challenge for their characterization.

The spectrometric characterization, developed by Meusel et. al, represents a precise method of determining the performance of sTSC for any given illumination spectrum by using a multi-source sun simulator. We apply this method to a state of the art vacuum deposited sTSC with complementary absorbers and compare it to the minimal requirements of the standard ASTM E2236-05 for characterizing multijunction photovoltaic devices. We show that in case of differing fill factors of the subcells of the sTSC it is not sufficient to use only a single source sun simulator, which does usually not yield correct results for the solar cell efficiency in accordance with the standard reporting conditions.

DS 6.3 Mon 15:30 EW 202

**Investigation of semiconducting polymers with thermally cleavable side chains for application in multilayer devices II: Spectroscopy** — ●SABINA HILLEBRANDT<sup>1,5</sup>, JANUSZ SCHINKE<sup>2,5</sup>, TORBEN ADERMANN<sup>3</sup>, ERIC MANKEL<sup>4,5</sup>, ROBERT LOVRINCIC<sup>2,5</sup>, MANUEL HAMBURGER<sup>3,5</sup>, TOBIAS GLASER<sup>1,5</sup>, WOLFRAM JAEGERMANN<sup>4</sup>, WOLFGANG KOWALSKY<sup>2,5</sup>, and ANNEMARIE PUCCI<sup>1,5</sup> — <sup>1</sup>Kirchhoff-Institut für Physik, Universität heidelberg — <sup>2</sup>Institut für Hochfrequenztechnik, Technische Universität Braunschweig — <sup>3</sup>Organisch-Chemisches Institut, Universität Heidelberg — <sup>4</sup>Institut für Materialwissenschaften, Technische Universität Darmstadt — <sup>5</sup>Innovationlab GmbH, Heidelberg

Conjugated polymers are a promising material class for solution processed organic electronic devices. A major challenge in solution processing of multi-layer devices is the limited number of options regarding orthogonal solvents. Therefore solubility alteration of the functional layers is crucial for facilitating device fabrication. In this talk the removal of side-chains of novel naphthalene tetracarboxydiimide based semiconducting polymers by thermal treatment is analyzed by infrared transmission spectroscopy, photoelectron spectroscopy and charge transport characteristics in organic field effect transistors. Side chain residuals in the films are correlated to temperature and duration of the thermal treatment. Solvent stability is tested by washing the films after thermal treatment. Our findings show that although side chains can be removed completely after washing the thermally treated

films, the charge transport strongly depends on the parameters used for this treatment.

DS 6.4 Mon 15:45 EW 202

**Understanding thickness dependent onset voltage shifts in OLED IV-characteristics I: Internal electric field distributions** — ●MAYBRITT KÜHN<sup>1,2</sup>, ERIC MANKEL<sup>1,2</sup>, CHRISTOP PFLUMM<sup>3</sup>, THOMAS MAYER<sup>1,2</sup>, and WOLFRAM JAEGERMANN<sup>1,2</sup> — <sup>1</sup>Technische Universität Darmstadt, Institute of Materials Science — <sup>2</sup>InnovationLab GmbH, Heidelberg — <sup>3</sup>Merck KGaA, Darmstadt

Steady-state IV measurements are used as important characterization method for organic light-emitting diodes (OLEDs). Surprisingly, in some OLED devices the current onset voltage increases significantly depending on the emission layer (EML) thickness by approximately 2.7V/100nm. For experimental investigations of this phenomenon we focus on a three layer device architecture, using two different isomers synthesized by Merck as transport material in the EML - one showing changes in onset voltage (EML-A) the other (EML-B) not. To investigate the onset voltage shift the mean electric fields in the respective layers are determined in dependence of the current density. Therefore, systematic layer thickness variations of the injection layers and both EML materials were performed and the respective IV characteristics were evaluated. In contrast to EML-B a large field enhancement in EML-A can be identified induced by discontinuities of the electric field at the EML-A contacts. Using a simple drift model both EML field distributions and the discontinuities can be described quantitatively. Furthermore they can be allocated to a lack of bulk charge carriers, probably induced by an energetic interface barrier or trapped interface charges. A further consideration of the topic will be done in part 2.

DS 6.5 Mon 16:00 EW 202

**Understanding thickness dependant onset voltage shifts in OLED IV-characteristics II: Equilibrium band alignments and their impact on the steady-state situation** — ●ERIC MANKEL<sup>1,2</sup>, MAYBRITT KÜHN<sup>1,2</sup>, CHRISTOP PFLUMM<sup>3</sup>, THOMAS MAYER<sup>1,2</sup>, and WOLFRAM JAEGERMANN<sup>1,2</sup> — <sup>1</sup>TU Darmstadt, Darmstadt — <sup>2</sup>InnovationLab GmbH, Heidelberg — <sup>3</sup>Merck KGaA, Darmstadt

Steady-state IV measurements are used as important characterization method for organic light-emitting diodes (OLEDs). Surprisingly, in some OLED devices the current onset voltage increases significantly depending on the emission layer (EML) thickness by approximately 2,7V/100nm. In part 1 we used two isomers - one showing changes in onset voltage (EML-A) the other (EML-B) not - and concluded that enhanced internal electric fields explain this unexpected behavior. Here in part 2 we present how interface band offsets (a), interface dipoles (b) and space charge regions (c) influence the field distribution under steady-state conditions. First we show the impact of a, b and c on the electric and the electrochemical potential distribution as well as the IV-characteristic of a two layer model device. Then we allocate these results to the measured interface discontinuities of the electric field shown in part 1. Finally we present the interface band diagrams of the EML layers and the respective contact layers measured by XPS layer-by-layer experiments. The values for a, b and c were used to model the IV-characteristics of both, EML-A and EML-B containing devices. The described onset voltage shift can successfully be reproduced.

DS 6.6 Mon 16:15 EW 202

**SWNT:Fullerene solar cells** — ●ALEXEY GAVRIK<sup>1</sup>, STEFAN VÄTH<sup>1</sup>, ANDREAS SPERLICH<sup>1</sup>, IMGE NAMAL<sup>2</sup>, FLORIAN SPÄTH<sup>2</sup>, TOBIAS HERTEL<sup>2</sup>, and VLADIMIR DYAKONOV<sup>1,3</sup> — <sup>1</sup>Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — <sup>2</sup>Physical and Theoretical Chemistry II, Julius Maximilian University of Würzburg, 97074 Würzburg — <sup>3</sup>ZAE Bayern, 97074 Würzburg

Single-wall carbon nanotubes (SWNTs) are a promising material for application in organic solar cells due to their attractive properties: solution processability, broadband absorption, high charge carrier mobility. Moreover, by selecting SWNTs of one chirality, it is possible to choose the energy gap, which determines the light absorption spectrum and therefore, solar cell performance.

In this study, solar cells were prepared using blends of (6,5)-SWNTs

and the soluble fullerene PC<sub>60</sub>BM. External quantum efficiency (EQE) spectra show spikes at ca. 570, 870 and 1000 nm, which correlates with absorption bands of SWNTs. This proves that charge carriers in SWNTs contribute to the photocurrent. Moreover, SWNTs are showing high performance of converting light into electricity: even at low SWNTs:fullerene ratios (1:100) the current from SWNTs in the EQE spectrum is comparable to the fullerenes' contribution.

This study shows the potential for the application of (6,5)-SWNTs as an active material in organic solar cells. While the device performance is still limited by film thickness and overall device characteristics, we were able to fabricate solar cells with reasonable efficiency.

DS 6.7 Mon 16:30 EW 202

**Effective injection barriers of organic Schottky diodes** — ●THORSTEN ARNOLD and FRANK ORTMANN — Institute for Mate-

rials Science and Dresden Center for Computational Material Science, TU Dresden, Germany

We describe electron transport through organic semiconductors connected to two metallic electrodes. The microscopic approach is based on a dynamic master-equation and Poisson equation describing the space charge potential. Disorder is modeled by a Gaussian site energy distribution. The current-voltage characteristic depends on the effective height of the injection barrier at the metal-semiconductor interface, which can be influenced by several effects, and the bulk properties.

The model is applied to a Schottky diode with different work functions of the electrodes. The influence of bulk and surface disorder on the rectification of the diode are analyzed for various temperatures. Furthermore, the influence of the space charge on the effective injection barrier height is investigated.

## DS 7: Organic photovoltaics and electronics - mostly properties of the absorber (jointly with CPP,DS)

Time: Monday 17:00–19:00

Location: EW 202

DS 7.1 Mon 17:00 EW 202

**Structural and electronic properties of planar organic heterojunction interfaces and their impact on diode characteristics** — ●A. OPITZ<sup>1</sup>, A. WILKE<sup>1</sup>, N. KOCH<sup>1,2</sup>, U. HÖRMANN<sup>3</sup>, W. BRÜTTING<sup>3</sup>, R. HANSSON<sup>4</sup>, and E. MOONS<sup>4</sup> — <sup>1</sup>Humboldt-Universität zu Berlin, Germany — <sup>2</sup>Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany — <sup>3</sup>University of Augsburg, Germany — <sup>4</sup>Karlstad University, Sweden

The structural and electronic properties of organic heterojunction interfaces are of paramount importance. Here two prototypical interfaces are discussed: diindenoperylene (DIP) combined with fullerene (C<sub>60</sub>) and copper-phthalocyanine combined with its perfluorinated analog. Angle dependent near edge X-ray absorption fine structure measurements were performed to determine the molecular orientation and compared to measurements of the frontier level alignment by ultraviolet photoelectron spectroscopy.

The orientation of the rod-like DIP molecules is unaffected upon deposition of spherical C<sub>60</sub> molecules on top and vacuum level alignment appears. In contrast, cofacial lying interface layers with  $\pi$ -orbital stacking of the two phthalocyanines is observed together with energy level bending. These results will be related to the solar cell performance [1,2]. The combined experimental approach results in a comprehensive model of the investigated interface. The presence of a  $\pi$ -orbital stacking is also of interest for ground-state charge transfer.

[1] J. Wagner et al., *Adv. Funct. Mater.* 20 (2010) 4295.

[2] A. Opitz et al., *Org. Electron.* 10 (2009) 1259.

DS 7.2 Mon 17:15 EW 202

**Unified model approach for hybrid charge transfer states in organic-organic heterostructures** — TINO MEISEL, ●PAUL BEYER, GEORG HEIMEL, NORBERT KOCH, and ANDREAS OPITZ — Humboldt-Universität zu Berlin, Germany

There are different electronic coupling mechanisms for organic-organic heterostructures, which ultimately determine the charge separation in solar cells or the doping efficiency in blended systems. Here, these charge transfer mechanisms are investigated in blends of diindenoperylene (DIP) with different acceptor materials, namely core functionalized perylene alkyldiimide with cyano groups (PDIR-CN<sub>2</sub>) and perfluoronaphthalene-diyldiene dimalononitrile (F6TCNNQ), which show compatible optical gaps. To scrutinize the interplay between these molecules a combination of atomic force microscopy (AFM), UV/Vis/NIR absorption spectroscopy and electrical conductivity measurements is used.

From absorption spectroscopy the formation of new absorption features is clearly seen in blends with both acceptors. An increase in electrical conductivity is observed for DIP:F6TCNNQ blends, which is absent in the DIP:PDIR-CN<sub>2</sub> case. The formation of distinct islands in AFM shows a difference in morphology between pristine and blended films. From these investigations we conclude the appearance of new charge transfer states and a unified hybridization model is applied to explain the different regimes of charge transfer behavior.

DS 7.3 Mon 17:30 EW 202

**New Insights on traps states in organic semiconductor devices using transient current measurements on metal-insulator-semiconductor capacitors** — HIPPOLYTE HIRWA and ●VEIT WAGNER — Jacobs University, Bremen, Germany

A Transient current measurement technique utilizing metal-insulator-semiconductor (MIS) capacitors is developed, which does not need a light stimulus. The technique offers insights on carrier trapping states such as capture time of trapping states and the attempt-to-escape frequency of trapped carriers. For the analysis of the measurements Fourier transformation of impedance-based circuit models to the time domain as well as direct numerical simulation of transient current of MIS capacitors were used. Numerical simulations allow to go beyond the usual assumptions of negligible extraction time for de-trapped carriers. It is shown, that re-trapping events are relevant in order to extract the proper band tail density of states and the corresponding characteristic parameters. For e.g. P3HT an exponential density of states with a total density of  $4 \cdot 10^{17} \text{ cm}^{-3}$  and a width of 50 meV was found to be representative for the band tail. Analyzing the multiple trap and release behavior in the numerical simulation, the average capture time and the attempt-to-escape frequency of band tail states were found to be  $10^{-10} \text{ s}$  and  $10^8 \text{ s}^{-1}$ , respectively.

DS 7.4 Mon 17:45 EW 202

**Influence of trap distribution on the electrical characteristics of organic solar cells** — ●ALEXANDER WAGENPFAHL, ROBERT HANFLAND, and CARSTEN DEIBEL — Chemnitz University of Technology, Institute of Physics, 09126 Chemnitz, Germany

Charge carrier traps have a strong impact on the performance of organic solar cell devices. It remains unclear, however, if either a Gaussian or an exponential distribution of the density of states (DOS) describes most organic photovoltaic devices better. In our work, we apply a macroscopic drift-diffusion simulation in combination with the multiple-trapping and release model to examine how the DOS distribution influences the current-voltage characteristics, diode ideality factor and effective charge carrier mobility of organic solar cells. We compare our findings to corresponding experimental data from different types of organic solar cells to determine the likely DOS shape. Its impact on the experimental device characteristics will be discussed.

DS 7.5 Mon 18:00 EW 202

**Investigation of DCV5T-Me Solar Cells on Presence of Traps** — ●NATALIA SERGEEVA<sup>1</sup>, JANINE FISCHER<sup>1</sup>, PAUL PAHNER<sup>1</sup>, LORENZO BURTONE<sup>1,2</sup>, CHRISTIAN KÖRNER<sup>1</sup>, KOEN VANDEWAL<sup>1</sup>, and KARL LEO<sup>1</sup> — <sup>1</sup>Institut für Angewandte Photophysik Technische Universität Dresden, Germany — <sup>2</sup>Globalfoundries, Dresden, Germany

Traps play an important role in the performance of organic solar cells (OSC). They influence the mobility, the amount of extracted charge carriers at the electrodes and lead to trap assisted recombination. Better understanding of traps is necessary to further improve the efficiency of OSC. We investigate bulk heterojunction OSC based on the donor material DCV5T-Me with regards to the presence of traps by performing Impedance spectroscopy (IS) and temperature stimulated currents (TSC) measurements. We discuss the observed impedance and TSC

spectra, evaluate the density and distribution of trap states and the attempt to escape frequency.

DS 7.6 Mon 18:15 EW 202

**Charge transport: Mobility in organic donor-acceptor blends for photovoltaics** — ●JOHANNES WIDMER, JULIA OELKER, JANINE FISCHER, CHRISTIAN KOERNER, and KARL LEO — IAPP (Institut für Angewandte Photophysik), TU Dresden, Germany

The charge carrier mobility  $\mu$  is the key parameter describing charge transport in semiconductors. In amorphous material with predominating hopping transport, the effective mobility is affected by disorder. The resulting  $\mu$  varies with electric field strength  $F$  and charge carrier density  $n$ , and is influenced by the layer morphology.

In this contribution, we analyze the mobility of various small molecule organic semiconductors in neat as well as blend layers. The mobility is measured by means of electric potential mapping (POEM), varying the thickness of single carrier devices and evaluating them at constant current density.[1] This measurement technique allows for resolving the field dependence and the density dependence of  $\mu(F, n)$  independently of each other, separately for electrons and holes.

Substrate heating during the deposition of donor-acceptor blend layers is known to substantially improve the device performance of solar cells, and we show which role the charge carrier mobility plays in this context. Furthermore, the influence of the blend ratio on  $\mu$  is investigated, which allows for a refined interpretation of the role of the acceptor phase in hole transport. These findings improve the understanding of charge transport in organic solar cells and inspire paths for efficient further improvement of device performance.

[1] Widmer et al., *OrgEl* 14, p. 3460 (2013)

DS 7.7 Mon 18:30 EW 202

**Mobility Relaxation in PTB7:PC<sub>70</sub>BM on nanosecond timescale** — ●ANDREAS FRITZE<sup>1</sup>, ANDREAS SPERLICH<sup>1</sup>, CARSTEN DEIBEL<sup>2</sup>, and VLADIMIR DYAKONOV<sup>1,3</sup> — <sup>1</sup>Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — <sup>2</sup>Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz — <sup>3</sup>ZAE Bayern, 97074 Würzburg

For photovoltaics, charge carrier lifetime is an essential parameter due to its influence on short circuit current, and thus on power conversion efficiency. In organic photovoltaics, for several material systems, charge carrier lifetime exceeds predictions from recombination

models by orders of magnitude. In literature, this phenomenon is discussed in the context of reduced Langevin recombination, for instance the high-efficiency bulk heterojunction polymer fullerene solar cell PTB7:PC<sub>70</sub>BM, it is shown that recombination is also reduced. However, the physical processes responsible for these low recombination rates, such as mobility relaxation, energetic traps, and morphological traps, are hard to observe separately. Here, we present simultaneous transient absorption (TA) and transient microwave conductivity (TRMC) measurements on PTB7:PC<sub>70</sub>BM films. From the experimental data we calculate time dependent mobility, since TA is sensitive to charge carrier density and TRMC is sensitive to conductivity. A relaxation of mobility on these time scales is measured the first time separately. Thus, we can distinguish mobility relaxation from other recombination influencing processes in PTB7:PC<sub>70</sub>BM.

DS 7.8 Mon 18:45 EW 202

**OTRACE: The technique to study charge carrier mobility and lifetime in organic thin film solar cells under real operating conditions** — ●ANDREAS BAUMANN<sup>1</sup>, ANDREAS ZUSAN<sup>2</sup>, and VLADIMIR DYAKONOV<sup>1,2</sup> — <sup>1</sup>Bayerisches Zentrum für Angewandte Energieforschung, Am Galgenberg 87, D-97074 Würzburg — <sup>2</sup>Experimentelle Physik 6, Julius-Maximilians-Universität Würzburg, Am Hubland, D-97074 Würzburg

For the development and design of new promising semiconducting materials for organic electronics material parameters like the mobility and the lifetime of photogenerated charge carriers need to be investigated and optimized. Usually, techniques such as TOF, SCLC, or photo-CELIV are used to study the charge carrier transport. Especially, the latter technique principally enables one to study both charge carrier mobility and lifetime. However, all of these techniques are not really suited to study real solar cell devices under ambient conditions. With our newly developed experimental method of open circuit corrected transient charge extraction (OTRACE)[1] it is feasible to easily determine the charge carrier mobility and lifetime under operating conditions of the solar cell device. In addition, the mobility determined by OTRACE is the most relevant one for organic solar cells at open circuit conditions without suffering from injected charge carriers, which would result in major RC limitations. In combination with IV measurement this technique can be easily used for material screening producing fast output of relevant solar cell parameters. [1] Baumann et. al., *AM*, 2012, 24(32): p. 4381-4386.

## DS 8: Application of Thin Films

Time: Monday 18:45–20:00

Location: H 0111

DS 8.1 Mon 18:45 H 0111

**Physics behind the growth of Multilayer Zone Plates** — ●CHRISTIAN EBERL<sup>1</sup>, FLORIAN DÖRING<sup>1</sup>, MARKUS OSTERHOFF<sup>2</sup>, HANS HOFSSÄSS<sup>3</sup>, TIM SALDITT<sup>2</sup>, and HANS-ULRICH KREBS<sup>1</sup> — <sup>1</sup>Institute for Materialphysics — <sup>2</sup>Institute for X-ray physics — <sup>3</sup>II. Institute of Physics, University of Göttingen, Germany

Due to the small wavelength and high penetration depth, X-ray microscopy is an auspicious technique for improved investigations of materials on nm-scale. For this, multilayer zone plates (MZP) with well-defined and smooth multilayers of low thickness grown on wires are promising focusing elements. We already have shown that high quality MZPs with sub-5nm focus size for hard x-rays can be fabricated using the combination of pulsed laser deposition (PLD) and focused ion beam (FIB) [1,2]. However, the growth of such multilayers onto wires with diameters of down to 500 nm is a challenging and ambitious project: During the multilayer growth occur stoichiometric changes, both element specific and angular dependent resputtering and backscattering as well as interfacial interactions. In order to control these effects, a deep understanding of the underlying processes is essential [2]. For this, detailed studies have been carried out using complementary methods such as X-ray diffraction (XRD), X-ray reflectivity (XRR), transmission electron microscopy (TEM) in cross-section as well as SDTrimSP simulations. Here, the most recent results obtained during growth of Ta<sub>2</sub>O<sub>5</sub>/ZrO<sub>2</sub>-multilayers leading to high quality MZPs are discussed. [1] Döring et al., *Opt. Expr.* 21 (2013); [2] Eberl et al., *Appl. Surf. Sci.* 307 (2014)

DS 8.2 Mon 19:00 H 0111

**Chromium/Scandium attosecond multilayer mirrors** — ●ALEXANDER GUGGENMOS<sup>1,2</sup>, STEFAN RADÜNZ<sup>1,2</sup>, MICHAEL JOBST<sup>2</sup>, MARCUS OSSIANDER<sup>2</sup>, JOHANN RIEMENSBERGER<sup>2</sup>, BERT NICKEL<sup>1</sup>, CHRISTINA SCHEU<sup>3</sup>, ERIC GULLIKSON<sup>4</sup>, REINHARD KIENBERGER<sup>2,5</sup>, FERENC KRAUSZ<sup>1,2</sup>, and ULF KLEINEBERG<sup>1,2</sup> — <sup>1</sup>LMU München, Fakultät für Physik, Garching, Germany — <sup>2</sup>MPQ, Garching, Germany — <sup>3</sup>LMU, Fakultät für Chemie, München, Germany — <sup>4</sup>CXRO, Lawrence Berkeley National Lab, Berkeley, USA — <sup>5</sup>TUM, Fakultät für Physik, Garching, Germany

Recent advances in the development of attosecond soft X-ray sources ranging into the water window spectral range, between the 1s states of carbon and oxygen (284 eV–543 eV), are also driving the development of suited broadband multilayer optics for steering and shaping attosecond pulses, enabling for the first time the unique investigation of ultrafast electronic processes within the core states of bio-molecules as proteins or other organic materials. Current attosecond experiments in the sub-200 eV range also benefit from this optic improvement. We present our achievements in optimizing ion-beam deposited Cr/Sc multilayer mirrors by a tailored material dependent deposition and interface polishing process, which offers attosecond mirrors from 140 eV up to 400 eV, thus present and future attosecond optics. Experimental results from measurements using X-ray reflectometry, XUV reflectometry as well as attosecond streaking characterization are shown and discussed.

DS 8.3 Mon 19:15 H 0111

**Fabrication of GDC membranes for electrical characterization** — ●FLORIAN KUHLMANN<sup>1,3</sup>, MATTHIAS T. ELM<sup>1,2</sup>, DANIEL REPPIN<sup>1</sup>, TORSTEN HENNING<sup>1</sup>, JÜRGEN JANEK<sup>2</sup>, STEFAN KOLLING<sup>3</sup>, and PETER J. KLAR<sup>1</sup> — <sup>1</sup>I. Physikalisches Institut, Justus Liebig University,

Heinrich-Buff-Ring 16, DE-35392 Giessen, Germany — <sup>2</sup>Physikalisch-Chemisches Institut, Justus Liebig University, Heinrich-Buff-Ring 58, DE-35392 Giessen, Germany — <sup>3</sup>Technische Hochschule Mittelhessen University of Applied Sciences Wiesenstrasse 14, DE-35390 Giessen, Germany

The oxygen-ion conductor GDC (gadolinium doped ceria) is an attractive material for the use as electrolyte in solid oxide fuel cells operating between 500 °C - 800 °C. Its rather high ionic conductivity is caused by oxygen vacancies which are formed when doping with gadolinium. For lowering the operation temperature of the SOFCs, miniaturization and reduction of the film thickness is needed. Another application of thin microfabricated GDC films may be their utilization as solid-state ion source.

For the fabrication of free-standing membranes, GDC thin films were deposited onto a Si-Wafer by CVD. Afterwards the silicon was partially removed by etching. The shape of the membranes is defined by the masking patterns in SiO<sub>2</sub>. In order to measure the electric properties using electrochemical impedance spectroscopy, Pt electrodes were deposited onto the free-standing membranes. Results of investigations of the correlation between the lateral dimensions of the membrane, its thickness and its total conductivity will be discussed.

DS 8.4 Mon 19:30 H 0111

**Spike-timing dependent plasticity in BiFeO<sub>3</sub> based artificial synapses** — ●N. DU<sup>1</sup>, T. YOU<sup>1</sup>, M. KIANI<sup>1</sup>, C. MAYR<sup>2</sup>, R. SCHUEFFNY<sup>3</sup>, D. BUERGER<sup>1</sup>, I. SKORUPA<sup>1,4</sup>, O. G. SCHMIDT<sup>1,5</sup>, and H. SCHMIDT<sup>1</sup> — <sup>1</sup>TU Chemnitz — <sup>2</sup>University of Zurich and ETH Zurich — <sup>3</sup>TU Dresden — <sup>4</sup>HZDR — <sup>5</sup>IFW Dresden

With the rapid progress in complementary metal-oxide-semiconductor (CMOS) integrated circuit technology, also a fast development of neuromorphic cognitive systems is expected. In this work spike-timing dependent plasticity (STDP) [1] with one pairing of a single presynaptic spike and of a single postsynaptic spike has been investigated in BiFeO<sub>3</sub>-based artificial synapses. The forming-free, nonvolatile, analog resistive switching of BiFeO<sub>3</sub> [2] allows to adjust the synaptic weight of BiFeO<sub>3</sub>-based artificial synapses in dependence on the time delay between the single pre- and postspike in classical STDP with 60-80 sin-

gle pairings [3] and in STDP with one single pairing. Due to the easy pulse sequence in one single pairing STDP, the time delay could be reduced to few microseconds, memory consolidation in delay learning could be investigated, and energy consumption per setting pulse could be reduced to only 4.5 pJ. Using BiFeO<sub>3</sub>-based artificial synapses with different flexible electrodes [4], we have realized STDP, Anti-STDP and both STDP/Anti-STDP within a single cell! [1] G. S. Snider, In Proc. IEEE Int. Symp. Nanoscale Architectures, 85-92 (2008) [2] Y. Shuai, N. Du et al., IEEE Elec. Dev. Lett. 34, 54-56 (2013) [3] C. Mayr, N. Du et al., Adv. Neural Inf. Process. Syst. 25, 1700-1708 (2012) [4] T. You, N. Du et al., Adv. Funct. Mater. 24, 3357-3365 (2014)

DS 8.5 Mon 19:45 H 0111

**Tip radius dependence of Young's modulus of 2D materials extracted via nanoindentation** — ●GERARD VERBIEST, JAN-FELIX MONEKE, and CHRISTOPH STAMPFER — JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany

Tow-dimensional (2D) materials are known for their remarkable electronic, optical, and mechanical properties. For example, graphene is only one atomic layer thick, but it is far stronger than steel and has an extremely high Young's Modulus of 1.02 TPa.

The standard way of determining the Young's Modulus of 2D materials is via nanoindentation experiments. In these experiments, a cantilever is used to indent a suspended part of the 2D material. From these measurements, one obtains the force on the 2D material as a function of the indentation depth into the 2D material. These curves strongly depend on the Young's modulus of the material. However, to extract the Young's modulus, one has to resort to an analytical model. Usually, one assumes a point load indenter in the center of the suspended 2D material.

Here we show that this model of a point load indenter in the center is not valid. Using the full nonlinear elasticity theory, we calculated the force vs. indentation depth for various tip radii of the cantilever and various indentation positions. Analyzing these curves with the point load model shows an overestimation of the Young's modulus by more than a factor 4 for a tip radius of 10 nm.

## DS 9: Focussed Session: Doped Si nanostructures (joint session with HL)

Time: Tuesday 9:30–13:00

Location: H 2032

### Invited Talk

DS 9.1 Tue 9:30 H 2032

**Electronic doping of crystalline silicon nanoparticles** — ●RUI N. PEREIRA — Walter Schottky Institut and Physik-Department, Technische Universität München, Germany — Department of Physics and I3N, University of Aveiro, 3810-193 Aveiro, Portugal

Crystalline silicon nanoparticles (NPs) have been attracting much research interest due to their remarkable electronic, optical, and chemical properties. Si NPs combine the processing advantages enabled by nanoparticles with the unique features of Si at the nanoscale such as wavelength tunable light emission and multiple exciton generation. The natural abundance of silicon and its dominant role in microelectronics industry may also facilitate the introduction of Si NPs in commercial products such as solar cells and light emitting devices. The essential role played by doping in semiconductor technology has in recent years triggered the study of doping of Si NPs with n- and p-type dopants. In this presentation a review of the current knowledge of doping in Si NPs will be given. Particular focus will be given to NPs synthesized from gas-phase in silane plasmas, with which most of the investigations reported so far have been carried out.

DS 9.2 Tue 10:00 H 2032

**Silicon nanocrystal thin films for solution-cast electronics** — ●WILLI AIGNER<sup>1</sup>, MARKUS WIESINGER<sup>1</sup>, STANISLAV ABRAMOV<sup>1</sup>, HARTMUT WIGGERS<sup>2</sup>, RUI N. PEREIRA<sup>1,3</sup>, and MARTIN STUTZMANN<sup>1</sup> — <sup>1</sup>Walter Schottky Institut and Physics Department, Technische Universität München, Garching, Germany — <sup>2</sup>Institute for Combustion and Gasdynamics - Reactive Fluids, Universität Duisburg-Essen, Duisburg, Germany — <sup>3</sup>Institute for Nanostructures, Nanomodelling and Nanofabrication, University of Aveiro, Aveiro, Portugal

In the last years, high-performance thin-film field-effect transistors (FETs) with an active layer of solution-processed semiconductor

nanocrystals (NCs) films were demonstrated. However, few studies apply Si NCs, which are environmentally favorable and offer controlled n- and p-type doping. Recently, FETs using intrinsic Si NCs [1], as well as Si NC films doped with an electronic coupling agent [2] have been reported. In this work, we carried out a comprehensive study on the morphology and its influence on the electrical properties of Si NC thin films deposited by spray-coating. The effect of film thickness and NC size was investigated studying the electrical characteristics of FETs such as current-voltage behavior, hysteresis and ambipolar conduction under illumination. As we observe a strong dependence on morphology, we optimized our deposition parameters and achieved FETs with field-effect mobilities one order of magnitude higher than reported in the literature so far [1,2].

[1] Z. C. Holman, *et al.* Nano Lett. **10**, 2661 (2010) [2] R. N. Pereira, *et al.* Nano Lett. **14**, 3817 (2014)

### Invited Talk

DS 9.3 Tue 10:15 H 2032

**Impurity doping of Si nanocrystals studied by single-quantum-dot spectroscopy** — ●JAN VALENTA<sup>1</sup>, ILYA SYCHUGOV<sup>2</sup>, JAN LINNROS<sup>2</sup>, and MINORU FUJII<sup>3</sup> — <sup>1</sup>Department of Chemical Physics & Optics, Charles University, Prague, Czechia — <sup>2</sup>Materials and Nano Physics, Royal Institute of Technology, Kista-Stockholm, Sweden — <sup>3</sup>Department of Electrical & Electronic Engineering, Kobe University, Nada, Japan

Recent research effort proved that doping of nanostructured semiconductors is much more complicated than in bulk due to the self-purification effect, increasing formation energy of substitutional doping sites etc. In order to get a deeper insight on impurity effects in Si nanocrystals (NCs) we applied single NC spectroscopy to study luminescence of two types of samples: (i) random quantum dots prepared by etching of highly doped (B, P, As, Sb) SOI wafers, (ii) highly B and P co-doped Si NCs formed by sputtering, annealing and etching. The

effect of B, P, As, and Sb impurities on individual emission spectra are determined by comparison with the undoped NCs. From the statistical analysis of the luminescence spectra, the donor ionization energies for NCs emitting in the range of 1.5-2 eV are estimated to be 140-200 meV, while the exciton-impurity binding energy for As and Sb-doped NCs is found to be about 40-45 meV. It means that both the donor ionization energy and the excitonic binding energy are increased by an order of magnitude compared to bulk Si. The luminescence spectra of heavily B,P co-doped Si NCs are characterized by a very broad emission band ( $>0.2\text{eV}$ ) even at low temperature (10 K).

**Invited Talk** DS 9.4 Tue 10:45 H 2032  
**Active Silicon Nanovolume Doping: Failure and Alternatives** — •DIRK KÖNIG — University of New South Wales, Sydney, Australia

We report on phosphorous (P) doping of SiNC/SiO<sub>2</sub> systems [1]. Relevant P configurations within SiNCs, at SiNC surfaces, within the sub-oxide interface shell and in the SiO<sub>2</sub> matrix were evaluated by hybrid (h-) DFT. Atom probe tomography (APT) and its statistical evaluation provide detailed spatial P distributions. We obtain ionization states of P atoms in SiNC/SiO<sub>2</sub> systems at room temperature using X-ray absorption near edge structure (XANES) spectroscopy. P K shell energies were confirmed by h-DFT. While P diffuses into SiNCs and predominantly resides on interstitial sites, its ionization probability is extremely low; free localized electrons to SiNCs are not provided.

As alternative, SiO<sub>2</sub> and Si<sub>3</sub>N<sub>4</sub> create substantial energy offsets of electronic states in SiNCs [2]. h-DFT, interface charge transfer and experimental verifications arrive at the same NC size below which the embedding dielectric dominates their electronic properties. An increased energy gap was found for Si NCs in Si<sub>3</sub>N<sub>4</sub> vs. SiO<sub>2</sub> by h-DFT and confirmed in experiment. We describe the interface impact as nanoscopic field effect and show that the energy offset is very robust and controllable. As application example, we propose an undoped CMOS-compatible and CMOS technology-compatible Si-Nanowire MISFET.

[1] D. König, S. Gutsch, H. Gnaser et al., *Nature Sci. Rep.*, accepted for publication (2014)

[2] D. König, D. Hiller, S. Gutsch et al., *Adv. Mater. Interf.* (2014); <http://onlinelibrary.wiley.com/doi/10.1002/admi.201400359/abstract>

15 min. break.

**Invited Talk** DS 9.5 Tue 11:30 H 2032  
**Doping issues in semiconductor field-effect transistors** — •JOACHIM KNOCH — Institute of Semiconductor Electronics, RWTH Aachen University, Aachen, Germany

The functionality of silicon devices such as transistors, solar cells etc. rely on the ability to create doping profiles. However, due to the continued downscaling of device dimensions doping becomes increasingly difficult due to a number of fundamental reasons. First, dopants will be statistically distributed within the silicon nanostructures leading to a dopant fingerprint that results in fluctuations of e.g. electronic transistor characteristics from device to device. Second, studying the resistivity of in-situ doped, VLS-grown nanowires we were able to show that with decreasing nanowire diameter the resistivity increases due to a deactivation of dopants. The reason for the deactivation was shown to be the modified effective dielectric environment if the nanowire diameter is scaled down. In turn, the deactivation results in larger parasitic re-

sistances of the contacts of e.g. transistors, substantially deteriorating their performance. Third, ultimately scaled conventional field-effect transistors (FETs) and in particular novel device architectures such as band-to-band tunnel FETs require extremely small nanowire diameters and eventually lead to one-dimensional (1D) electronic transport. While 1D transport is beneficial to conventional FETs, in the case of tunnel FETs the 1D density of states leads to an inability of appropriate doping (even if deactivation and the statistical dopant distribution could be avoided). The effects will be discussed particularly with respect to their impact on device functionality.

**Invited Talk** DS 9.6 Tue 12:00 H 2032  
**Probing composition and conductivity in 3D-structures and confined volumes.** — •WILFRIED VANDERVORST — Imec, Kapeldreef 75, B-3001 Leuven, Belgium

Developing and implementing next technology nodes is a complex task involving innovation in materials engineering, process development and device design. The down scaling of devices into non-planar structures has led to physical phenomena which can only be seen in 3D-structures and confined volumes such that the metrology is now pushed into dealing with analysis on a scale commensurate with device dimensions. Concepts like Atomprobe tomography with its inherent 3D-resolution are obviously a potential solution although its routine application is still hampered by localization problems, reconstruction artifacts due to inhomogeneous evaporation, sensitivity due to the limited statistics, poor tip yield, etc. On the other hand concepts like scanning probe microscopy are inherently 2D can be extended towards 3D appear either by the design of dedicated tests structures or by novel approaches such as mechanical scalping. Recent applications of Scalpel SPM have unraveled the filament formation in RRAM-devices and highlighted the conduction paths in NAND devices. Despite the apparent 1D-nature of Secondary Ion Mass Spectrometry, novel concepts like Self-focusing SIMS enable to probe layer composition within trenches as narrow as 20 nm.

**Invited Talk** DS 9.7 Tue 12:30 H 2032  
**Silicon Nanowire Devices and Applications** — •THOMAS MIKOLAJICK<sup>1,2,3</sup> and WALTER WEBER<sup>1,3</sup> — <sup>1</sup>NaMLab gGmbH, Nöthnitzer Str. 64, 01187 Dresden — <sup>2</sup>Institut für Halbleiter und Mikrosystemtechnik, TU Dresden, 01062 Dresden — <sup>3</sup>Center for Advancing Electronics Dresden (CFAED), TU Dresden, 01062 Dresden

Due to the quasi 1-dimensional nature of nanowires the controllability of electrical fields and currents are significantly enhanced. Therefore silicon nanowires are in development in the semiconductor industry as a very promising option for end of roadmap CMOS devices. Additionally new device concepts that are hard to realize in planar structures are enabled [1]. In this talk, first the fabrication of silicon nanowires and related device structures are explained. In the second part interesting transport properties that enable new device options will be shown. Based on these observations the most important nanowire device concepts will be deduced. The reconfigurable field effect transistor (RFET) will be explained as one interesting example that makes use of the specific advantage of the nanowire geometry. Finally an outlook to other applications of silicon nanowires like chemical sensing will be given.

[1] T. Mikolajick et al., *Silicon nanowires - a versatile technology platform*, *Phys. Status Solidi RRL* 7, No. 1, p. 793-799 (2013)

## DS 10: Thermoelectric materials

Time: Tuesday 9:30–11:00

Location: H 0111

DS 10.1 Tue 9:30 H 0111

**Complete thermoelectric material characterization at high temperatures** — ●HENDRIK KOLB<sup>1</sup>, TITAS DASGUPTA<sup>2</sup>, JOHANNES DE BOOR<sup>1</sup>, KNUD ZABROCKI<sup>1</sup>, and ECKHARD MÜLLER<sup>1,3</sup> — <sup>1</sup>Institute of Materials Research, German Aerospace Center — <sup>2</sup>Dept. of Metallurgical Engineering and Materials Science, Indian Institute of Technology Bombay — <sup>3</sup>Institute of Inorganic and Analytical Chemistry, Justus-Liebig-Universität Gießen

Thermoelectricity is the direct conversion of thermal energy into electrical energy and can be used for the recovery of waste heat into electrical power. For an efficient research process a quick characterization is crucial to see the effects of the material manufacturing process on the thermoelectric properties. The three thermoelectric key quantities can strongly be temperature dependent, which makes a complete characterization over a wide temperature range necessary. The special feature of our system is the additional direct  $zT$  measurement by the Harman method independently from the single measurements to verify the results. The better comparability of the measured properties is one main advantage in a simultaneous measurement, because all quantities are measured at one temperature step. Additionally the measurement uncertainty which can easily reach more than 20% in the  $zT$  measurement due to methodical or geometrical differences in different setups is reduced. We show results for a complete high temperature characterization of thermoelectric materials up to 650 K and show good agreement with reference data. Also, we demonstrate the influence of radiation losses on thermal conductivity measurement.

DS 10.2 Tue 9:45 H 0111

**Enhanced transport properties of rutile oxides** — ●DENIS MÜSIC and JOCHEN M. SCHNEIDER — Materials Chemistry, RWTH Aachen University, Kopernikusstr. 10, 52074 Aachen, Germany

Oxide based thermoelectrics offer potential for high efficiency thermoelectric conversion for harvesting electricity from heat, but suffer from a low power factor due to the low electrical conductivity. We used quantum mechanical calculations to identify alloying elements for RuO<sub>2</sub> with enhanced Seebeck coefficient. We probed all 3d and 4d transition metals as well as all lanthanides and identified Fe and La to be the most promising candidates as a manifold increase in Seebeck coefficient was predicted. This materials design proposal was then critically evaluated by measuring the Seebeck coefficient of sputter-deposited thin films. Furthermore, the electrical and thermal conductivity was measured. Saturated RuO<sub>2</sub> with Fe and La exhibit not only a four-fold increase in the Seebeck coefficient, but also a decrease in thermal conductivity. This yields the highest power factor reported for RuO<sub>2</sub> despite a twofold decrease in the electrical conductivity. Hence, the ab initio predictions regarding the Seebeck coefficient are validated by experiments. Furthermore, Fe and La lead to grain refinement and a more porous morphology. Our results suggest that maximizing the structural distortion of RuO<sub>2</sub> by dilute alloying with selected transition metals and lanthanides can increase the Seebeck coefficient and decrease the thermal conductivity by fostering quantum confinement and phonon scattering, respectively. Other rutile oxides, such as MnO<sub>2</sub>, will also be discussed.

DS 10.3 Tue 10:00 H 0111

**Reduced thermal conductivity of TiNiSn/HfNiSn superlattices** — ●PAULINA HOLUJ<sup>1,3</sup>, CHRISTOPH EULER<sup>1</sup>, TINO JAEGER<sup>1</sup>, BENJAMIN BALKE<sup>2</sup>, and GERHARD JAKOB<sup>1,3</sup> — <sup>1</sup>Institute of Physics, University of Mainz, Staudinger Weg 9, 55128, Germany — <sup>2</sup>Institute of Inorganic and Analytical Chemistry, University of Mainz, Staudinger Weg 9, 55128, Germany — <sup>3</sup>Graduate School Materials Science in Mainz, Staudinger Weg 9, 55128, Germany

Thermoelectric materials possess the ability to convert unused heat to electricity. The efficiency of their operation depends on the dimensionless figure of merit  $ZT = \frac{S^2\sigma}{\kappa}$  that contains only material dependent parameters ( $S$  - Seebeck coefficient,  $\sigma$  - electrical conductivity,  $\kappa$  - thermal conductivity). The goal of our work is to reduce thermal conductivity and doing so we aim to enhance  $ZT$ . Reduction of  $\kappa$  is achieved by scattering of phonons at interfaces of superlattices (SL) made out of TiNiSn and HfNiSn half-Heusler materials. Based on x-ray diffraction we assume to have sharp interfaces between constituent layers. In the current study we observe a systematic reduction of the

thermal conductivity as the period of the SLs is decreasing with a clear minimum at about 3 nm and a further increase of  $\kappa$  due to formation of an artificial crystal.

We gratefully acknowledge financial support by DFG (Ja821/4-2) and the Graduate School of Excellence Material Science in Mainz (GSC 266).

DS 10.4 Tue 10:15 H 0111

**Nanostructured SiGe thin films obtained through MIC processing** — ●MARC LINDORF<sup>1</sup>, HARTMUT ROHRMANN<sup>2</sup>, and MANFRED ALBRECHT<sup>1</sup> — <sup>1</sup>University of Augsburg, Universitätsstraße 1, 86159 Augsburg, Germany — <sup>2</sup>Oerlikon Advanced Technologies AG, Iramali 18, 9496 Balzers, Liechtenstein

In times of growing energy consumption thermoelectric devices pose an opportunity for energy harvesting. However commercially available thermoelectric materials show a deficit in efficiency governed by low  $ZT$  values. New approaches like nanostructuring [1] try to increase the efficiency, but often lack industrial applicability due to high cost and low production speed. This work presents results on sputter deposited multilayer stacks of Si<sub>80</sub>Ge<sub>20</sub> (10 nm)/[Al( $d_{Al}$ )/Si<sub>80</sub>Ge<sub>20</sub> (10 nm)]<sub>50</sub>/SiO<sub>2</sub> (200 nm)/Si. Crystallization and Al dopant activation is achieved by post-annealing through metal induced crystallization (MIC) [2]. This approach allows grain size control via annealing temperature and Al interlayer thickness  $d_{Al}$  in the nanometer regime. Results will be presented regarding structural and thermoelectric properties.

[1] Y. Lan et al., *Adv. Funct. Mater.* **20**, 357-376 (2010).[2] Z. M. Wang et al., *Phys. Rev. Lett.* **100**, 125503 (2008)

DS 10.5 Tue 10:30 H 0111

**The Influence of a Distinct Diameter Variation on the Thermal Conductivity of Individual Bismuth Telluride Nanowires** — ●DANNY KOJDA<sup>1</sup>, RÜDIGER MITTDANK<sup>1</sup>, ANNA MOGILATENKO<sup>2</sup>, WILLIAM TÖLLNER<sup>3</sup>, ZHI WANG<sup>4</sup>, MICHAEL KRÖNER<sup>4</sup>, PETER WOIAS<sup>4</sup>, KORNELIUS NIELSCH<sup>3</sup>, and SASKIA F. FISCHER<sup>1</sup> — <sup>1</sup>AG Neue Materialien, Humboldt-Universität zu Berlin, D-10099 Berlin — <sup>2</sup>Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, D-12489 Berlin — <sup>3</sup>Institut für Angewandte Physik, Universität Hamburg, D-20355 Hamburg — <sup>4</sup>Laboratory for Design of Microsystems, University of Freiburg - IMTEK, D-79110 Freiburg

Calculations on indented nanowires (NWs) have shown that surface morphology can affect the thermal conductivity  $\lambda$  by phonon backscattering [1]. In order to determine the role of a distinct diameter variation, two Bi<sub>0.39</sub>Te<sub>0.61</sub> NWs from the same batch are investigated by means of a combined full-thermoelectrical, structural and chemical characterization. Both NWs have the same chemical composition and the same direction of growth along the [110] direction. The NWs differ in their morphology. One NW shows a strong diameter variation between 190 nm and 320 nm and the other has a diameter of 187 nm with smooth sidewalls. At room temperature  $\lambda$  was determined by the  $3\omega$ -method and a reduction in the indented NW by about 50% with respect to the smooth NW was observed. Hence, NW-vacuum interfaces perpendicularly arranged to the direction of transport can lead to a reduced  $\lambda$  in NWs [2]. [1] A. Moore et al., 2008 APL, **93** 083112. [2] D. Kojda et al., 2014 Semicond. Sci. Technol., **29** 124006.

DS 10.6 Tue 10:45 H 0111

**Enhanced thermoelectric efficiency of  $p$ -type Half-Heuslers by intrinsic phase separation and carrier concentration optimization.** — ●ELISABETH RAUSCH<sup>1,2</sup>, CLAUDIA FELSER<sup>2</sup>, and BENJAMIN BALKE<sup>1</sup> — <sup>1</sup>Institut für Anorganische und Analytische Chemie, Johannes Gutenberg-Universität, Mainz, Germany — <sup>2</sup>Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany

State of the art  $p$ -type Half-Heusler compounds (space group F43m) for thermoelectric applications are found in the  $M\text{CoSb}_{0.8}\text{Sn}_{0.2}$  ( $M = \text{Ti}/\text{Zr}/\text{Hf}$ ) system. The outstanding properties are achieved by a nanostructuring approach via ball milling followed by a rapid consolidation method. We, herein report on an alternative approach to reduce the thermal conductivity, which is by an intrinsic phase separation. A optimum ratio of Ti to Hf in combination with an adjustment of carrier concentration via Sn substitution lead to a record thermoelectric figure of merit  $ZT = 1.15$  for Ti<sub>0.25</sub>Hf<sub>0.75</sub>CoSb<sub>0.85</sub>Sn<sub>0.15</sub>. Our

study is complemented by a long-term stability test under thermal cycling conditions in the interesting temperature range for automotive

applications.

## DS 11: Transport: Topological Insulators 2 (joint session with DS, HL, MA, O)

Time: Tuesday 9:30–13:00

Location: H 3005

DS 11.1 Tue 9:30 H 3005

**How electron-electron interactions may lead to a spontaneous time reversal symmetry breaking in (fractional) topological insulators** — •TOBIAS MENG<sup>1,2</sup> and ERAN SELA<sup>3</sup> — <sup>1</sup>Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — <sup>2</sup>Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland — <sup>3</sup>Raymond and Beverly Sackler School of Physics and Astronomy, Tel-Aviv University, Tel Aviv, 69978, Israel

We analyze the consequences of strong electron-electron interactions in topological insulators. Naively, topological insulators can be thought of as two copies of quantum Hall states for spin up and spin down electrons at opposite magnetic field, hence maintaining time reversal symmetry. Using an extension of the coupled-wire construction of quantum Hall states to systems with zero magnetic field, we find that interactions between electrons of spin up and spin down can stabilize a large family of fractional topological phases with broken time reversal invariance. The latter is manifest by a spontaneous spin polarization, a finite Hall conductivity, or by both. This suggests the possibility that strongly correlated fractional topological insulators may be unstable to spontaneous symmetry breaking.

DS 11.2 Tue 9:45 H 3005

**Emergence of surface conductivity at low temperatures in FeSi** — •MICHAEL WAGNER, RALF KORNTNER, ANDREAS BAUER, and CHRISTIAN PFLEIDERER — Physik-Department, Technische Universität München, D-85748 Garching, Germany

We report a comprehensive study of the influence of the sample quality on the Hall-conductivity in the correlated semiconductor FeSi. For our study three high-quality Fe<sub>1+x</sub>Si single crystals with slightly different Fe concentrations  $x$  were grown by optical float zoning under ultra-high vacuum compatible conditions. While the magnetic properties vary sensitively for the samples studied, the transport properties display several key features that are independent of the Fe concentration. As our main result we find, that the Hall-conductivity of FeSi can be described in terms of a Drude-model. For low temperatures a second transport channel emerges besides bulk conductivity, which can be assigned unambiguously to the sample surface. Remarkably, the mobility of this surface conduction is extraordinarily high as compared to similar effects in conventional semiconductors, being quantitatively consistent with topological insulators such as Bi<sub>2</sub>Te<sub>3</sub> where they are viewed as the signature of topologically protected transport channels.

DS 11.3 Tue 10:00 H 3005

**Spin transport in 3d-topological insulator nanostructures** — •MATTHIAS STOSIEK, SVEN ESSERT, COSIMO GORINI, and KLAUS RICHTER — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

The spin-momentum locking for charge carriers on the surface of three-dimensional topological insulators holds promising prospects for spintronics applications. In this predominantly numerical study, we investigate the transport properties of nanostructures of 3d-TIs with ferromagnetic leads using model Hamiltonians. We also explore the influence of external electric and magnetic fields.

DS 11.4 Tue 10:15 H 3005

**Tunnel Magnetoresistance scan of surface states of 3D topological insulators** — •SHITADHI ROY — Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany

The Fermi-surface of surface states of a 3D topological insulator (TI) has zero magnetization owing to time reversal symmetry, but an arbitrary segment of the full Fermi surface has a unique magnetic moment consistent with the type of spin-momentum locking. A three-terminal set up is proposed which directly couples to the magnetization of a chosen segment of a Fermi surface, hence leading to a finite tunnel magnetoresistance (TMR) response of the non-magnetic TI surface states, when coupled to spin polarized STM probe. This multi-terminal TMR

reconstructs the in-plane momentum locked spin texture and also the out-of-plane spin polarization of hexagonally warped Fermi surfaces relevant for materials like Bi<sub>2</sub>Te<sub>3</sub>. This proposal is further extended to surfaces exposed by cleaving crystals at arbitrary angles to the crystal growth axis, and it shown that the TMR response not only probes and distinguishes these surfaces uniquely but the study of the spin textures for different surfaces put together acts like a hologram of the bulk band structure of the material.

DS 11.5 Tue 10:30 H 3005

**Weak Antilocalization of 3DTI Surface States in the Presence of Spin-Orbit Impurities** — •PIERRE ADROGUER<sup>1</sup>, WEIZHE LIU<sup>2</sup>, DIMITRIE CULCER<sup>2</sup> und EWELINA HANKIEWICZ<sup>1</sup> — <sup>1</sup>Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Deutschland — <sup>2</sup>School of Physics, The University of New South Wales, Sydney, Australia

The recent realization of three dimensional topological insulators (3DTIs) allows to probe the coherent transport of Dirac systems. In the presence of scalar disorder, weak antilocalization (WAL) is observed. However, TIs are materials where spin-orbit plays a crucial role, and the effect of spin-orbit impurities on coherent transport had not been studied yet.

In conventional electron gases where electrons have a parabolic dispersion, the concentration of spin-orbit impurities is of significant importance. Indeed, when the concentration of spin-orbit impurities is increased, the sign of the quantum correction to conductivity changes, going from weak localization to weak antilocalization (WAL).

In this work, we derive with the standard diagrammatic technique the quantum correction to conductivity when we add spin-orbit impurities to the diffusion of Dirac fermions in a disordered potential. We show that for every concentration of the spin-orbit impurities we remain in the symplectic class of WAL. We also derive the value of this quantum correction to conductivity in the presence of a transverse magnetic field, and we show that fits with the conventional theory have to be revisited in the view of our results.

DS 11.6 Tue 10:45 H 3005

**SmO thin films: a flexible route to correlated flat bands with nontrivial topology** — •DEEPA KASINATHAN<sup>1</sup>, KLAUS KOEPERNIK<sup>2</sup>, LIU HAO TJENG<sup>1</sup>, and MAURITS HAVERKORT<sup>1</sup> — <sup>1</sup>Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany — <sup>2</sup>IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

Using density functional theory based calculations, we show that the correlated mixed-valent compound SmO is a 3D strongly topological semi-metal as a result of a  $4f-5d$  band inversion at the X point. We also show that the topological non-triviality in SmO is very robust and prevails for a wide range of lattice parameters, making it an ideal candidate to investigate topological nontrivial correlated flat bands in thin-film form. Moreover, the electron filling is tunable by strain. In addition, we find conditions for which the inversion is of the  $4f-6s$  type, making SmO to be a rather unique system. The similarities of the crystal symmetry and the lattice constant of SmO to the well studied ferromagnetic semiconductor EuO, makes SmO/EuO thin film interfaces an excellent contender towards realizing the quantum anomalous Hall effect in a strongly correlated electron system.

15 min. break.

Invited Talk

DS 11.7 Tue 11:15 H 3005

**Interacting Topological Insulators** — •STEPHAN RACHEL — Institut für Theoretische Physik, Technische Universität Dresden

The physics of electronic correlations in systems with topological band structures is a young and exciting field. In this talk, I will give an overview of the most relevant and interesting interaction effects in 2D and 3D topological insulators. Specifically, I will address the physics of the Kane-Mele-Hubbard model, the prototypical model of a correlated

topological insulator, and its descendants in 2D as well as topological Mott insulators emerging in 3D topological band structures. Eventually, I will explain how strong interactions can affect the surface states of strong topological insulators and lead to even more exotic phases.

DS 11.8 Tue 11:45 H 3005

**Interplay of topology and interactions in the quantum Hall regime of two-dimensional topological insulators** — ●STEFAN JÜRGENS, MAXIM KHARITONOV, and BJÖRN TRAUZETTEL — Institute of Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany

We study a class of two-dimensional topological insulators, in which the single-particle edge states are preserved in the presence of the magnetic field by a symmetry (e.g., crystalline) other than time-reversal. We focus on the vicinity of the crossing point between the zero-mode Landau levels. At half-filling, Coulomb interactions become particularly strong and lead to the formation of the quantum Hall "ferromagnetic" state with gapped charge excitations in the bulk. We identify the phases of this state that have gapped or gapless collective charge edge excitations and are characterized by the presence or absence of spontaneous symmetry breaking. The transitions between these phases can occur either continuously (via second order) or abruptly (via first order), depending on the parameters of the system. These transitions are accompanied by the corresponding behavior of the edge gap, which could be detected in transport measurements. Our findings provide an example of the interplay of topological and interaction-induced (spontaneous symmetry breaking) phenomena in the strong coupling regime.

DS 11.9 Tue 12:00 H 3005

**Superconducting proximity effect in three-dimensional topological insulators in the presence of external magnetic fields** — ●PABLO BURSET, GRIGORY TKACHOV, EWELINA HANKIEWICZ, and BJÖRN TRAUZETTEL — Institute for Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany

The proximity induced pair potential in a topological insulator-superconductor hybrid features an interesting superposition of conventional spin-singlet potential from the superconductor and spin-triplet pairing induced by the surface state of the topological insulator. We theoretically describe ballistic junctions between superconductors and topological insulators under external magnetic fields. We use Green functions techniques to calculate experimentally relevant transport signatures like normal-superconductor tunnel spectroscopy, local density of states, and Josephson current. Additionally, we consider the effect of both topological order and an external magnetic field in the superconducting correlations. We associate the unconventional transport signatures with the symmetry of the singlet and triplet components of the pair potential.

DS 11.10 Tue 12:15 H 3005

**Non-universal conductance fluctuations in 3D topological insulator nanowires.** — ●EMMANOUIL XYPAKIS<sup>1</sup>, JENS H BARDARSON<sup>1</sup>, LOUIS VEYRAT<sup>2</sup>, JOSEPH DUFOULEUR<sup>2</sup>, and ROMAIN GIRAUD<sup>2</sup> — <sup>1</sup>Max-Planck-Institut fuer Physik Komplexer Systeme, Noethnitzer Straße 38, D-01187 Dresden, Germany — <sup>2</sup>Leibniz Institute for Solid State and Materials Research, IFW Dresden, D-01069 Dresden, Germany

## DS 12: Transport: Graphene (joint session with DS, DY, HL, MA, O)

Time: Tuesday 9:30–12:15

Location: A 053

DS 12.1 Tue 9:30 A 053

**Observation of supercurrent in graphene-based Josephson junction** — ●LIBIN WANG<sup>1</sup>, CHUAN XU<sup>2</sup>, SEN LI<sup>1</sup>, WENCAI REN<sup>2</sup>, and NING KANG<sup>1</sup> — <sup>1</sup>Key Laboratory for the Physics and Chemistry of Nanodevices and Department of Electronics, Peking University, Beijing 100871, China — <sup>2</sup>Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China

Josephson junctions with a normal metal region sandwiched between two superconductors (S) are known as superconductor-normal-superconductor (SNS) structures. It has attracted significant attention especially when changing the normal metal with graphene, which allow for high tunability with the gate voltage and to study the prox-

imity effect of the massless Dirac fermions. Here we report our work on graphene-based Josephson junction with a new two dimensional superconductor crystal, which grown directly on graphene, as superconducting electrodes. At low temperature, we observe proximity effect induced supercurrent flowing through the junction. The temperature and the magnetic field dependences of the critical current characteristics of the junction are also studied. The critical current exhibits a Fraunhofer-type diffraction pattern against magnetic field. Our experiments provided a new route of fabrication of graphene-based Josephson junction.

DS 11.11 Tue 12:30 H 3005

**How dephasing and charge puddles affect the edge transport in 2d-topological insulators** — ●SVEN ESSERT, VIKTOR KRUECKL, and KLAUS RICHTER — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

State of the art 2d-TI material systems show a length dependent non-quantized conductance for sample sizes larger than one micron. This feature is so far not well understood: Coherent elastic backscattering is symmetry forbidden and the observed weak temperature dependence does not seem to match the predictions for inelastic backscattering. We analytically and numerically investigate the effects of a third mechanism which was proposed to play a major role for the edge resistance: The combined effect of dephasing and elastic backscattering in charge puddles which are known to exist in the experimental samples.

We extract a range of dephasing times which are consistent with the experimental results. In addition, we make predictions for experiments on artificial charge puddles from which the real dephasing time scale could be determined.

DS 11.12 Tue 12:45 H 3005

**Anderson localization at the edge of a 2D topological insulator** — ●ESLAM KHALAF and PAVEL OSTROVSKY — Max Planck institute for solid state research, Stuttgart, Germany

We study transport via edge modes in a 2D topological insulator. Topological protection prevents complete localization of the edge states; however, quantum interference effects are still relevant for the transport properties at finite length scales. We mainly focus on the two most experimentally relevant cases: (i) a junction between two quantum Hall insulators with different filling factors and hence an imbalance in the number of right- and left-propagating modes (symmetry class A) and (ii) a relatively thick HgTe quantum well in the insulating state with an arbitrary number of edge modes (symmetry class AII). We derive the distribution of transmission probabilities as a function of the distance between leads. This allows us to demonstrate topological effects in the average conductance and the shot noise of the setup. We also consider mesoscopic fluctuations and compute the variance of conductance. This quantity is strongly influenced by topology in the quantum Hall case. All the calculations are carried out assuming localization effects are weak, i.e., in the short length limit. Technically, this amounts to studying 1D non-linear sigma model with a proper topological term and source fields on the semiclassical level. Remarkably, the semiclassical limit of the 1D sigma model can be exactly mapped onto a fully quantum 0D sigma model of a different symmetry class. This allows us to identify the distribution of transmission probabilities with the spectrum of a certain random matrix.

DS 12.2 Tue 9:45 A 053

**Magnetoresistance of nanocrystalline and ion-irradiated graphene** — ●PAUL LINSMAIER<sup>1</sup>, LORENZ WEISS<sup>1</sup>, ARMIN

SHAUKAT<sup>1</sup>, CHRISTIAN BÄUML<sup>1</sup>, DANIEL STEININGER<sup>1</sup>, INA SCHNEIDER<sup>1</sup>, MATTHIAS BÜENFELD<sup>2</sup>, NILS-EIKE WEBER<sup>2</sup>, ANDREY TURCHANIN<sup>2</sup>, MIRIAM GROTHE<sup>3</sup>, THOMAS WEIMANN<sup>3</sup>, FERDINAND KISSLINGER<sup>4</sup>, HEIKO B. WEBER<sup>4</sup>, and CHRISTOPH STRUNK<sup>1</sup> — <sup>1</sup>Inst. f. Exp. and Appl. Physics, University of Regensburg — <sup>2</sup>Fac. of Physics, University of Bielefeld — <sup>3</sup>Physikalisch-Technische Bundesanstalt, Braunschweig — <sup>4</sup>Fac. of Physics, F.-A. University Erlangen-Nürnberg

We investigate the magnetotransport in Hall bar structures of nanocrystalline graphene [1] compared to Ar<sup>+</sup>-bombarded epitaxial graphene [2]. We measured the resistance  $R(T)$  and  $R(B)$  for samples with different sheet resistance (10-40 k $\Omega$ /sq at  $T = 300$ K). The I-V characteristics of both types show strong non-linear behavior at low temperatures. Low resistive samples of nanocrystalline graphene show positive magnetoresistance (MR) with values up to + 60 % in perpendicular magnetic field for temperatures below a crossover temperature. Above this temperature the MR becomes negative. The perpendicular MR in the ion-bombarded graphene was always negative. In parallel magnetic field the MR exhibits large positive values up to + 700 % in the nanocrystalline graphene. Strongly non-monotonic behavior of the MR was observed in the ion-bombarded sample in parallel field.

[1] A. Turchanin et al., ACS Nano 5 (2011).

[2] K. V. Emtsev et al., Nat. Mat. 8, 203 - 207 (2009).

DS 12.3 Tue 10:00 A 053

**Aharonov-Bohm effect in a graphene ring encapsulated in hexagonal boron nitride** — ●JAN DAUBER<sup>1,2</sup>, MARTIN OELLERS<sup>1</sup>, ALEXANDER EPPING<sup>1,2</sup>, KENJI WATANABE<sup>3</sup>, TAKASHI TANIGUCHI<sup>3</sup>, FABIAN HASSLER<sup>4</sup>, and CHRISTOPH STAMPFER<sup>1,2</sup> — <sup>1</sup>JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, Aachen, Germany — <sup>2</sup>Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, Jülich, Germany — <sup>3</sup>National Institute for Materials Science, 1-1 Namiki, Tsukuba, Japan — <sup>4</sup>JARA-Institute for Quantum Information at RWTH Aachen University, Aachen, Germany

Recent developments in the van der Waals assembly of heterostructures of two-dimensional materials enable the fabrication of graphene on substrate with very high quality. Outstanding charge carrier mobility and mean free path have been reported for micrometer sized samples of graphene encapsulated in hexagonal boron nitride (hBN). These unique electronic properties offer opportunities for the observation of rich mesoscopic transport phenomena in sub-micron sized graphene-hBN devices. Here, we present low-temperature magnetotransport measurements on a high mobility graphene ring encapsulated in hexagonal boron nitride. We observe the co-existence of weak localization, Aharonov-Bohm (AB) oscillations and universal conductance fluctuations. We investigate the periodicity of the AB oscillations as a function of charge carrier density and find clear evidence of the AB effect even at very low carrier densities. Finally, we report on the investigation of the AB oscillations in the cross over regime of emerging quantum Hall effect at reasonable magnetic fields.

DS 12.4 Tue 10:15 A 053

**Ab-initio simulations of local current flows in functionalized graphene flakes and ribbons** — ●MICHAEL WALZ<sup>1</sup>, JAN WILHELM<sup>2</sup>, ALEXEI BAGRETS<sup>1</sup>, and FERDINAND EVERS<sup>3</sup> — <sup>1</sup>Institute of Nanotechnology, Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany — <sup>2</sup>Institute of Physical Chemistry, University of Zürich, CH-8057 Zürich, Switzerland — <sup>3</sup>Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany

Using our DFT-based transport framework AITRANSS [1], we calculate the transmission and the local current density in graphene flakes functionalized by adsorbed atoms, such as nitrogen or hydrogen. We find that even a single nitrogen atom can almost completely suppress the conductance of a (gated) graphene armchair nano-ribbon. In this situation local ring currents emerge that result in local (orbital) magnetic moments.

In addition, the current flow shows a highly inhomogeneous structure. In the absence of any scatters, the current flows along parallel streamlines that exhibit a strong lateral modulation [2]. In the presence of scattering centers, such as 20% hydrogen adsorbants, we observe a filamentary pattern of streamlines. It exhibits local ring currents (“ed-dies”) that go along with sizeable local magnetic fields,  $\mathbf{B}(\mathbf{r})$ . [3]

In the future, we plan to study the statistics of local currents of such large flakes and its dependency on the impurity concentration.

[1] A. Arnold, F. Weigend, F. Evers, J. Chem. Phys. 126 (2007)

[2] J. Wilhelm, M. Walz, F. Evers, Phys. Rev. B 89 (2014)

[3] M. Walz, J. Wilhelm, F. Evers, Phys. Rev. Lett. 113 (2014)

DS 12.5 Tue 10:30 A 053

**Fabry-Pérot interference in monolayer and bilayer graphene devices** — ●MING-HAO LIU and KLAUS RICHTER — Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany

Recent progress on high-quality graphene device fabrications has made submicron- or even micron-scale phase-coherent phenomena in graphene experimentally observable. Hence reliable quantum transport simulations for ballistic graphene devices are nowadays highly demanded. In this talk we give an overview on how such simulations can be accurately and efficiently performed. Concrete examples of Fabry-Pérot interference in single pn junctions in suspended monolayer graphene [1], multiple pn junctions in monolayer graphene on substrate [2], and pnp junctions in bilayer graphene encapsulated by hexagonal boron nitride [3] will be briefly shown, as well as further studies of “electron optics” in graphene.

[1] P. Rickhaus, R. Maurand, M.-H. Liu, M. Weiss, K. Richter, and C. Schönberger, Nature Comm. 4, 2342 (2013); M.-H. Liu, et. al., arXiv:1407.5620 (2014).

[2] M. Drienovsky, F.-X. Schrettenbrunner, A. Sandner, D. Weiss, J. Eroms, M.-H. Liu, F. Tkatschenko, and K. Richter, Phys. Rev. B 89, 115421 (2014).

[3] A. Varlet, M.-H. Liu, V. Krueckl, D. Bischoff, P. Simonet, K. Watanabe, T. Taniguchi, K. Richter, K. Ensslin, and T. Ihn, Phys. Rev. Lett. 113, 116601 (2014).

DS 12.6 Tue 10:45 A 053

**Substrate-Induced doping of supported graphene: an ab initio study** — ●AREZOO DIANAT<sup>1</sup>, RAFAEL GUTIERREZ<sup>1</sup>, ZHONGQUAN LIAO<sup>2</sup>, MARTIN GALL<sup>2</sup>, EHRENFRIED ZSCHECH<sup>2</sup>, and GIANAURELIO CUNIBERTI<sup>1</sup> — <sup>1</sup>Institute for Materials Science, Technische Universität Dresden, D-01062 Dresden, Germany — <sup>2</sup>Fraunhofer Institute for Ceramic Technologies and Systems, D-01109 Dresden, Germany

A major challenge for applications of graphene in nanoelectronics is the absence of a band gap in its low energy spectrum. One possibility of gap opening is doping and there are various methods to achieve it: evaporation, thermal treatment, and plasma doping. In this study, using ab initio molecular dynamics, we investigate graphene doping mediated by substrate-induced mechanisms. More specifically, we address graphene on a B-doped Si(100) surface. Our ab initio total energy calculations show that B atoms prefer to locate on the surface layer of Si(100). Further, intercalation of B atoms into vacancy positions of graphene is only found for temperatures larger than 700 K. In a second step, the electrical transport properties of B-doped graphene are studied using the non-equilibrium Green’s function approach.

15 min. break.

DS 12.7 Tue 11:15 A 053

**Density of states of graphene with vacancies** — ●SOUMYA BERA — MPI-PKS, Dresden

We numerically calculate the density of states (DOS) of graphene in the presence of compensated vacancy disorder. The model belongs to the BDI class of Atland-Zirnbauer symmetry classification of disordered metals, where the non-linear Sigma model predicts a Gade-type singularity in the DOS  $\rho(E) \sim E^{-1} \exp(-|\log(E)|^{-1/2})$ . We show that in the pre-asymptotic regime this is indeed true, however, at even lower energies the Gade-type behavior gives away to a stronger singularity of the form  $\rho(E) \sim E^{-1} |\log(E)|^{-x}$  with  $2 > x \geq 1$  in agreement with recent analytical work (Ostrovsky et al., PRL 113, 186803). We conclude that the generic Sigma model of the BDI class does not apply for strong (unitary) scatterers; the nature of disorder is of important to determine the low energy behaviour of disordered graphene.

[1] PRL 113, 186802 (2014).

DS 12.8 Tue 11:30 A 053

**Nonlocal optical excitations and dynamic shear viscosity of graphene** — ●JULIA LINK, PETER P. ORTH, and JÖRG SCHMALIAN — Institute for Theoretical Condensed Matter physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe

We study the dynamic shear viscosity of the interacting electronic fluid of graphene in the finite frequency, collision-less regime, relevant for nonlocal optical properties. We determine the frequency dependence of the dynamic shear viscosity for non-interacting graphene and study

the influence of the long-range Coulomb interaction. Finally we discuss a setup where the viscosity can be spectroscopically measured.

DS 12.9 Tue 11:45 A 053

**Transport phenomena in deformed graphene: Magnetic field versus curvature** — THOMAS STEGMANN<sup>1,2</sup> and NIKODEM SZPAK<sup>1</sup> — <sup>1</sup>Fakultät für Physik, Universität Duisburg-Essen, Duisburg, Germany — <sup>2</sup>Instituto de Ciencias Físicas, Universidad Nacional Autónoma de México, Cuernavaca, México

The current flow in deformed graphene nanoribbons is studied theoretically. Using a tight-binding model, we apply the nonequilibrium Green's function (NEGF) method to investigate how a localized deformation and a perpendicular magnetic field affect the current flow. At long wavelengths, the eikonal approximation applied to the effective Dirac equation leads to the Mathisson-Papapetrou equations describing trajectories of a spinning point-like particle in a curved space. We show that these trajectories are compatible with the current flow paths of the NEGF calculations. The deformation has two-fold effect on them: First, via a pseudo-magnetic field, with sixfold symmetry of attractive and repulsive regions, which acts differently on electrons and holes, but changes its sign when going from the K to the K' point. Second, via an attractive force due to the curvature of the ribbon, which treats electrons and holes equivalently. We conclude with an outlook on how to use deformed graphene ribbons for geometrical focusing of the current flow.

DS 12.10 Tue 12:00 A 053

**Merging of the Dirac points in electronic artificial graphene** — JURAJ FEILHAUER<sup>1,2</sup>, WALTER APEL<sup>1</sup>, and LUDWIG SCHWEITZER<sup>1</sup> — <sup>1</sup>Physikalisch-Technische Bundesanstalt (PTB), Braunschweig, Germany — <sup>2</sup>Institute of Electrical Engineering, Slovak Academy of Sciences, Bratislava, Slovakia

Artificial graphene (AG) is a man-made electron system which has a similar bandstructure as normal graphene, i.e. in the low-energy part of the electronic spectrum, two bands touch and form a pair of Dirac cones. We study analytically and numerically the bandstructure of electronic AG under uniaxial strain. Here, AG is created from the two-dimensional electron gas by applying a repulsive triangular potential and the effect of strain is modeled by tuning the distance between the repulsive potentials along the armchair direction. In normal graphene, the theory based on nearest-neighbour tight-binding approximation predicts that due to the change of the hopping integrals by applying uniaxial strain, both Dirac cones are shifted away from the corners of the Brillouin zone and also becomes elliptical instead of circular. With increasing compressive strain, the Dirac cones move along the edge of Brillouin zone towards each other until they merge. We show that such a merging of the Dirac cones also exists in uniaxially compressed AG. With applied strain, we find the Dirac cones are also tilted and that can be simulated by the presence of a next-nearest-neighbour hopping in the tight-binding hamiltonian. We discuss a possible realization of our theoretical results in a recent experiment with molecular graphene.

## DS 13: Interfaces and Thin Films I (joint session with CPP)

Time: Tuesday 10:00–12:30

Location: C 243

DS 13.1 Tue 10:00 C 243

**What is the result of a tensiometer measurement to do with the surface tension?** — MARKUS BIER — Max Planck Institute IS and University of Stuttgart, Germany

The surface tension of liquids is routinely measured with various types of tensiometers under ambient pressure conditions [1]. For, e.g., water at room temperature this leads to the well-known value of 0.07 N/m [1]. However, the surface tension is strictly defined only under conditions of liquid-vapour bulk coexistence, whereas, e.g., water at room temperature and ambient pressure is deep in the one-phase region of the phase diagram, far away from phase coexistence. Hence the above-mentioned tensiometer measurements are actually performed at interfaces under non-equilibrium conditions. This leads to the question whether it is legitimate at all to identify the result of a tensiometer measurement of a non-equilibrium interface with the surface tension. This contribution gives an answer to that question [2].

References:

- [1] D.R. Lide (ed.), *CRC Handbook of Chemistry and Physics, 82nd edition* (CRC Press, Boca Raton, 2001).
- [2] M. Bier and D. Arnold, *Phys. Rev. E* **88**, 062307 (2013).

DS 13.2 Tue 10:15 C 243

**Morphometric thermodynamics and interface conventions** — ANDREAS REINDL, MARKUS BIER, and S. DIETRICH — Max Planck Institute IS, University of Stuttgart, Germany

Several model fluids with small number densities in contact with planar, spherical and cylindrical walls are investigated within density functional theory. The dependence of the interfacial tension on the curvature of spherical and cylindrical walls is examined and compared to the expression derived within the framework of morphometric thermodynamics. Particular attention is paid to the influence of the choice of the interface location, which underlies the definition of the interfacial tension. We found that morphometric thermodynamics is never exact for the considered systems and that its quality as an approximation depends on the choice of the interface.

DS 13.3 Tue 10:30 C 243

**The surface tension anomaly of water** — MARCELLO SEGA<sup>1</sup>, GEORGE HORVAI<sup>2</sup>, and PAL JEDLOVSKY<sup>3</sup> — <sup>1</sup>University of Vienna, Institut für Computergestützte Biologische Chemie, Vienna, Austria — <sup>2</sup>MTA-BME Research Group of Technical Analytical Chemistry, Budapest, Hungary — <sup>3</sup>Department of Chemistry, EKF Training School, Eger, Hungary

The surface tension of water is characterised by an anomalous dependence on the temperature that manifests itself in the form of an inflection point [1]. So far, a microscopic explanation of this phenomenon was missing. By using intrinsic surface analysis on the liquid/vapour interface, simulated using six different water models, we managed to establish a link between the surface tension inflection and the topological properties of the hydrogen-bond network of the surface layer. We discovered that the inflection temperature coincides with the percolation threshold of the hydrogen bond network in the first molecular layer at the liquid/vapour interface. This provides strong evidence that the sudden breakup of the network, which takes place at the percolation threshold, is the underlying microscopic mechanism at the origin of this surface tension anomaly of water [2,3].

- [1] J. S. Rowlinson and B. Widom. *Molecular Theory of Capillarity*; Dover Publications: Mineola, NY, 2002; p 11.
- [2] M. Sega, G. Horvai and P. Jedlovsky, *Langmuir* **30**, 2969 (2014)
- [3] M. Sega, G. Horvai and P. Jedlovsky, *J. Chem. Phys.* **141**, 054707 (2014)

DS 13.4 Tue 10:45 C 243

**Liquid drops on a surface: comparing results from microscopic density functional theory (DFT) with mesoscopic modelling and a method for calculating the binding potential** — ADAM HUGHES<sup>1</sup>, UWE THIELE<sup>2</sup>, and ANDREW ARCHER<sup>1</sup> — <sup>1</sup>Department of Mathematical Sciences, Loughborough University, Loughborough, LE11 3TU, UK — <sup>2</sup>Westfälische Wilhelms-Universität Münster, Institut für Theoretische Physik, Wilhelm-Klemm-Str. 9, 48149 Münster, Deutschland

We present a microscopic DFT based method for calculating the binding potential  $g(h)$  for a film of liquid on a solid surface, where  $h$  is the thickness of the liquid film. The form of  $g(h)$  determines whether or not the liquid wets the surface. We study in detail the effect on  $g(h)$  of truncating the range of the dispersion forces, both those between the fluid molecules and those between the fluid and wall. We find this can have a significant effect on the form of  $g(h)$  and therefore also on whether the liquid is predicted to wet the surface or not. We also calculate density profiles for liquid drops on a surface, using both DFT and also from inputting  $g(h)$  into a mesoscopic free energy. Comparing quantities such as the contact angle and the shape of the drops, we find good agreement between the two methods.

15 min. break

DS 13.5 Tue 11:15 C 243

**Crack-Free Hierarchical Wrinkle Patterns** — ●BERNHARD GLATZ and ANDREAS FERY — Physical Chemistry II, University of Bayreuth, Universitätsstraße 30, 95447 Bayreuth, Germany

Wrinkling is a mechanical instability phenomenon of thin films: Wrinkles form, if a system consisting of a hard, thin layer in strong adhesive contact with a soft, thick elastomer is subject to in plane compression. Under these conditions, a buckling instability results in a periodic surface corrugation with well-defined wavelength. In that regard PDMS is a well-established elastomer since it allows the in-situ generation of a glassy layer by oxidization processes as plasma or UVO. It comprises however side features as cracks and line defects, which form in most wrinkling process and are not predictable yet. We demonstrate a crack-free method where line defects are arranged by modifying the substrate: A stiffness gradient between two covalently linked PDMS phases induces a change in the wrinkle periodicity along the border of both. We tuned the ratio of the phases and so received several hierarchical line defect patterns. Furthermore computer simulations helped us to understand the observed structures. Such crack-free wrinkles with predictable defect positions allow applications as channel junctions in microfluidics or templates for particle alignment.

[1] B. A. Glatz and co-workers (in preparation)

DS 13.6 Tue 11:30 C 243

**Condensation of methane in metal organic frameworks (MOFs): Novel phase transitions** — ●NICOLAS HÖFT and JÜRGEN HORBACH — Institut für Theoretische Physik II: Soft Matter, Heinrich-Heine-Universität Düsseldorf, Germany

Metal-Organic frameworks (MOFs) are nanoporous crystalline materials where metal oxide complexes are connected to each other by organic linkers. Due to the large inner surface, MOFs are well-suited for applications associated with gas adsorption. Experimentally, adsorption isotherms have been studied for molecules such as CH<sub>4</sub>, CO<sub>2</sub>, H<sub>2</sub>O, etc., indicating the possibility of a phase-transition in various MOF structures. However, the nature of these transitions is not well understood, in particular with respect to the interplay between layering on the inner surface and gas-liquid coexistence in the porous structure.

We use grand canonical Monte Carlo simulations in conjunction with successive umbrella sampling to study the condensation of CH<sub>4</sub> in the MOF systems IRMOF-1, IRMOF-8, and IRMOF-16. We find a very rich phase behaviour in these systems and analyse in detail the occurring coexisting phases as well as the critical behaviour.

DS 13.7 Tue 11:45 C 243

**Extreme Surface Propensity of Halide Ions in Water** — ●ELLEN H.G. BACKUS<sup>1</sup>, LUKASZ PIATKOWSKI<sup>2</sup>, ZHEN ZHANG<sup>1</sup>, HUIB J. BAKKER<sup>2</sup>, and MISCHA BONN<sup>1</sup> — <sup>1</sup>Max Planck Institute for Polymer Research, Mainz, Germany — <sup>2</sup>FOM Institute AMOLF, Amsterdam, the Netherlands

The dominant part of water on earth is not pure water; it contains salts. Moreover, especially in atmospheric chemistry the ions present at the interface are important for various reactions occurring at these interfaces. These ions are potentially reactive and/or determine the water structure, thereby influencing the surface reactivity. Experimentally, it is very challenging to determine the local concentration of ions in the outermost molecular monolayer region of aqueous solutions. Here, we show how two-dimensional sum frequency generation spectroscopy can be used to determine this concentration by measuring the energy

transfer rate between water molecules. The presence of ions leads to a reduction of this transfer rate. The data reveal a high surface propensity for iodide anions corresponding to a surface concentration three times higher than the bulk concentration.

DS 13.8 Tue 12:00 C 243

**Pressure induced adsorption of lysozyme at the solid-liquid interface** — ●PAUL SALMEN<sup>1</sup>, JULIA NASE<sup>1</sup>, SUSANNE DOGAN<sup>1</sup>, HOLGER GÖHRING<sup>1</sup>, IRENA KIESEL<sup>1,3</sup>, JOHANNES MÖLLER<sup>1,2</sup>, CHRISTOPHER WEIS<sup>1</sup>, FLORIAN WIRKERT<sup>1</sup>, MICHAEL PAULUS<sup>1</sup>, and METIN TOLAN<sup>1</sup> — <sup>1</sup>Fakultät Physik/DELTA, TU Dortmund, 44221 Dortmund, Germany — <sup>2</sup>ESRF - The European Synchrotron, 71 Avenue des Martyrs, F-38043 Grenoble, France — <sup>3</sup>Institut Laue-Langevin, 71 Avenue des Martyrs, 38000 Grenoble, France

The pressure-induced adsorption of proteins at hydrophilic and hydrophobic interfaces was studied by x-ray reflectivity measurements. In our custom-built cell for x-ray reflectivity (XRR) measurements [1], we are able to apply pressures up to 5 kbar and study the solid/liquid interface in-situ with Angstrom resolution. As hydrophobic surfaces, silicon wafers covered with octadecyltrichlorosilane (OTS) were used, while bare silicon wafers with a native silicon dioxide layer provide charged, hydrophilic interfaces. Lysozyme was used in 20 mM BisTris buffer (pH 7.1) at a concentration of 0.1 mg/ml. The measurements were performed at the synchrotron light sources DELTA (Dortmund, Germany), ESRF (Grenoble, France) and SLS (Villigen, Switzerland) using high energy x-ray radiation. At low pressures, only a monolayer of lysozyme adsorbs at both interfaces. When pressure is increased, a second layer of lysozyme adsorbs. Because the thickness of the first layer decreases in this process, we suppose a partial collapse of the first lysozyme layer. [1] F. J. Wirkert et al., Journal of Synchrotron Radiation 2014 (21) doi:10.1107/S1600577513021516

DS 13.9 Tue 12:15 C 243

**A Standing-Wave Approach in Ambient Pressure Photoemission: Chemical State and Depth Resolved Concentration Profiles of Solid/Liquid and Liquid/Gas Interfaces** — ●SLAVOMIR NEMSAK<sup>1</sup>, HENDRIK BLUHM<sup>2</sup>, CHARLES FADLEY<sup>3</sup>, and CLAUS SCHNEIDER<sup>1</sup> — <sup>1</sup>Peter Grünberg Institut 6, Forschungszentrum Jülich, 52425 Jülich, Germany — <sup>2</sup>Chemical Sciences Division, Lawrence Berkeley National Laboratory, 94720 Berkeley, CA, USA — <sup>3</sup>Department of Physics, University of California, 95616 Davis, CA, USA

A standing wave approach in the ambient pressure photoelectron spectroscopy is a new and powerful technique to study heterogeneous processes in solid/gas, liquid/gas and solid/liquid interfaces [1]. Advantages of the technique, such as superb depth resolution and chemical sensitivity, are demonstrated on several model systems with relevance to energy research, heterogeneous catalysis, electrochemistry, and atmospheric and environmental science. A strong standing-wave is generated using a multi-layer Si/Mo mirror as a substrate and phase of the standing wave is tailored through the interface of interest by rocking the sample around the Bragg angle. Photoemission signal from different species is then analyzed in order to provide their spatial arrangement, as well as local potential variations, along the direction perpendicular to the interface with sub-nm accuracy. Pros and cons of using harder X-ray excitation are discussed in terms of a photoemission signal strength and a standing wave effects amplitude.

[1] Nemsak et. al, Nature Communications 5, 2014.

## DS 14: Plasmonics and nanooptics: Structure, fabrication and characterization (joint session with O)

Time: Tuesday 10:30–13:15

Location: MA 043

DS 14.1 Tue 10:30 MA 043

**Large-area spectrally selective plasmonic perfect absorber sensor fabricated by laser interference lithography** — ●SHAHIN BAGHERI, NIKOLAI STROHFELDT, ANDREAS TITTL, and HARALD GIESSEN — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

We employ laser interference lithography to create homogeneous wire and rectangle arrays and utilize them for manufacturing of large-area plasmonic perfect absorbers [1]. Geometry and periodicity of such tailored nanostructures can be precisely controlled by adjusting the interference conditions in single- and double-exposure processes, resulting in spectrally selective perfect absorption of light from the visible to the mid-infrared wavelength range. We also demonstrate the applicability of our fabrication method for detection schemes by measuring the hydrogen sensing performance of a palladium-based perfect absorber operating in the visible wavelength range. Due to the large-area and fast fabrication process, our method offers a great potential for low-cost commercial nanophotonic and plasmonic devices in industrial applications.

[1] S. Bagheri et al., *Adv. Opt. Mater.* **2**, 1050-1056 (2014)

DS 14.2 Tue 10:45 MA 043

**Light trapping and enhanced absorption in femtosecond-laser materials processed amorphous thin-film silicon** — DOMINIK DIFFERT<sup>1</sup>, ●WALTER PFEIFFER<sup>1</sup>, BABAK SOLEYMANZADEH<sup>1</sup>, and HELMUT STIEBIG<sup>1,2</sup> — <sup>1</sup>Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany — <sup>2</sup>Institut für Innovationstransfer an der Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany

Efficient thin-film solar cells balance the reduced absorption in thin absorber layers by means of various photon management strategies that often involve nanotextured interfaces. We report broadband absorption enhancement in femtosecond (fs) laser materials processed thin amorphous silicon. The absorption of a single amplified fs laser pulse (30 fs, 795 nm, 75 mJ cm<sup>-2</sup>) creates a thin nanotextured microcrystalline surface layer. Coherent scattered light micro-spectroscopy in combination with spectral interferometry reveals that incident radiation is trapped for about 100 fs in localized photonic modes in the laser processed area. This trapping explains the enhanced absorption and the observed local Raman yield enhancement. The lateral correlation length of the light trapping modes indicates very efficient light scattering in the processed layer that leads to strong localization of light in the absorber layer. Consequently, fs materials processing offers an interesting pathway towards advanced photon management in amorphous silicon based thin-film solar cells.

DS 14.3 Tue 11:00 MA 043

**Extreme Ultraviolet Proximity Lithography for fast, flexible and large-scale fabrication of infrared antennas** — ●GEORG KUNKEMÖLLER<sup>1,3</sup>, TOBIAS W.W. MASS<sup>2</sup>, ANN-KATRIN U. MICHEL<sup>2</sup>, HYUN-SU KIM<sup>3</sup>, SASCHA BROSE<sup>1</sup>, SERHIY DANYLYUK<sup>1</sup>, THOMAS TAUBNER<sup>2</sup>, and LARISSA JUSCHKIN<sup>3</sup> — <sup>1</sup>TOS, RWTH Aachen University — <sup>2</sup>I. Institute of Physics (IA), RWTH Aachen University — <sup>3</sup>Chair for Experimental Physics of Extreme-Ultraviolet EUV, RWTH Aachen University

Recently, several lithographic approaches to improve throughput and costs for the fabrication of infrared antennas by using parallel processes were presented [1-4]. In this contribution, we present Extreme ultraviolet (EUV) proximity lithography as a comparable advantageous technique for the fabrication of large arrays of infrared antennas. Using Fresnel-diffraction, this method offers the potential of a great variety of structures [5]. Depending on exposure time and gap between mask and resist, different dumbbell-shaped structures can be fabricated using only a single mask-geometry. Characterization via SEM imaging and FTIR spectroscopy show a good agreement to lithography- and FDTD simulations and turns this fabrication method to a promising tool for a large-area fabrication of infrared nanostructures.

[1] Hoffmann et al. *J. Phys. Chem. C* **2013** 117, 11311-11316

[2] Cataldo et al. *ACS Nano* **2012** 6, 979-985

[3] Aksu et al. *Nano Lett.* **2010** 10, 2511-2518

[4] Bagheri et al. *Adv. Opt. Mat.* **2014** 2, 1050-1056

[5] Danylyuk et al. *J. Vac. Sci. Technol. B* **2013** 31, 021602

DS 14.4 Tue 11:15 MA 043

**Fabrication and Characterization of Plasmonic Nanocone Antennas for Strong Spontaneous Emission Enhancement** — ●BJÖRN HOFFMANN<sup>1</sup>, SIMON VASSANT<sup>1</sup>, XUE-WEN CHEN<sup>1</sup>, STEPHAN GÖTZINGER<sup>1,2</sup>, VAHID SANDOGHDAR<sup>1,2</sup>, and SILKE CHRISTIANSEN<sup>1,3</sup> — <sup>1</sup>Max Planck Institute for the Science of Light, Erlangen, Germany — <sup>2</sup>Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — <sup>3</sup>Helmholtz Centre Berlin for Materials and Energy, Berlin, Germany

Plasmonic nano-antennas have attracted remarkable attention due to their ability to strongly modify the excitation and emission channels of quantum emitters. Metallic nanocones are a promising candidate for a strong enhancement of spontaneous emission while keeping high quantum efficiencies. Here, we report on the precise fabrication of gold nanocones with tunable dimensions to tailor their plasmon resonance to specific applications. Therefore, we developed a focused ion beam (FIB) etching procedure that offers precise control over the height, diameter and tip radius of the cones. We measured the plasmon resonance spectra of gradually etched cones and were able to reproduce the spectra by BOR-FDTD simulations. The cones show reproducible plasmon resonances between 580 - 700 nm and exhibit theoretical radiative Purcell factors above 500, which renders them promising structures for spontaneous emission enhancement.

DS 14.5 Tue 11:30 MA 043

**Creating metallic nanostructures by electron beam induced deposition (EBID) for plasmonic applications** — ●CASPAR HAVERKAMP<sup>1</sup>, KATJA HÖFLICH<sup>1</sup>, and SILKE CHRISTIANSEN<sup>1,2</sup> — <sup>1</sup>Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — <sup>2</sup>Max Planck Institute for the Science of Light, Erlangen, Germany

During EBID a gas-injection system (GIS) inserts a precursor Gas into the vacuum chamber of an scanning electron microscope (SEM). The molecules which adsorb, desorb and diffuse at the substrate surfaces and are locally decomposed by the electron beam. While the volatile part is pumped out the non-volatile part forms the deposit onto the substrate. By controlling the electron beam movement via a patterning engine various shapes can be realized. As precursor gas the metal-organic compound dimethyl-(acetylacetonate) Gold(III), short Me<sub>2</sub>Au(acac) is used, resulting in nanometer-sized gold particles embedded in a carbonaceous matrix. Since the metal content of this material is very low, two approaches are discussed how to overcome this drawback. The first one is to decrease the carbon content of the structure by an in-situ post-treatment with water vapor irradiated by the electron beam. The splitting of the water molecules by the electron beam results in reactive oxygen species which react with the carbon of the EBID structure creating volatile carbon oxides. The second approach is to use the EBID structure as template and achieving the plasmonic response by a metallic coverage .

DS 14.6 Tue 11:45 MA 043

**Cathodoluminescence of sharp Au- and Ag-tips in the vicinity of a Au-film** — ●MARTIN GRÜSSER, XINZHOU MA, and ROLF SCHUSTER — Institute of Physical Chemistry, Condensed Matter Division, Karlsruhe Institute of Technology (KIT), Germany

Sharp metal tips acting as optical antennas play an important role in many experimental applications. The locally enhanced electromagnetic field allows, e.g., for tip-enhanced raman spectroscopy [1, 2] on the single molecule level. In addition to the lightning-rod effect, also surface plasmons localized at the tip apex and gap plasmons between a tip and a sample surface [3] contribute to the field enhancement.

To investigate the local excitation of surface plasmons and gap plasmons in the tip-surface system we employ, cathodoluminescence upon electron irradiation in a scanning electron microscope (SEM), which accesses the radiative modes of the electron excited plasmons. The distance between tip and surface is controlled by a scanning tunneling microscope, mounted inside the vacuum chamber of the SEM. We observed enhanced photon emission upon electron irradiation near the tip-surface gap, on both the tip as well as on the sample side. Spectra upon irradiation of tip or sample show strong differences in intensity

and peak position, e.g. a redshift for smaller tip-surface distances and evolution of additional peaks, which may depend on the formation of gap plasmons.

[1] R. M. Stöckle et al., *Chem. Phys. Lett.* 2000, 318, 131. [2] B. Pettinger et al., *Annu. Rev. Phys. Chem.* 2012, 63, 379. [3] Z. Yang, J. Aizpurua, H. Xu, *J. Raman Spectrosc.* 2009, 40, 1343.

DS 14.7 Tue 12:00 MA 043

**Nanowire-film gap plasmon waveguides for spaser resonators**

— ●FRIEDEMANN GÄDEKE, GÜNTER KEWES, and OLIVER BENSON — AG Nano Optik, Institut für Physik, Humboldt-Universität zu Berlin

Surface plasmon amplification by stimulated emission of radiation (spaser) might be an essential part of future nano-photonic devices. Spasers are subwavelength sized light sources and could be used in quantum information technology or nano-lithography [1].

We report on numerical and experimental investigations on an ultracompact resonator design for spasers. We use organic gain media in a waveguide which is formed by a gap between a gold film and a gold nanowire. The design follows Ref. [2] and [3] and includes emitter-free spacing layers between active medium and metal [4] which will be beneficial to achieve lower spasing thresholds. We optimize our design towards a well defined energy distribution in the gap and low propagation losses. We present a feasible fabrication technique based on relatively simple and quick methods like spin-coating, ellipsometry and stamping as well as first fluorescence studies.

[1] Stockman, M. L., *Journal of Optics* 12, 024004 (2010) [2] Oulton, R. F. et al., *Nature* 461, 629-632 (2009) [3] Russell, K. J. et al., *Nature Photonics* 6, 459-462 (2012) [4] Kewes, G. et al., *Arxiv* 1408.7054 (2014)

DS 14.8 Tue 12:15 MA 043

**Material contrasts of layered Phase Change Materials in s-SNOM**

— ●MARTIN LEWIN, BENEDIKT HAUER, ANN-KATRIN U. MICHEL, and THOMAS TAUBNER — Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

Phase Change Materials (PCM) show at least two stable states in the solid phase with significantly different physical properties. They can be switched reversibly by optical or electrical means, which enables their use for storage and logical applications [1].

Scattering-type Scanning Near-field Optical Microscopy (s-SNOM) is based on an illuminated metal coated tip being scanned over a sample. Due to the local detecting approach, the optical properties of the sample can be analysed wavelength-independently on a nm-scale [2].

Hence, s-SNOM can be used to investigate the switching in nanometre sized phase change devices: We could show that it is possible to distinguish amorphous and crystalline regions of AgInSbTe even below 100 nm of capping layer. Firstly, the material contrasts of a bare 30 nm thick layer of AgInSbTe with and without capping layer are analysed. Secondly, correlative TEM and s-SNOM analyses are performed of a sandwiched amorphous layer with crystalline spots. The found complex material contrasts are explained by theoretical calculations taking into account the layered structure of the sample.

[1] M. Wuttig and N. Yamada, *Nature Mater.* 6, pp. 824-832 (2007) [2] F. Keilmann and R. Hillenbrand, *Phil. Trans. R. Soc. Lond. A* 362, pp. 787-805 (2004)

DS 14.9 Tue 12:30 MA 043

**Surfactant-Controlled Kinetic Overgrowth of Gold Rods into Gold-Core Silver-Shell Rods to Induce Controlled Internal Mirror Charges**

— ●TOBIAS KÖNIG, MORITZ TEBBE, MARTIN MAYER, CHRISTIAN KUTTNER, and ANDREAS FERY — Physical Chemistry II, University of Bayreuth, 95447 Bayreuth, Germany

We present the surfactant-controlled overgrowth of gold nanorods into gold-core silver-shell nanoparticles (rodboids) to gain low growth rates for full control of the kinetic process. In gold-core silver-shell rod-

boids not much attention has been paid to the overlap region of the intraband gaps of gold and silver (326 to 515 nm). In this optical region, the gold core acts as a retarding element because of the much higher damping in the core compared to the silver shell. Electromagnetic simulations show that the silver shell induces mirror charges at the core/shell interface which results in a similar signature as an anti-bonding mode. An excitation outside the overlap region yields in-phase oscillations of the surface charges (signature of a bonding mode). In contrast to plasmonic hybridization, the energetic splitting of the two modes is weaker so that both modes are present in the optical spectrum. Consequently, full control over the kinetic process allows for precise tailoring of the resonance wavelengths of both modes. Tailored rodboids represent ideal candidates as a building block for metamaterials and are suitable for application as optical sensor, light harvesting, and information technology.

DS 14.10 Tue 12:45 MA 043

**Strongly Coupled Plasmonic Modes of Self-Assembled Particles Lines in the Context of Ensemble-Averaging and Disorder**

— ●CHRISTIAN KUTTNER, CHRISTOPH HANSKE, MORITZ TEBBE, TOBIAS KÖNIG, and ANDREAS FERY — Physical Chemistry II, University of Bayreuth, 95447 Bayreuth, Germany

We present ensembles of gold nanoparticle arranged in single and double lines on solid substrates.[1] These linear assemblies were formed by template-assisted self-assembly[2,3] of monodisperse protein-coated gold nanoparticles in wrinkle templates. The substrates exhibit high structural regularity on centimeter-squared areas which allow for characterization of their extinction cross-sections by conventional UV/vis/NIR spectroscopy.

Modeling based on electrodynamic simulations shows a clear signature of strong plasmonic coupling with an interparticle spacing of 1-2 nm. We find evidence for well-defined plasmonic modes of quasi-infinite chains.[1] Beyond elementary simulations on the individual chain level, we introduce an advanced model taking parameters like the chain length distribution, ensemble-averaging, as well as interchain disorder into account.[1]

[1] C. Hanske et al. *Nano Lett.* 2014, in press.

[2] C. Lu et al. *Soft Matter*, 2007, 3, 1530-1536.

[3] N. Pazos-Perez et al. *Chem. Sci.*, 2010, 1, 174-178.

DS 14.11 Tue 13:00 MA 043

**New details about monocrystalline goldflakes for plasmonic applications**

— ●THORSTEN FEICHTNER<sup>1</sup>, MUHAMMAD BASHOUTI<sup>1</sup>, BJÖRN HOFFMANN<sup>1</sup>, ACHMED SALAHELDIN<sup>2</sup>, MIRZA MAČKOVIĆ<sup>3</sup>, CHRISTEL DIEKER<sup>3</sup>, PETER RICHTER<sup>4</sup>, OVIDIU GORDAN<sup>4</sup>, DIETRICH ZAHN<sup>4</sup>, ERDMANN SPIEKER<sup>3</sup>, and SILKE CHRISTIANSEN<sup>1,5</sup> — <sup>1</sup>Max Planck Institute for the Science of Light (MPL), 91058 Erlangen, Germany — <sup>2</sup>Universität Erlangen-Nürnberg, Institute of Particle Technology, 91058 Erlangen, Germany — <sup>3</sup>Universität Erlangen-Nürnberg, Center for Nanoanalysis and Electron Microscopy (CENEM), 91058 Erlangen, Germany — <sup>4</sup>Semiconductor Physics, Technische Universität Chemnitz, 09107 Chemnitz, Germany — <sup>5</sup>Helmholtz Centre Berlin for Materials and Energy (HZB), 14109 Berlin, Germany

Wet-chemical synthesis of nm-thin, large area gold flakes is a viable method to realize a flat, monocrystalline raw material for fabricating high quality plasmonic devices. Transmission electron microscopy (TEM) proved the gold flakes being single crystalline except for twin boundary formation parallel to the flake surface. Micro-ellipsometry allowed to determine their complex dielectric constant for the first time. The flakes were polished by focused ion beam (FIB) milling and analyzed with electron backscatter diffraction (EBSD). The gold flakes remain monocrystalline down to a thickness of  $\approx 10$  nm allowing state-of-the-art nanofabrication processing to obtain nano-antennas or other desired plasmonic structures at sizes and structure perfections impossible with evaporated, poly-crystalline gold thin films.

## DS 15: High-k and Low-k Dielectrics (joint session with DF)

Time: Tuesday 11:15–12:15

Location: H 0111

DS 15.1 Tue 11:15 H 0111

**Broadband dielectric response of doped rutile: intrinsic or extrinsic colossal dielectric constants?** — ●MARTIN WOHLAUER, STEPHAN KROHNS, PETER LUNKENHEIMER, and ALOIS LOIDL — Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg (Germany)

Materials exhibiting so-called colossal effects have an enormous potential for future use in correlated electronics, including capacitors for energy storage and integrated circuits. The search for functional ceramics showing colossal dielectric constants (CDC) is still an active field of research<sup>1</sup>. Different phenomena, e.g., charge-order or internal as well as external electrical heterogeneities can lead to CDCs<sup>2</sup>. For the most prominent ceramic,  $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$ , the mechanism giving rise to a dielectric permittivity of up to  $10^5$  is of extrinsic nature, e.g. interface polarisation. The discovery of CDCs in indium- and niobium-doped rutile at room temperatures recently also attracted high scientific interest<sup>3</sup>. In this talk, broadband dielectric measurements on various doped rutile ceramics will be presented. The results will be thoroughly discussed, especially emphasizing the contributions of external and internal interface effects influencing the permittivity. We demonstrate, that extrinsic interface effects are responsible for the CDCs in doped rutile.

<sup>1</sup>S. Krohns *et al.*, *Nat. Mat.*, **10**:899 (2011).

<sup>2</sup>P. Lunkenheimer *et al.*, *Eur. Phys. J. Special Topics*, **180**:61 (2010).

<sup>3</sup>W. Hu *et al.*, *Nat. Mat.*, **12**:821 (2013).

DS 15.2 Tue 11:30 H 0111

**Structuring and interface manipulation of ultra-thin silicate films on a  $\text{Si}(001)$  surface** — ●SHARIFUL ISLAM<sup>1</sup>, KARL HOFMANN<sup>2</sup>, and HERBERT PFNÜR<sup>1</sup> — <sup>1</sup>Institut für Festkörperphysik (ATMOS), Leibniz Universität Hannover — <sup>2</sup>Inst. f. Bauelemente der Mikroelektronik, Leibniz Universität Hannover

The dielectric-substrate interface plays a very important role on the growth condition and on the chemical, structural and kinetic properties of dielectric layers. Some very important properties like the sharpness of the interface, trap densities and band alignment also influenced by the cleanliness of substrate surface. We found the crystalline high-k silicate ( $\text{Ba}_{0.8}\text{Sr}_{0.2}\text{SiO}_4$  and  $\text{Ba}_2\text{SiO}_4$ ) to have dielectric constants  $\sim 18$  and  $\sim 20$  respectively. We studied the silicates elaborately both on structured and unstructured  $\text{Si}(001)$  surface after depositing both at room and at high temperature ( $650^\circ\text{C}$ ). In addition to the spectroscopic measurements (XPS, SPA-LEED, EELS, AFM and TEM) we performed electrical measurements (C-V & I-V) of the silicate as an alternate gate dielectric in a MOS diode to study the dielectric-substrate interface in detail. The crystalline orthorhombic  $\text{Ba}_2\text{SiO}_4$  grown here has a band gap of  $E_G = 5.7\text{eV}$ , an interface trap density  $D_{it} \sim 10^{12}\text{eV}^{-1}\text{cm}^{-2}$ , very low hysteresis  $< 0.5\text{mV}$ , band offset

$> 2\text{eV}$ , leakage current  $< 6\text{mA}/\text{cm}^2$  at  $+1\text{V}$ ; additional structural and electrical properties will be discussed.

DS 15.3 Tue 11:45 H 0111

**k-restore Process with Plasma Enhanced Fragmentation for Damaged ULK Materials — A DFT and MD Study** — ●ANJA FÖRSTER<sup>1,5</sup>, CHRISTIAN WAGNER<sup>2</sup>, JÖRG SCHUSTER<sup>1</sup>, SIBYLLE GEMMING<sup>3,4</sup>, and STEFAN SCHULZ<sup>1,2</sup> — <sup>1</sup>Fraunhofer ENAS, Chemnitz — <sup>2</sup>Center for Microtechnologies, TU Chemnitz, Chemnitz — <sup>3</sup>Institute of Physics, TU Chemnitz, Chemnitz — <sup>4</sup>Helmholtz-Zentrum Dresden-Rossendorf, Dresden — <sup>5</sup>cfad, TU Dresden, Dresden

Because of their low dielectric constant (k-value) ultra-low-k (ULK) materials are used for isolating the interconnects in integrated circuits. However, during the manufacturing process the k-value lowering methyl groups are replaced by hydroxyl groups and hydrogen atoms. This process is called OH- and H-damage.

In our simulation study we use fragmented silylation molecules (OMCTS, DMADMS) to repair the OH- and H-damages and restore the k-value of the ULK material by reinserting lost methyl groups. The fragmentation of DMADMS and OMCTS is investigated as a function of the reaction temperature using DFT on the PBE/DNP-level.

The repair behavior of the so obtained fragments are studied with two model systems: an assortment of small ULK-fragments and a silica cluster. We show that larger repair fragments with two and three methyl groups are energetically favorable.

DS 15.4 Tue 12:00 H 0111

**Dissipative hydrogen two-level systems in  $\text{Al}_2\text{O}_3$**  — ●HAZEM ABU-FARSAKH<sup>1,2</sup>, LUKE GORDON<sup>1</sup>, ANDERSON JANOTTI<sup>1</sup>, and CHRIS G. VAN DE WALLE<sup>1</sup> — <sup>1</sup>Materials Department, University of California, Santa Barbara — <sup>2</sup>Prince Sultan University, Riyadh, Saudi Arabia

Superconducting qubits based on Josephson tunnel junctions are promising candidates for quantum computing. A limiting factor for their performance is the resonant absorption by two-level systems (TLSs) in the dielectric material. However, the microscopic nature of these TLSs has not been identified. In this work we propose that hydrogen interstitial atoms are the main source of TLSs in  $\text{Al}_2\text{O}_3$ . Using *ab-initio* calculations employing hybrid functionals we identify H binding sites and show that a hydrogen atom forms a H-bond in  $\text{Al}_2\text{O}_3$  and feels a double potential well, resulting in a tunneling effect. We map the three-dimensional potential energy of an interstitial H atom and calculate its tunneling frequency by solving the corresponding Schrödinger equation. Our results show that the tunneling of H atoms gives rise to a resonant absorption in the 10 GHz region, in agreement with experimental observations. This work was supported by IARPA.

## DS 16: Atomic Layer Deposition

Time: Tuesday 12:15–13:00

Location: H 0111

DS 16.1 Tue 12:15 H 0111

**$\text{SiO}_2$ -,  $\text{Al}_2\text{O}_3$ -, and  $\text{TiO}_2$ -nanotubes synthesized by ALD in etched ion-track membranes** — ●ANNE SPENDE<sup>1,2</sup>, NICOLAS SOBEL<sup>2</sup>, CHRISTIAN HESS<sup>2</sup>, MANUELA LUKAS<sup>2</sup>, BERND STÜHN<sup>2</sup>, JOSEF M MONTERO MORENO<sup>3</sup>, ROBERT ZIEROLD<sup>3</sup>, KORNELIUS NIELSCH<sup>3</sup>, CHRISTINA TRAUTMANN<sup>1,2</sup>, and MARIA EUGENIA TOIMIL-MOLARES<sup>1</sup> — <sup>1</sup>Materialforschung, GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt — <sup>2</sup>Technische Universität Darmstadt — <sup>3</sup>Universität Hamburg

Nanochannels and nanotubes of tailored dimensions and surface coatings are of great interest for basic research and applications e.g. in nanofluidics or sensoric. By combining ion-track nanotechnology with atomic layer deposition (ALD), we present a novel approach to fabricate inorganic nanotubes and surface modified nanochannels with aspect ratios above 3000.  $30\ \mu\text{m}$  thick polycarbonate foils are irradiated with GeV Au ions at the UNILAC accelerator of GSI. Subsequent chemical etching converts the ion tracks into open, cylindrical chan-

nels, with smallest achievable diameter presently down to 18 nm. We further reduced channel diameters of etched ion-track membranes in a controlled manner by applying ALD to coat the surface with  $\text{SiO}_2$ ,  $\text{Al}_2\text{O}_3$ , and  $\text{TiO}_2$ . By dissolving the polymer template, nanotubes with well defined wall thickness were obtained. ALD-coated membranes and released nanotubes were analysed by small-angle x-ray spectroscopy, electron microscopy and EDX. The coating is shape conformal and highly homogeneous along the entire channel length. XPS shows the stoichiometric composition of the deposited films.

DS 16.2 Tue 12:30 H 0111

**Atomic Layer Deposition and characterization of Ga-doped  $\text{Sb}_2\text{Te}_3$  thin films at low temperatures.** — ●CHRISTOPH WIEGAND<sup>1</sup>, MONIKA RUSEK<sup>2</sup>, JOHANNES GOOTH<sup>1</sup>, ROBERT ZIEROLD<sup>1</sup>, STEPHAN SCHULZ<sup>2</sup>, and KORNELIUS NIELSCH<sup>1</sup> — <sup>1</sup>Institut für Nanostruktur- und Festkörperphysik, Universität Hamburg — <sup>2</sup>Institut für Anorganische Chemie, Universität Duisburg-

Essen

Semiconductors of the  $V_2VI_3$ -type have recently become in the focus of a new type of material class, called topological insulators (TIs). TIs are bulk insulators that offer time-reversal symmetry protected highly conductive surface states.

We demonstrate the growth of antimony telluride and gallium telluride thin films via ALD at temperatures below 100 °C, which is relatively low compared to CVD or comparable techniques. In super-cyclic approach depicted  $Ga_xSb_{2-x}Te_3$  compounds and nanolaminates have been synthesized and have led to an understanding of the crystallization behavior of  $Sb_2Te_3$  in dependence of the Ga-content and the underlying substrate. We were able to determine the minimum Ga-content needed for single-crystalline growth of  $Ga_xSb_{2-x}Te_3$  thin films. Moreover, actual studies are performed on the measurement of the electrical transport properties of these  $Ga_xSb_{2-x}Te_3$  films using a micron-sized hall-bar device fabricated by standard photolithography and lift-off processing.

The authors acknowledge financial support from the DFG through the SPP 1666 project "Topological Insulators".

DS 16.3 Tue 12:45 H 0111

**Encapsulation of Silver Nanowires in Transparent Conductive Oxides by Atomic Layer Deposition** — ●MANUELA GÖBELT<sup>1</sup>,

RALF KEDING<sup>1</sup>, BJÖRN HOFFMANN<sup>1</sup>, SEBASTIAN SCHMITT<sup>1</sup>, SARA JÄCKLE<sup>1</sup>, MICHAEL LATZEL<sup>2</sup>, and SILKE CHRISTIANSEN<sup>1,3</sup> — <sup>1</sup>Max Planck Institute for the Science of Light, Günther-Scharowsky-Str. 1/Bau 24, Erlangen, Germany — <sup>2</sup>Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Institute of Optics, Information and Photonics, Staudtstr. 7/B2, Erlangen, Germany — <sup>3</sup>Helmholtz Center Berlin for Energy and Materials, Hahn-Meitner-Platz 1, Berlin, Germany

Aluminum doped ZnO (AZO) has become a promising material for transparent electrodes due to its high abundance and its suitable electrical and optical properties. However, the sheet resistance of AZO is rather high to adapt as transparent electrode. Silver nanowire (AgNW) networks encapsulated in an AZO layer hold the promise to significantly decrease its resistivity, but the encapsulation of high aspect ratio structures is rather difficult to achieve by conventional deposition techniques. Atomic layer deposition (ALD) is a useful technique to deposit homogenous and uniform layers e.g. on nanostructures used in third generation solar cell concepts. This deposition technique is based on a self-limiting reaction mechanism, which guarantees excellent film deposition conformity and atomic-scale thickness control. The encapsulation of AgNWs by ALD is shown and optimization routes for its conductivity and transparency are pointed out. Furthermore, the application of AgNW/AZO-TCOs for silicon solar cells is discussed.

## DS 17: Transport: Topological Insulators 3 (joint session with DS, HL, MA, O)

Time: Tuesday 14:00–16:00

Location: H 0110

DS 17.1 Tue 14:00 H 0110

**Helical Surface States In Strained HgTe** — ●JAN BOETTCHER and EWELINA M. HANKIEWICZ — Universität Würzburg, Faculty for Physics and Astronomy, TP IV

Strained HgTe is a 3D topological insulator with negligible bulk conductivity, where the transport is dominated by the surface states for a wide density range [1]. We analytically show the existence of a topologically protected surface state within the framework of a simplified 6x6 Kane Hamiltonian defined on the half-space. Strained HgTe is different from other 3D TIs due to an additional coupling of the surface states, forming between the light-hole and electron-like (S) bands, to the heavy-hole bands. This coupling causes an avoided crossing between these bands and, therefore, opens a large gap in the surface state spectrum by which the topological protection is not affected. Furthermore, we investigate the spin texture of the surface states. In the presence of an external magnetic field, we study the Landau level spectrum and discuss the experimental signatures which would be a consequence of our model.

We acknowledge grant HA 5893/4-1 within SPP 1666.

[1] Brüne et al., arXiv:1407.6537 (to be published in PRX 2014).

DS 17.2 Tue 14:15 H 0110

**Transport signatures of a Zeeman-split quantum dot coupled to a helical edge state** — ●BENEDIKT PROBST<sup>1</sup>, PAULI VIRTANEN<sup>2</sup>, and PATRIK RECHER<sup>1</sup> — <sup>1</sup>Institut für Mathematische Physik, TU Braunschweig, 38106 Braunschweig, Germany — <sup>2</sup>O.V. Lounasmaa Laboratory, Aalto University School of Science, Finland

We investigate the transport signatures of a Zeeman-split quantum dot (QD) containing a single spin 1/2 weakly coupled to a helical Luttinger liquid (HLL) within a generalized master equation approach. The HLL induces a tunable magnetization direction on the QD controlled by an applied bias voltage when the quantization axes of the QD and the HLL are noncollinear. This tunability allows to extract characteristic signatures of a HLL and the spin dynamics of the QD via the backscattering conductance and the current noise.

DS 17.3 Tue 14:30 H 0110

**Effects of random Rashba spin-orbit coupling and magnetic impurities on edge state transport in topological insulators** — LUKAS KIMME<sup>1</sup>, ●BERND ROSENOW<sup>1</sup>, and ARNE BRATAAS<sup>2</sup> — <sup>1</sup>Institut für Theoretische Physik, Universität Leipzig, D-04103, Leipzig, Germany — <sup>2</sup>Department of Physics, Norwegian University of Science and Technology, NO-7491 Trondheim, Norway

CdTe/HgTe quantum-wells that exceed a critical thickness host topologically protected edge states, which give rise to a quantized conductance. Despite the topological protection, experimentally a mean free

path of a few microns is found [1]. The experimentally observed weak temperature dependence of the mean free path challenges proposed theoretical explanations, many of which predict power law behaviors. We here consider a model where edge electrons experience spatially random Rashba spin-orbit coupling, and are also coupled to a magnetic impurity. Using a rate equation model, we determine the steady state of the impurity spin in the finite bias regime, and compute both linear and nonlinear resistances. For a finite density of impurity spins, we obtain a weak temperature dependence of the mean free path, in agreement with experimental findings.

[1] M. König, S. Wiedmann, C. Brüne, A. Roth, H. Buhmann, L. W. Molenkamp, X.-L. Qi, and S.-C. Zhang, Science 318, 766 (2007).

DS 17.4 Tue 14:45 H 0110

**Spin-based Mach-Zehnder interferometry in topological insulator p-n junctions** — ●FERNANDO DE JUAN<sup>1,2</sup>, RONI ILAN<sup>1</sup>, and JOEL E. MOORE<sup>1</sup> — <sup>1</sup>University of California, Berkeley — <sup>2</sup>Freie Universität Berlin

A p-n junction, an interface between two regions of a material populated with carriers of opposite charge, is a basic building block of solid state electronic devices. From the fundamental physics perspective, it often serves as a tool to reveal the unconventional transport behavior of novel materials. In this work, we show that a p-n junction made from a three dimensional topological insulator (3DTI) in a magnetic field realizes an electronic Mach-Zehnder interferometer with virtually perfect visibility. This is owed to the confinement of the topological Dirac fermion state to a closed two-dimensional surface, which offers the unprecedented possibility of utilizing external fields to design networks of chiral modes wrapping around the bulk in closed trajectories, without the need of complex constrictions or etching. Remarkably, this junction also acts as a spin filter, where the path of the particle is tied to the direction of spin propagation. It therefore constitutes a novel and highly tunable spintronic device where spin polarized input and output currents are naturally formed and could be accessed and manipulated separately.

DS 17.5 Tue 15:00 H 0110

**Broken-gap topological insulators in magnetic fields** — RAFAŁ SKOLASINSKI<sup>1</sup>, DIMITRY PIKULIN<sup>2</sup>, and ●MICHAEL WIMMER<sup>1</sup> — <sup>1</sup>Delft University of Technology, The Netherlands — <sup>2</sup>University of British Columbia, Canada

Two-dimensional topological insulators have helical edge channels protected by time-reversal symmetry, leading to a quantized conductance within the topological gap. A magnetic field breaks time-reversal symmetry, and thus is expected to break the quantization of conduc-

tance. Yet, recent experiments on topological insulators in broken-gap InAs/GaSb quantum wells have found very little dependence on magnetic field [1]. We discuss the effects of the orbital and the Zeeman part of the magnetic field on broken-gap quantum wells, and consider in which regime quantized conductance can be preserved.

[1] L. Du et al., arXiv:1306.1925

DS 17.6 Tue 15:15 H 0110

**Cherenkov effect in topological insulators** — ●SERGEY SMIRNOV — Institute for theoretical physics, Regensburg University, 93040 Regensburg, Germany

The Cherenkov radiation discovered experimentally by Cherenkov in optics of transparent media and theoretically explained later by Tamm and Frank reappears in solids where particles move faster than sound and, as a result, excite lattice vibrations or phonons. In both cases the photons or phonons are distributed within a forward cone centered around the momentum of the particle producing the Cherenkov light or sound.

Here we demonstrate that at high energies helical particles on surfaces of topological insulators excite anomalous Cherenkov sound outside the forward cone when the anisotropy of the surface states exceeds a critical value. The sound features many outstanding properties. In particular, at strong anisotropy it localizes into a few forward and backward beams propagating along specific directions [1].

At low energies we predict that an in-plane magnetic field applied to a surface of a topological insulator will asymmetrically reverse the Cherenkov sound. This asymmetric Cherenkov acoustic reverse may be of practical relevance in design of low energy electronic devices such as acoustic ratchets or, in general, in low power design of electronic circuits with an external control of the Cherenkov dissipation [2].

[1] S. Smirnov, Phys. Rev. B 88, 205301 (2013).

[2] S. Smirnov, Phys. Rev. B 90, 125305 (2014).

DS 17.7 Tue 15:30 H 0110

**One-dimensional Dirac electrons on the surface of weak topological insulators** — ●ALEXANDER LAU<sup>1</sup>, CARMINE ORTIX<sup>1</sup>, and JEROEN VAN DEN BRINK<sup>1,2</sup> — <sup>1</sup>Institute for Theoretical Solid State Physics, IFW Dresden, Germany — <sup>2</sup>Department of Physics, TU Dresden, Germany

We show that a class of weak three-dimensional topological insulators feature one-dimensional Dirac electrons on their surfaces. Their hallmark is a line-like energy dispersion along certain directions of the surface Brillouin zone. Interestingly, these one-dimensional Dirac line degeneracies are topologically protected by a symmetry that we refer to as in-plane time-reversal invariance. As an example, we demonstrate how this invariance leads to Dirac lines in the surface spectrum of stacked Kane-Mele systems.

DS 17.8 Tue 15:45 H 0110

**Fractional quantization of the topological charge pumped in a 1D superlattice** — ●PASQUALE MARRA<sup>1</sup>, ROBERTA CITRO<sup>1,2</sup>, and CARMINE ORTIX<sup>3</sup> — <sup>1</sup>CNR-SPIN, I-84084 Fisciano (Salerno), Italy — <sup>2</sup>Dipartimento di Fisica “E. R. Caianiello”, Università di Salerno, I-84084 Fisciano (Salerno), Italy — <sup>3</sup>Institute for Theoretical Solid State Physics, IFW Dresden, D-01069 Dresden, Germany

A one-dimensional quantum charge pump transfers a quantized charge in each pumping cycle. This quantization is topologically robust being analogous to the quantum Hall effect. The charge transferred in a fraction of the pumping period is instead generally not quantized. We show, however, that with specific symmetries in parameter space the charge transferred at well-defined fractions of the pumping period is quantized as integer fractions of the Chern number. We illustrate in details this fractional quantization in a one-dimensional Harper-Hofstadter model for both periodic and open boundary conditions, and discuss its relevance for cold atomic gases in optical superlattices.

[1] arxiv:1408.4457 [cond-mat]

## DS 18: Interfaces and Thin Films II (joint session with CPP)

Time: Tuesday 14:00–16:00

Location: C 243

### Invited Talk

DS 18.1 Tue 14:00 C 243

**Structure formation at interfaces: breath figures and beyond** — ●MASOUD AMIRKHANI — Institut für Experimentelle Physik Universität Ulm Albert-Einstein-Allee 11 89081 Ulm, Germany

The interaction of two (or more) different materials in contact is crucial for basic science as well as for practical purposes. At the micro and nano regime, the number of molecules at the interface is comparable to that of bulk molecules so the interaction at the interface governs the overall structure and functionality of the system. The interface interaction is particularly crucial for the formation of emulsions, microemulsions and surface micelles. Additionally, the existence of a large interface does directly affect the adsorption of polymer on the surface and the performance of many systems such as ionic polymer metal composites (IPMC). One should note that the interface interaction can be altered using various physical and chemical stimuli. For example amphiphilic and amphiphilic-like molecules are able to modify surfaces and interface properties and also form self-assembled structures. In this talk, we present the investigation of the size and structure of surface emulsion and microemulsions under the influence of different additives. Additionally, the conformation and configuration of diblock copolymer on the substrate under the influence of solvent vapor annealing and electric field will be discussed.

DS 18.2 Tue 14:30 C 243

**Simulations of solvent vapor annealing of cylinder-forming blockcopolymer thin films** — ●ANATOLY V. BEREZKIN<sup>1</sup>, IGOR I. POTEKIN<sup>2</sup>, and CHRISTINE M. PAPADAKIS<sup>1</sup> — <sup>1</sup>Technische Universität München, Physik Department, München, Germany — <sup>2</sup>Lomonosov Moscow State University, Physics Department, Moscow, Russian Federation

Ordered block copolymer films are promising as functional templates for lithography, molecular biology, colloid science etc. Using dissipative particle dynamics, we simulated the solvent vapor annealing (SVA) that is used to relax morphological defects, and control domain orientation in these films. The drying of films was considered in case of intermediate A/B block segregation and fast solvent evaporation. Un-

der these conditions, the SVA transforms equilibrium morphology of lying cylinders to hexagonally ordered perpendicular cylinders in the wide parameter range. The best conditions for this were a moderate initial solvent concentration in the film, and a selectivity of the solvent to the major block. This is probably necessary to compensate entropy-driven adsorption of the short blocks at the film surfaces, revealed in other works. Too weak or too strong block segregation, or solvent selectivity result in disordered morphologies. First disordered microdomains are formed, and then after evaporation of the half of the solvent, the domains reorient along the gradient of solvent concentration. This may be explained by the Gibbs-Marangoni effect. Such mechanism of microdomain ordering notably distinguishes from those observed in other recent simulations.

DS 18.3 Tue 14:45 C 243

**Instabilities in PS-PVP polymer blends thin films driven by surface tension and temperature effects** — ●MARLENA FILIMON<sup>1</sup>, JEAN-NICOLAS AUDINOT<sup>2</sup>, PATRICK GRYSAN<sup>2</sup>, JÖRG BALLER<sup>1</sup>, and ROLAND SANCTUARY<sup>1</sup> — <sup>1</sup>Laboratory for the Physics of Advanced Materials, University of Luxembourg, Luxembourg — <sup>2</sup>Department of Science and Analysis of Materials, Centre de Recherche Public-Gabriel Lippmann, Belvaux, Luxembourg

In thin supported films of polymer blends, in addition to composition and molecular weight of components, the structure is dependent on the surface energies of the components and on geometrical constraints induced by confinement in a thin film. Two-dimensional patterns attributed to the Marangoni instability and dependence of the Gibbs free energy of mixing components were observed for an interesting polymer blend ( polystyrene/poly(vinylpyrrolidone) (PS-PVP)) thin films. As tools for investigating the nano-size domains structures of thin polymer blends (~150 nm), we exploited Tapping-Mode Atomic Force Microscopy (TM-AFM) and Nano-dynamic Secondary Ion Mass Spectrometry technique (Nano-SIMS 50). Additionally, wetting properties of the substrate and influences of these instabilities are studied using wetting measurements - contact angle. We propose a possible formation mechanism for presented patterns and show that the mechanism

is relevant to the Marangoni instability. The relevant variables which can affect the morphological evolution such as surface enrichment and temperature dependence were also discussed.

DS 18.4 Tue 15:00 C 243

**Morphological Changes of Surface Immobilized Responsive Micelles** — ●INNA DEWALD<sup>1</sup>, JULIA GENSEL<sup>1</sup>, JOHANN ERATH<sup>1</sup>, EVA BETTHAUSEN<sup>2</sup>, AXEL H. E. MÜLLER<sup>2,3</sup>, and ANDREAS FERY<sup>1</sup> — <sup>1</sup>University of Bayreuth, Physical Chemistry II — <sup>2</sup>University of Bayreuth, Macromolecular Chemistry II — <sup>3</sup>Johannes Gutenberg University Mainz, Institute of Organic Chemistry

In recent years, formation of a multitude of smart coatings made from macromolecular building blocks has been demonstrated. Typical examples are brush type architectures or films formed by layer-by-layer self assembly (LbL-SA). In our work, we investigate multicompartment micelles formed from amphiphilic ABC triblock terpolymers as building blocks for responsive coatings. The application of such colloidal units for thin films has several advantages from a material-science perspective, e.g. stimulus-responsivity and multi-functionality on a single particle level and simple preparation of coatings by physisorption. Besides, using LbL-SA allows forming hierarchically structured coatings with novel properties and collective stimulus response of the integrated nanostructures.[1] Here, we investigate the effects of pH and salt on properties of these films [2] and explore the accompanying morphological changes of the surface immobilized micelles as a function of their composition, i.e. properties of each block and the succession they are connected to each other. 1.Gensel J., Dewald I., Erath J., Betthausen E., Müller A. H. E., Fery A., Chem. Sci., 2013, 4, 325. 2.Gensel J., Betthausen E., Hasenöhr C., Trenkenschuh K., Hund M., Boulmedais F., Schaaf P., Müller A. H. E. and Fery A., Soft Matter, 2011, 7, 11144.

DS 18.5 Tue 15:15 C 243

**Polymer-solid interphases and glass transition probed by positron annihilation lifetime spectroscopy** — CHRISTIAN OHRT, TÖNJES KOSCHINE, ●KLAUS RÄTZKE, and FRANZ FAUPEL — University of Kiel, Chair for Multicomponent Materials, D-24143 Kiel, Germany

The properties of materials involving polymer-solid interfaces are not only determined by the constituents but also by the interfacial region of the polymer near the solid, the so-called interphase. This interphase is particularly important in polymer-based nanocomposites. Here we report on positron annihilation lifetime spectroscopy (PALS) measurements of the free volume near the interface with a moderated positron beam. First investigations from the polymer side indicated a reduced free volume in Teflon AF / Si samples [1] but no quantitative information. Analysis from substrate side with a focused beam through a hole showed a significant average density increase in an interphase region with a width of about 10 nm. Additionally, the glass transition temperature as a probe for chain dynamics was determined as function of distance to the interface in a Teflon AF / SiN sample with depth resolved PALS. Within error margins, no change in the glass transition

temperature could be detected in the interfacial region.

[1] S. Harms, K. Rätzke, V. Zaporozhchenko, F. Faupel W. Egger, L. Ravelli, Polymer, 52 (2011) 505

DS 18.6 Tue 15:30 C 243

**Conjugated diblock copolymer/fullerene bulk heterojunction system in organic photovoltaic application** — ●RUI WANG<sup>1</sup>, ZHENYU DI<sup>1</sup>, HENRICH FRIELINGHAUS<sup>1</sup>, PETER MÜLLER-BUSCHBAUM<sup>2</sup>, and DIETER RICHTER<sup>1</sup> — <sup>1</sup>Jülich Center for Neutron Science, outstation at FRM II, Lichtenbergstr. 1, 85747 Garching — <sup>2</sup>TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

In order to achieve an optimum energy conversion efficiency for polymer based organic solar cells an interpenetrating bulk heterojunction (BHJ) network is needed, which has a nanoscale morphology on the order of the exciton diffusion length. The interpenetrating network provides larger interface area for exciton dissociation as well. Diblock copolymers are very promising for achieving well controlled nanoscale morphologies. In the present work, we blend the conjugated diblock copolymer P3HT-b-PS with the fullerene derivative PCBM. By applying grazing incidence small angle neutron scattering (GISANS) we investigate the active layer, GISANS had proven to give good contrast conditions for polymer:PCBM films in previous investigations. We present the determined structures in terms of phase information, size of structural length scales and molecular miscibility between the components.

DS 18.7 Tue 15:45 C 243

**Controlling Nanostructures by Templated Templates: Inheriting Molecular Orientation in Binary Heterostructures** — ●TOBIAS BREUER and GREGOR WITTE — AG Molekulare Festkörperphysik, Philipps-Universität Marburg, Deutschland

Precise preparation strategies are required to fabricate nanostructures of specific arrangement. In bottom-up approaches, where nanostructures are gradually formed by piecing together individual parts to the final structure, the self-ordering mechanisms of the involved structures are utilized. In order to achieve the desired structures regarding morphology, grain size and orientation of the individual moieties, templates can be applied, which influence the formation process of subsequent structures. However, this strategy is of limited use for complex architectures, as the templates only influence the structure formation at the interface between the template and the first compound. Here, we discuss the implementation of so-called templated templates and analyze, in which extent orientations of initial layers are inherited in top layers of another compound to enable structural control in binary heterostructures. To that purpose we have prepared crystalline templates of the organic semiconductors pentacene and perfluoropentacene in different exclusive orientations. We observe that for templates of both individual materials the molecular orientation is inherited in the top layers of the respective counterpart.

## DS 19: Ion and electron beam induced processes

Time: Wednesday 9:30–12:15

Location: H 2032

### Invited Talk

DS 19.1 Wed 9:30 H 2032

**Ferromagnetic shape memory alloys: From ion-beam assisted synthesis to plasma-aided functionalization for biomedical applications** — ARIYAN ARABI-HASHEMI<sup>1,2</sup>, UTA ALLENSTEIN<sup>1,3</sup>, FLORIAN SZILLAT<sup>1</sup>, ASTRID WEIDT<sup>3</sup>, MAREIKE ZINK<sup>3</sup>, and ●STEFAN G. MAYR<sup>1,2,3</sup> — <sup>1</sup>Leibniz-Institut für Oberflächenmodifizierung e.V. (IOM), Leipzig — <sup>2</sup>Translationszentrum für regenerative Medizin — <sup>3</sup>Fakultät für Physik und Geowissenschaften, Universität Leipzig

Yielding magnetically switchable strains of several percent, ferromagnetic shape memory alloys bear enormous potential for contact-less actuators in biomedical applications. We report about recent progress in synthesis and characterization of freestanding Fe-Pd based ferromagnetic shape memory membranes. Energetic ion beams provide a powerful tool to precisely tune materials properties, including phase, the martensite-austenite transformation and magnetic behavior. Employing atomistic computer simulations, we unveil the underlying physics, which is dominated by changes in short range order and defect insertion. We also discuss latest plasma-aided functionalization strategies

resulting in covalently-attached and crosslinked amino acids for mechanical coupling to biological cells and tissue. Density functional theory (DFT) calculation unravel the details of bonding, resulting in flexible, but highly durable polypeptide coatings.

[1] T. Edler, S.G. Mayr, Adv. Mater. 22, 4969 (2010).

[2] A. Arabi-Hashemi, S.G. Mayr, Phys. Rev. Lett. 109, 195704 (2012).

[3] M. Zink, F. Szillat, U. Allenstein, S. G. Mayr, Adv. Funct. Mat. 23, 1383 (2013).

### Invited Talk

DS 19.2 Wed 10:00 H 2032

**Writing magnetic patterns using ion-beams** — ●RANTEJ BALI — Helmholtz-Zentrum Dresden-Rossendorf e.V, Bautzner Landstraße 400, 01328 Dresden.

In certain binary alloys, a large increase of the saturation magnetization can be triggered by subtle chemical disordering [1]. This phenomenon is linked to an increase in the number of nearest-neighbor magnetic atoms and local variations in the electronic band-structure due to the existence of disorder sites. An approach to induce disorder

is to irradiate a chemically ordered precursor with energetic noble-gas ions; collision cascades formed by the ions knock atoms from their ordered sites and the concomitant vacancies are filled randomly *via* thermal diffusion of atoms. The ordered structure thereby undergoes a transition into a metastable solid solution. We consider the case of  $\text{Fe}_{60}\text{Al}_{40}$  where the chemically ordered (B2) structure is paramagnetic; and the chemically disordered (A2) structure is ferromagnetic [2]. Such phase transitions can be deployed to pattern localized ferromagnetic regions, for instance, by irradiation through lithographed masks, or by direct writing using an ion-beam stylus. We demonstrate experimentally, the patterning of highly-resolved magnetic nanostructures embedded within topographically flat thin films. Materials in which the magnetic behavior can be tuned *via* ion-induced phase transitions may allow the fabrication of novel spin-transport and memory devices, such as lateral spin-valves, using existing patterning tools. [1] R. Bali *et al.*, Nano Lett. 14, 435 (2014). [2] J. Fassbender *et al.*, Phys. Rev. B 77, 174430 (2008).

DS 19.3 Wed 10:30 H 2032

**Tailoring the magnetic easy axis of cobalt ferrite films by He implantation** — ●ANDREAS HERKLOTZ<sup>1</sup>, ANTONY WONG<sup>1</sup>, STEFANIA FLORINA RUS<sup>2</sup>, and THOMAS ZAC WARD<sup>1</sup> — <sup>1</sup>Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA — <sup>2</sup>National Institute for Research and Development in Electrochemistry and Condensed Matter, 300569 Timisoara, Romania

Heteroepitaxial strain engineering is an essential tool in the strongly correlated systems for investigating fundamental coupling effects and for more practical control of thin film properties. Recently, we have explored a new technique of strain control by the implantation of He into the film lattice. Here, we demonstrate the tuning of the magnetic anisotropy of  $\text{CoFe}_2\text{O}_4$  (CFO) films through He doping by the use of a commercial ion gun. Compressively strained thin films of CFO are grown coherently on MgO substrates and show pronounced out-of-plane magnetic anisotropy. It is shown that He dosing of coherent films results in an expansion of the out-of-plane lattice parameter while the in-plane lattice stays epitaxially locked to the substrate. Simultaneously we observe a continuous rotation of the magnetic easy axis towards the film plane. The results demonstrate that He implantation is an elegant path to tune the magnetic anisotropy of oxide films and, more generally, desired characteristics of transition metal oxide thin films. This work was supported by the U. S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division.

DS 19.4 Wed 10:45 H 2032

**Strong vortex matching effects in YBCO films with periodic modulations of the superconducting order parameter fabricated by masked ion irradiation** — LT HAAG<sup>1</sup>, G ZECHNER<sup>1</sup>, W LANG<sup>1</sup>, ●M DOSMAILOV<sup>2</sup>, MA BODEA<sup>2</sup>, and JD PEDARNIG<sup>2</sup> — <sup>1</sup>University of Vienna, Faculty of Physics, Electronic Properties of Materials, Boltzmanngasse 5, A-1090 Wien, Austria — <sup>2</sup>Johannes-Kepler-University Linz, Institute of Applied Physics, Altenbergerstrasse 69, A-4040 Linz, Austria

We report on measurements of the magnetoresistance and of the critical current in thin films of the high-temperature superconductor  $\text{YBa}_2\text{Cu}_3\text{O}_{7-d}$  (YBCO). A square array of regions with suppressed superconducting order parameter has been created in these films by introducing point defects via irradiation with  $\text{He}^+$  ions through a silicon stencil mask. In such a structure distinct peaks of the critical current can be observed at commensurate arrangements of magnetic flux quanta with the artificial defect lattice. Concurrently, the magnetoresistance shows pronounced minima. Both observations demonstrate that the strong intrinsic pinning in YBCO can be overcome by a periodic array of ion-damage columns with 300 nm spacing [1].

[1] L.T. Haag, M. Dosmailov *et al.*, Physica C 503 (2014) 75-81.

Acknowledgements: This work was supported by the Research Network "Nanoscience and Engineering in Superconductors (NES)" of the European Science Foundation and the COST Action MP-1201.

DS 19.5 Wed 11:00 H 2032

**Modelling ion-induced pattern formation based on theories of erosion and mass redistribution using the crater function formalism** — ●HANS HOFSSÄSS — II. Physikalisches Institut, Universität Göttingen, Göttingen, Germany

The Bradley-Harper (BH) and Carter-Vishnyakov (CV) theories with their recent extensions [1,2] are evaluated with regard to a quantita-

tive prediction of ion-induced pattern formation on elemental and compound surfaces. The crater function formalism is applied and moments of the crater function were calculated using Monte Carlo simulations with the program SDTrimSP. The extensions to the linear theories give rise to additional curvature coefficients which have relevant impact on the formation of parallel ripples. The thickness dependence leads to a stabilizing contribution at intermediate angles. The curvature dependence of the crater function leads to a stabilizing contribution, except for larger angles where it becomes strongly destabilizing. With these extensions, the combination of BH and CV theory is able to quantitatively predict the angular regime for parallel ripple formation, the ripple wavelength and the initial growth rates. In particular, the extended theories are able to explain the absence of pattern formation in certain cases.

[1] M.P. Harrison, R.M. Bradley, Phys. Rev. B 89, 245401 (2014).

[2] H. Hofssäss, Appl. Phys. A 114 401 (2014).

DS 19.6 Wed 11:15 H 2032

**Particle redeposition during ion-beam erosion can stabilize well-ordered nanostructures** — ●CHRISTIAN DIDDENS<sup>1</sup> and STEFAN J. LINZ<sup>2</sup> — <sup>1</sup>Eindhoven University of Technology, The Netherlands — <sup>2</sup>Institut für Theoretische Physik, WWU Münster

We present a detailed analysis of a continuum model for the redeposition mechanism during the self-organized nanopatterning by ion-beam erosion. In particular, we investigate (i) the distribution of reattaching particles on the surface, (ii) an approximation of the latter as a function of the surface height and (iii) spatio-temporal evolutions of two-dimensional surfaces subject to combined erosion and redeposition. The most important finding is that redeposition can be an essential mechanism for the emergence of self-organized nanopatterns. This stabilizing effect can be observed for a wide range of the entering parameters.

[1] C. Diddens and S. J. Linz, EPL, 104 (2013) 17010

[2] C. Diddens and S. J. Linz, Eur. Phys. J. B, 86 (2013) 397

[3] C. Diddens and S. J. Linz, (in preparation)

DS 19.7 Wed 11:30 H 2032

**Interaction of Slow Highly Charged Ions with Ultrathin Membranes - Potential Sputtering, Energy Loss and Charge Exchange** — ●RICHARD A. WILHELM<sup>1</sup>, ELISABETH GRUBER<sup>2</sup>, ROBERT RITTER<sup>2</sup>, RENÉ HELLER<sup>1</sup>, STEFAN FACSKO<sup>1</sup>, and FRIEDRICH AUMAYR<sup>2</sup> — <sup>1</sup>Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — <sup>2</sup>Technische Universität Wien, Wien, Austria

Slow highly charged ions (HCI) are known as an efficient tool for surface nano structuring of various insulating and semi-conducting surfaces. We show here that slow HCI can also be used to perforate a free-standing carbon nano membrane (CNM) with a thickness of only 1 nm. Round pores with sizes of up to 15 nm in diameter and corresponding sputter yields of up to a few thousand atoms are observed. Recent energy loss and charge exchange measurements on ions transmitted through a 1 nm thick CNM and free-standing Graphene reveal a strong dependence of the ion energy loss on charge exchange. Surprisingly, two distinct exit charge state distributions are observed, i.e. one part of the ions is almost neutralized and the other part remains in very high charge states after transmission. The ions potential and kinetic energy dependence on pore formation is discussed in terms of charge exchange and energy loss.

DS 19.8 Wed 11:45 H 2032

**Epitaxial GaN films deposited on ion-beam structured Si(111) with  $\text{SiN}_x$  intermediate layer** — ●ANNEMARIE FINZEL, JÜRGEN W. GERLACH, FRANK FROST, RENATE FECHNER, MARC TEICHMANN, ANDRIY LOTNYK, and BERND RAUSCHENBACH — Leibniz-Institut für Oberflächenmodifizierung e.V. (IOM Leipzig), Permoserstraße 15, D-04318 Leipzig, Germany

In this study, Si(111) substrates were structured by using a Kr ion beam in order to obtain nanometric ripple or terrace-like surface structures. After cleaning and oxide etching, the pristine as well as the ion-beam structured substrates were irradiated with hyperthermal nitrogen ions ( $E_{kin} \leq 25$  eV) at elevated temperatures to create a thin  $\text{SiN}_x$  intermediate layer for preventing melt-back etching of the Si substrate surface by Ga. Immediately afterwards, thin GaN films were deposited on these pre-treated substrates by ion-beam assisted molecular-beam epitaxy (IBA-MBE). The characterization of the samples by (S)TEM and AFM shows that the 1-2 nm thin  $\text{SiN}_x$  intermediate layer is sufficient to protect the Si from melt-back etching. Although the layer is partially amorphous, it is possible to grow GaN films epitaxially on the

SiN<sub>x</sub> layer (FWHM of the c-plane XRD rocking curve: 2°). Furthermore, the findings reveal on the one hand a higher wettability of the ion-beam structured Si substrates, leading to more compact and dense films in comparison to the non-structured ones. On the other hand, the GaN films deposited on the structured Si substrates exhibit a higher mosaicity (FWHM of the XRD rocking curves: 2.8-3.0°). The results will be discussed.

DS 19.9 Wed 12:00 H 2032

**LMIS-Injector-Module including a beam formation unit for the generation of high mono- and polyatomic ion currents** — ●PHILIPP LAUFER<sup>1</sup>, DANIEL BOCK<sup>1</sup>, WOLFGANG PILZ<sup>1</sup>, LOTHAR BISCHOFF<sup>2</sup>, and MARTIN TAJMAR<sup>1</sup> — <sup>1</sup>Technische Universität Dresden, 01062 Dresden — <sup>2</sup>Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstr. 400, 01328 Dresden

A high current Liquid Metal Ion Source (LMIS) module including ion optics for beam formation is developed. This spin-off from aerospace

research for ion propulsion units enables ion currents in the order of 100  $\mu\text{A}$  [1]. A reservoir of more than 1 g propellant is used to guarantee long-term operation. The small module has a length and a diameter of 8 cm each. The ion optical components are designed and optimized by state-of-art simulation-tools to focus the highly divergent ion beam to a nearly parallel beam of about 2 mm diameter. About 10% of the total emitted current are cluster ions [2]. Together with a mass separating system the module will offer high polyatomic ion currents, which can be used to manufacture nanostructured or smooth surfaces on  $\text{cm}^2$  area. Moreover, the module can be applied as a sputter tool for analysis of solid surfaces. As the majority of the sputtered particles are neutral the combination with an Electron Beam Ion Source (EBIS) [3] would enable to ionize these particles for mass analysis or to generate highly charged ions.

[1] M. Tajmar, et al., Ultramicroscopy 111 (2010)

[2] L. Bischoff, et al., Nucl. Instr. and Meth. B 272 (2012) 198

[3] M. Schmidt, et al., 12th Int. Symp. on EBIS a. Traps (EBIST'14)

## DS 20: Focused Session: In-situ optical spectroscopy

Time: Wednesday 9:30–13:00

Location: H 0111

### Invited Talk

DS 20.1 Wed 9:30 H 0111

**Differential Optical Spectroscopy for Surface Science** — ●PETER ZEPPENFELD — Institut für Experimentalphysik, Johannes Kepler Universität Linz, Austria

Conceptually very simple optical methods, namely Reflectance Difference Spectroscopy (RDS/RAS) and Differential Reflectance Spectroscopy (DRS), can provide valuable insight into the structure and growth of ultrathin films in straight correlation with their electronic, optical and other physical or chemical properties. Notably, differential optical spectroscopies can achieve sub-monolayer sensitivity and are capable of monitoring kinetic processes on surfaces in real time. This will be illustrated in selected examples dealing with the fabrication and optical characterization of functional layers, such as reconstructed surfaces [1,2], graphene nanoribbons [3], and ultrathin molecular films [4,5]. While the spatial resolution in the UV-VIS range is naturally limited, microscopic information on the structure and electronic properties can be obtained with complementary surface science techniques such as STM and Photoemission Electron Microscopy (PEEM). As an outlook, I will describe how optical spectroscopy and PEEM can be combined into a single experiment, thus enabling truly parallel optical and photoelectron spectroscopy at a local scale.

[1] L.D. Sun et al., Phys. Rev. B 69, 045407 (2004)

[2] M. Bachmann et al., Appl. Surf. Sci. 258, 10123 (2012)

[3] R. Denk et al., Nat. Commun. 5:4253 (2014)

[4] L.D. Sun et al., Phys. Chem. Chem. Phys. 14, 13651 (2012)

[5] L.D. Sun et al., Phys. Rev. Lett. 110, 106101 (2013)

### Invited Talk

DS 20.2 Wed 10:00 H 0111

**In situ Raman monitoring of Potassium intercalation in Manganese Phthalocyanine** — ●OVIDIU D. GORDAN<sup>1</sup>, MICHAEL LEDEMANN<sup>1,2</sup>, FRANZISKA LÜTTICH<sup>1</sup>, DMYTRO SOLONENKO<sup>1</sup>, PHILIPP SCHÄFER<sup>1</sup>, and DIETRICH R.T. ZAHN<sup>1</sup> — <sup>1</sup>Semiconductor Physics, Technische Universität Chemnitz, D-09107 Chemnitz — <sup>2</sup>now at Anatec Instruments AG, D-08606 Oelsnitz (V)

Charge redistribution in the molecular orbitals of organic molecules can be used to adjust their optical, electrical, and magnetical properties. In the case of metal phthalocyanines (MPc) this can be done by e.g. potassium intercalation. However, the effects of additional charges on the molecule geometry and the corresponding rearrangement of the molecular orbitals as well as the question whether the charge is electrically active or not are theoretically hard to predict. The entire picture gets more complicated by the formation and coexistence of several charged states between the organic molecule and dopant. Here the intercalation process is studied by *in situ* Raman monitoring. The corresponding Raman spectra reveal extremely strong changes when ultra-thin layers of MnPc prepared by organic molecular beam deposition in ultra-high vacuum are exposed to potassium. These changes can directly be related to the formation of distinct charged phases. The results presented thus beautifully illustrate that *in situ* Raman spectroscopy is a powerful tool for monitoring the dynamics of the intercalation process. Moreover, using organic field effect structures in the Raman experiment the different charged stages can be related to

changes in the conductivity.

### Invited Talk

DS 20.3 Wed 10:30 H 0111

**Infrared surface and interface studies - vibrational analysis and beyond** — ●ANNEMARIE PUCCI — Kirchhoff-Institut für Physik der Universität Heidelberg

Various excitations can be studied in the infrared, vibrational spectra, low-energetic electron transitions, and plasmonic behaviour. With careful referencing, such excitations can be observed also on surfaces and in ultrathin layers. The excitation spectra deliver information on the atomic level and, furthermore, on collective behaviour. In the talk examples for ultra-high vacuum studies will be presented, for example, charge transfer at organic-inorganic interfaces and plasmonic excitations in low-dimensional systems.

### Invited Talk

DS 20.4 Wed 11:00 H 0111

**Correlation of IR spectra with thin film structure at solid-water interfaces** — ●KARSTEN HINRICHS — Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., 12489 Berlin, Germany

A crucial point for infrared characterizations at solid/liquid interfaces in electrochemistry, polymer science and biosensing is the understanding of spectra-structure correlations. Optical layer calculations are required for quantitative conclusions on the structure from measured infrared spectra, in particular in the range of water vibrational bands. For infrared measurements of thin films in a flow cell spectroscopic ellipsometry was adapted. Exemplarily the stimuli-responsive properties of polymer brushes will be discussed, e. g. swelling degree, water content, and molecular interactions and dissociation of functional groups within an ultrathin polymer layer as well as the pH- and temperature-responsive adsorption and desorption of proteins. Current work is related to reduce the needed volume of liquids by use of microfluidic cells, to increase the lateral resolution by infrared microscopy, to enhance the detection limit by nano/microstructured substrates and to complement the optical layer simulations by optical calculations (e.g. using rigorous coupled-wave analysis (RCWA), finite-difference time-domain method (FDTD)).

### Invited Talk

DS 20.5 Wed 11:30 H 0111

**In-situ characterization of electronic materials by optical second-harmonic generation** — ●MICHAEL DOWNER — University of Texas at Austin, USA

Optical second-harmonic generation (SHG) uniquely enables sensitive, noninvasive, in-situ monitoring of centrosymmetry-breaking features of electronic materials, including surface and buried interface discontinuities, and bulk strain gradients and other bond distortions. I will describe several emerging applications of SHG that exploit these unique diagnostic capabilities, and that can be implemented with a compact, single-wavelength femtosecond light source. These include sub-micron imaging of anti-phase boundary defects in GaAs films on Si substrates, detection of "improper" ferroelectricity in advanced double-perovskite materials, detection of strain gradients in 3D integrated circuit struc-

tures, and non-spectroscopic fingerprinting of surface bonds during epitaxial film growth. Tunable femtosecond light sources add spectroscopic capability to SHG. I will describe applications of spectroscopic SHG to measurement of band offsets of ultrathin high-K dielectric films with silicon substrates, and to the characterization of unique bond structures at the interfaces of silicon nanocrystals.

DS 20.6 Wed 12:00 H 0111

**Microfluidic cells in IR-microscopy for biosensing** — ●CHRISTOPH KRATZ<sup>1</sup>, TOM W. H. OATES<sup>1</sup>, DIRK JANASEK<sup>2</sup>, and KARSTEN HINRICHS<sup>1</sup> — <sup>1</sup>Leibniz-Institut für Analytische Wissenschaften -ISAS- e.V., 12489 Berlin, Germany — <sup>2</sup>Leibniz-Institut für Analytische Wissenschaften -ISAS- e.V., 44139 Dortmund, Germany

A novel flow cell platform system for investigations of solid/liquid-interfaces combining expertise in the fields of in situ IR-spectroscopy, enhancement substrates and microfluidics will be presented.

The versatile investigation technique of in situ IR spectroscopy which has been applied in various studies of technologically relevant thin films as e.g. smart polymer brushes will be supported by surface enhanced methods (surface enhanced infrared absorption, SEIRA) to increase sensitivity for biosensing. The high potential of the presented technique lies in a label-free investigation with the possibility e.g. to monitor chemical and structural changes of molecules and proteins via the interpretation of absorption bands of specific molecular vibrations using adequate optical.

DS 20.7 Wed 12:15 H 0111

**in-situ-ATR-FTIR characterization of thin films deposited from dopamine solutions** — ●MARTIN MÜLLER<sup>1,2</sup> and BIRGIT URBAN<sup>1</sup> — <sup>1</sup>Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Straße 6, 01069 Dresden, — <sup>2</sup>Technische Universität Dresden, 01062 Dresden, Germany

in-situ-ATR-FTIR data on reactive deposition of catecholamines like dopamine (DA) at model surfaces aiming at structure and deposition mechanism of such bioinspired melanin like films are presented. The process initially observed by Lee is related to mussel adhesion via L-DOPA rich proteins and caused by a sequence of reaction steps suggesting transformation of DA into indole like moieties followed by polymerization to PDA. An ATR-FTIR pseudo-double-beam device and a thermostatable homebuilt flow cell were used. Germanium (Ge) internal reflection elements (IRE) were contacted with DA solutions allowing presence or absence of oxygen to certain degree. DA deposition was followed in dependence of either time or concentration. Via significant increases of characteristic IR bands from phenolic and aromatic species the formation of thin PDA films (SFM: 50 nm) at Ge could be followed in-situ. These bands revealed similar thermodynamic and kinetic adsorption behavior with rate constants of  $k=0.013$  min<sup>-1</sup>. The comparison of ATR-FTIR and transmission-FTIR data on PDA films, on the blackish PDA phase above and on original melanin suggested, that surface and bulk phase initiated PDA material is different.

Furthermore, application oriented studies revealed sustained release of model drugs and low protein adsorption at PDA films.

DS 20.8 Wed 12:30 H 0111

**Correlation Between Structure and Optical Properties in Organic Mixtures: A Real-Time Study During Thin Film Growth** — ●ALEXANDER HINDERHOFER, KATHARINA BROCH, ALEXANDER GERLACH, CHRISTOPHER LORCH, JOHANNES DIETERLE, JIŘÍ NOVÁK, and FRANK SCHREIBER — Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen

An understanding of the structure-property relation in binary blends of organic semiconductors is relevant for device optimization as well as for fundamental research [1]. Due to transient effects, post growth studies are often not sufficient for a detailed characterization of these complex systems [2,3]. Using grazing incidence X-ray diffraction simultaneously with optical spectroscopy techniques we follow the growth of binary blends of perfluoropentacene and diindenoperylene in situ and in real-time. Comparing the results obtained for the different mixing ratios, we find significant differences in the structure formation during growth of the mixed films as well as pronounced transient effects in the absorption spectra. We discuss these observations in the context of the competing effects of favorable intermolecular interaction and steric incompatibilities [4].

[1] A. Hinderhofer and F. Schreiber, *ChemPhysChem* 13, (2012), [2] U. Heinemeyer et al., *Phys. Rev. Lett.* 104, (2010), [3] R. Forcker and T. Fritz, *Phys. Chem. Chem. Phys.* 11, (2009), [4] K. Broch et al., *J. Chem. Phys.* 139, (2013).

DS 20.9 Wed 12:45 H 0111

**Space and Time Resolved Transmission Spectroscopy of Tungsten Oxide Thin Films** — ●SIMON BURKHARDT, SABRINA DARMAWI, MATTHIAS T. ELM, and PETER J. KLAR — I. Physikalisches Institut, Justus-Liebig-Universität, Heinrich-Buff-Ring 16, 35392 Gießen

Tungsten-IV oxide (WO<sub>3</sub>) is of great interest for numerous applications due to its electrochromic behavior, where the intercalation of ions results in a change of the optical properties. Although the electrochromism of WO<sub>3</sub> has been studied intensively during the last decades, the details of the ion intercalation mechanism and the corresponding coloration are still under discussion. In order to provide some new insights, WO<sub>3</sub> thin films were investigated by a combination of electrochemical and optical measurement techniques. The thin films were obtained by the depositions of WO<sub>3</sub> powder onto TCO-coated glass substrates via electron beam evaporation. Using transmission spectroscopy the coloration was monitored during the intercalation of hydrogen ions. The results obtained are correlated with structural changes of the thin films during the intercalation, which were investigated using XPS and XRD. Furthermore, similar measurements on laterally patterned WO<sub>3</sub> thin films are presented, which were performed in order to investigate and simulate the diffusion of the ions during the intercalation process.

## DS 21: Multiferroics I (joint session with DF)

Time: Wednesday 9:30–13:00

Location: EB 107

DS 21.1 Wed 9:30 EB 107

**Magnetoelectric domain control in multiferroic TbMnO<sub>3</sub>** — ●SEBASTIAN MANZ<sup>1</sup>, MASAKAZU MATSUBARA<sup>1,2</sup>, MASAHIITO MOCHIZUKI<sup>3,4</sup>, TERESA KUBACKA<sup>1</sup>, AYATO IYAMA<sup>5</sup>, NADIR ALIOUANE<sup>6</sup>, TSUYOSHI KIMURA<sup>5</sup>, STEVEN JOHNSON<sup>1</sup>, DENNIS MEIER<sup>1</sup>, and MANFRED FIEBIG<sup>1</sup> — <sup>1</sup>ETH Zürich — <sup>2</sup>Tohoku University — <sup>3</sup>Aoyama Gakuin University — <sup>4</sup>Japan Science and Technology Agency — <sup>5</sup>Osaka University — <sup>6</sup>Paul Scherrer Institute

Spin-spiral multiferroics exhibit a strong coupling between the electric and magnetic subsystems which is of potential interest for technological applications. Although these systems have been investigated for more than a decade, the magnetoelectric domain evolution under external fields is still largely unknown. Using optical second harmonic generation we resolve how electric and magnetic fields affect the multiferroic domains in the archetypal spin-spiral multiferroic TbMnO<sub>3</sub>. In consecutive electric switching cycles, varying multi-domain patterns emerge before a single-domain state is obtained. This observation reflects that the domain walls can easily move without being pinned by,

e.g., structural defects. In striking contrast to the electric-field response, multi-domain patterns persist when the polarization direction is flopped by applied magnetic fields. Here, a uniform polarization rotation is observed within all domains, which incorporates a transformation of neutral into nominally charged domain walls. Our results are explained based on numerical Landau-Lifshitz-Gilbert simulations and provide first evidence for the scalability of macroscopic magnetoelectric properties onto the level of domains.

DS 21.2 Wed 9:45 EB 107

**Critical behavior at the order-disorder transition in multiferroic DyMnO<sub>3</sub>** — ●MARKUS SCHIEBL, ALEXEY SHUVAEV, ANNA PIMENOV, GRAEME EGIN JOHNSTONE, ULADZISLAW DZIOM, and ANDREI PIMENOV — Institute for Solid State Physics, Vienna University of Technology, 1040 Vienna Austria

We present the results of detailed dielectric investigations of the relaxation dynamics in DyMnO<sub>3</sub> multiferroic manganite. In addition to known domain wall relaxation a second strong mode is observed at low frequencies. We provide an experimental evidence that the new relax-

ation mode is coupled to the chirality switching of the spin cycloid.

We demonstrate that the relaxation dynamics in  $\text{DyMnO}_3$  is typical for an order-disorder phase transition. Therefore,  $\text{DyMnO}_3$  follows an order-disorder transition scenario implicating that a short range cycloidal order of Mn-spins exists above  $T_C$ . The results suggest that the paramagnetic sinusoidal phase should be explained as a dynamic equilibrium between the clockwise and counterclockwise cycloidal magnetic orders. The short range order in the paraelectric phase is transformed to a long range cycloid at the ferroelectric transition temperature.

DS 21.3 Wed 10:00 EB 107

**Biquadratic and four-spin ring interactions in orthorhombic perovskite manganites** — ●NATALYA FEDOROVA, ANDREA SCARAMUCCI, CLAUDE EDERER, and NICOLA A. SPALDIN — ETH Zurich, Materials Theory, Wolfgang-Pauli-Strasse 27, CH-8093, Zurich, Switzerland

We use *ab initio* electronic structure calculations, based on DFT within the GGA+U approximation, to estimate the microscopic exchange interactions in the series of orthorhombic perovskite manganites ( $o\text{-RMnO}_3$ ), in order to find a model Hamiltonian which can provide an accurate description of the magnetism in these materials. At low temperatures  $o\text{-RMnO}_3$  with small radii of  $R$  cations (therefore, large octahedral tiltings) demonstrate a spiral or E-type antiferromagnetic orderings (E-AFM), which drive their multiferroic properties. Usually the establishment of such magnetic orderings is explained within the framework of a Heisenberg model with competing nearest-neighboring (NN) and next-nearest-neighboring exchange interactions. However, we find that the mapping the results of *ab initio* calculations onto the Heisenberg Hamiltonian for  $o\text{-RMnO}_3$  show a clear deviation from the Heisenberg-like behavior. We demonstrate that this deviation can be explained only by the presence of biquadratic and four-spin ring exchange couplings and show that they have the strongest effect in compounds where NN exchange interactions are weakened, for example, due to large octahedral tiltings.

DS 21.4 Wed 10:15 EB 107

**Time resolved polarized neutron scattering and dielectric spectroscopy reveal multiferroic domain dynamics in  $\text{MnWO}_4$  and  $\text{TbMnO}_3$**  — ●JONAS STEIN<sup>1</sup>, DANIEL NIERMANN<sup>1</sup>, CHRISTOPH GRAMS<sup>1</sup>, MAX BAUM<sup>1</sup>, TOBIAS CRONERT<sup>1</sup>, JEANNIS LEIST<sup>2</sup>, KARIN SCHMALZL<sup>3</sup>, A AGUNG NUGROHO<sup>4</sup>, ALEXANDER C KOMAREK<sup>5</sup>, GÖTZ ECKOLD<sup>2</sup>, PETRA BECKER<sup>6</sup>, LADISLAV BOHATÝ<sup>6</sup>, JOACHIM HEMBERGER<sup>1</sup>, and MARKUS BRADEN<sup>1</sup> — <sup>1</sup>II. Physikalisches Institut, Uni Köln — <sup>2</sup>Institut für Phys. Chemie, Uni Göttingen — <sup>3</sup>JCNS at ILL, France — <sup>4</sup>Institut Teknologi Bandung, Indonesia — <sup>5</sup>MPI Dresden — <sup>6</sup>Institut für Kristallographie, Uni Köln

Multiferroic materials are promising for future memory devices with low power consumption. The rise time between two states is a crucial parameter for a possible application and was investigated in the spin spiral multiferroics  $\text{TbMnO}_3$  and  $\text{MnWO}_4$ . Polarized neutron diffraction is able to determine the ratio of chiral domains, which can be controlled by an electric field. Using the stroboscopic technique we follow the reversion of chiral domains in the timescale of a few hundred microseconds to hours. In  $\text{TbMnO}_3$  we find a simple logarithmic relation between the rise time and temperature that is fulfilled over 5 decades. Broadband linear and nonlinear dielectric spectroscopy revealed the domain dynamics in the MF phase of  $\text{MnWO}_4$ . The rise time reaches values in the minute range in the middle of the multiferroic temperature regime at  $T \approx 10$  K but unexpectedly decays again on approaching the lower, first-order phase boundary at  $T_{N1} \approx 7.6$  K.

[1] Niermann et al. **PRB** **89**,134412 [2] Baum et al. **PRB** **89**,144406

DS 21.5 Wed 10:30 EB 107

**Polarization control at spin-driven ferroelectric domain walls** — ●NAËMI LEO<sup>1</sup>, ANDERS BERGMANN<sup>2</sup>, ANDRES CANO<sup>3</sup>, NARAYAN POUDEL<sup>4</sup>, BERND LORENZ<sup>4</sup>, MANFRED FIEBIG<sup>1</sup>, and DENNIS MEIER<sup>1</sup> — <sup>1</sup>ETH Zurich, Switzerland — <sup>2</sup>Uppsala University, Sweden — <sup>3</sup>University Bordeaux, France — <sup>4</sup>University of Houston, USA

As was recently demonstrated, domain walls in ferroelectric materials show emergent electronic properties, like enhanced conductivity tunable by the relative orientation of the polarisation in the adjacent domains. Here, multiferroic materials with a coexistence of magnetic and electric order offer a new route for the control of such localised functionalities at domain boundaries.

Using spatially-resolved optical second harmonic generation we demonstrate the magneto-electric-field control of the multiferroic domains in Co-doped  $\text{MnWO}_4$ . In particular, the obtained domain distri-

bution remains unchanged upon the magnetic-field-induced continuous 90°-rotation of the ferroelectric polarization.

This stability implies that multiferroic domain walls can accommodate for varying local polarisation configurations leading to local charging and discharging. We discuss the microscopic structure of the domain walls using micro-magnetic simulations.

DS 21.6 Wed 10:45 EB 107

**Tuning order-by-disorder multiferroicity in  $\text{CuO}$  by doping** — ●JOHAN HELLSVIK<sup>1,2</sup>, MARCELLO BALESTIERI<sup>1</sup>, TOMOYASU USUI<sup>3</sup>, ALESSANDRO STROPPA<sup>2</sup>, ANDERS BERGMAN<sup>4</sup>, LARS BERGQVIST<sup>5</sup>, DHARMALINGAM PRABHAKARAN<sup>6</sup>, OLLE ERIKSSON<sup>4</sup>, SILVIA PICOZZI<sup>2</sup>, TSUYOSHI KIMURA<sup>3</sup>, and JOSÉ LORENZANA<sup>1,2</sup> — <sup>1</sup>ISC-CNR, Rome, Italy — <sup>2</sup>CNR-SPIN, L'Aquila, Italy — <sup>3</sup>Osaka University, Osaka, Japan — <sup>4</sup>Uppsala University, Uppsala, Sweden — <sup>5</sup>KTH, Stockholm, Sweden — <sup>6</sup>University of Oxford, Oxford, United Kingdom

The high Curie temperature multiferroic compound  $\text{CuO}$  has a quasidegenerate magnetic ground state that makes it prone to manipulation by the so-called "order-by-disorder" mechanism. First principle computations supplemented with Monte Carlo simulations and experiments show that isovalent doping allows us to stabilize the multiferroic phase in nonferroelectric regions of the pristine material phase diagram with experiments reaching a 250% widening of the ferroelectric temperature window with 5% of Zn doping. Our results allow us to validate the importance of a quasidegenerate ground state on promoting multiferroicity on  $\text{CuO}$  at high temperatures and open a path to the material engineering of multiferroic materials. In addition we present a complete explanation of the  $\text{CuO}$  phase diagram and a computation on the incommensurability in excellent agreement with experiment without free parameters.

[1] J. Hellsvik et al., *Phys. Rev. B* **90**, 014437 (2014) [2] T. Kimura et al., *Nature Mat.* **7**, 291 (2008) [3] G. Giovannetti et al., *Phys. Rev. Lett.* **106**, 026401 (2011)

DS 21.7 Wed 11:00 EB 107

**Dielectric properties and electrical switching behavior of the spin-driven multiferroic  $\text{LiCuVO}_4$**  — ●ALEXANDER RUFF<sup>1</sup>, STEPHAN KROHNS<sup>1</sup>, PETER LUNKENHEIMER<sup>1</sup>, ANDREY PROKOFIEV<sup>2</sup>, and ALOIS LOIDL<sup>1</sup> — <sup>1</sup>Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany — <sup>2</sup>Solid State Physics, Vienna University of Technology, Austria

The spin-1/2 chain cuprate  $\text{LiCuVO}_4$  exhibits both ferroelectric and magnetic order at low temperatures. This so-called multiferroic behavior is of great scientific interest due to the underlying complex physical mechanisms, especially in the case of strong magnetoelectric coupling. Here we thoroughly discuss the multiferroic properties of the prototypical spin-driven ferroelectric material  $\text{LiCuVO}_4$ . At temperatures below about 2.5 K, it exhibits a three dimensional helical spiral spin order, with propagation in the  $b$  direction and a spin helix in the  $ab$  plane, which induces via an inverse Dzyaloshinskii-Moriya interaction a ferroelectric polarization in the  $a$  direction. In an external magnetic field, the direction of the spin spiral and thus the direction of the electrical polarization can be switched. This switching behavior of the polarization was demonstrated via dielectric spectroscopy on a single crystalline sample oriented in two different directions in magnetic fields up to 9 T. Detailed magnetic-field and temperature-dependent ferroelectric hysteresis-loop measurements imply the electric control of the spin helicity [1]. This rarely documented feature indicates the close coupling of electric and magnetic order of  $\text{LiCuVO}_4$ .

[1] A. Ruff et al., *J. Phys.: Condens. Matter*, **26**:485901 (2014).

## 15 min coffee break

DS 21.8 Wed 11:30 EB 107

**Emergence of ferroelectricity in multiferroic  $\text{h-YMnO}_3$**  — ●MARTIN LILIENBLUM<sup>1</sup>, THOMAS LOTTERMOSER<sup>1</sup>, SEBASTIAN MANZ<sup>1</sup>, SVERRE M. SELBACH<sup>2</sup>, ANDRES CANO<sup>3</sup> and MANFRED FIEBIG<sup>1</sup> — <sup>1</sup>Department of Materials, ETH Zurich, Vladimir-Prelog-Weg 4, 8093 Zurich, Switzerland — <sup>2</sup>Department of Material Science and Engineering, NTNU, N-7491 Trondheim, Norway — <sup>3</sup>CNRS, Université de Bordeaux, ICMCB, UPR 9048, F-33600 Pessac, France

Universal scaling laws, interfacial nano-electronics, and topological defects are currently studied using hexagonal manganites  $\text{RMnO}_3$  ( $R = \text{Sc}, \text{Y}, \text{Dy-Lu}$ ) as model system. In spite of the remarkably broad interest in the system, surprisingly little is known about the origin of the ferroelectric state. Here we solve the controversy about the emergence

of the spontaneous polarization and its coupling to the underlying structural distortion by applying scanning probe microscopy (SPM) and optical second harmonic generation (SHG). We trace the spontaneous polarization by SHG from 100 K to 1450 K directly and contact-free. We find that only a single transition exists in which the polarization arises slower than expected as by-product of the structural distortion. By thermal treatments close to the structural transition and subsequent SPM scans, we show that the exceptionally robust ferroelectric domain pattern is determined only by the structural distortion. In summary we reveal that the ferroelectric order results from an interplay of electric polarization, topological effects, and temperature.

DS 21.9 Wed 11:45 EB 107

**Monte Carlo approach to the ferroelectric phase transition in hexagonal manganites** — •THOMAS LOTTERMOSER<sup>1</sup>, MARTIN LILIEBLUM<sup>1</sup>, ANDRES CANO<sup>2</sup>, and MANFRED FIEBIG<sup>1</sup> — <sup>1</sup>ETH Zurich, Zurich, Switzerland — <sup>2</sup>Université de Bordeaux, Pessac, France

Despite several experimental and theoretical efforts in recent years the nature of the structural high temperature phase transition in the hexagonal manganites and its relation to the occurrence of a ferroelectric polarization in this materials is still not fully understood. Experimental data give two contradicting answers to this problem. Some experiments indicate a simultaneous appearance of the polarization in a single structural phase transition while others hint to a second phase transition several hundred Kelvin below the structural transition. In order to clarify these contradictions we performed Monte Carlo simulations based on the so-called clock model. In this model the six trimerization states of the manganite crystal structure are represented by six clock vectors in the complex plane. From the simulation data we calculated the temperature dependence of the complex structural order parameter and the induced ferroelectric polarization. The results point to a single phase transition with a strongly suppressed polarization contribution at high temperatures. This is experimentally confirmed by direct measurements of the ferroelectric polarization using optical second harmonic generation. Contradictions with other experimental data can be explained as finite size effects depending on the length scale of the experimental probe.

DS 21.10 Wed 12:00 EB 107

**Magnon-phonon interactions in hexagonal multiferroic YMnO<sub>3</sub>** — •ANDREAS KREISEL<sup>1</sup>, SHANTANU MUKHERJEE<sup>1</sup>, BRIAN M. ANDERSEN<sup>1</sup>, TURI SCHÄFFER<sup>1</sup>, SONJA HOLM<sup>1</sup>, KIM LEFMANN<sup>1</sup>, NIELS C.R. MOMSEN<sup>1</sup>, JACOB LARSEN<sup>2</sup>, AMY FENNELL<sup>3</sup>, UWE STUHR<sup>3</sup>, and ZAHRA YAMANI<sup>4</sup> — <sup>1</sup>Niels Bohr Institute, University of Copenhagen, Denmark — <sup>2</sup>Institute of Physics, Technical University of Denmark — <sup>3</sup>Laboratory of Neutron Scattering, Paul Scherrer Institute, Switzerland — <sup>4</sup>Chalk River National Laboratory, Canada

The multiferroic material YMnO<sub>3</sub> is known to show a large spin lattice coupling such that the spin and lattice degrees of freedom influence various properties, as for example the thermal conductivity that is found to have an anomalous contribution. The magnetoelastic modes have been measured recently in neutron diffraction experiments and linked to certain spectral features in Raman signals. Starting from a Heisenberg model on a triangular lattice with single ion anisotropies, we investigate the spin-phonon coupling via the magnetostriction mechanism and derive a coupled magnon-phonon model valid in the entire Brillouin zone. Within a spin-wave approach, where the coupling yields a hybrid magnon-phonon mode, we calculate the dynamic structure factor and compare to recent experimental neutron results.

DS 21.11 Wed 12:15 EB 107

**Stability of magnetic and electric domains against chemical doping in hexagonal manganites** — •EHSAN HASSANPOUR YESAGHI, VIKTOR WEGMAYR, JAKOB SCHAAB, DENNIS MEIER, and MANFRED FIEBIG — Department of Materials, ETH Zürich, Zürich, Switzerland

The unique properties of magnetoelectric multiferroics are, to a large

extent, determined by the coexistence and interaction of magnetic and electric domains. A major challenge towards future applications is to optimize the properties of these domains, such as their transport, without weakening or even losing the existing multiferroic order. Here, we present our study of ferroelectric and antiferromagnetic domains in chemically doped hexagonal manganites. We show that the electronic conductance of ErMnO<sub>3</sub> can be enhanced or suppressed by introducing either divalent (Ca<sup>2+</sup>) or tetravalent (Zr<sup>4+</sup>, Ti<sup>4+</sup>) ions into the system. Using piezoresponse force microscopy (PFM) and optical second harmonic generation (SHG) we monitor the corresponding changes on the level of domains. We find that the RMnO<sub>3</sub>-characteristic domain topography, as well as the multiferroic transition temperature, are robust against the applied ionic alteration, which demonstrates the usability of chemical doping for non-perturbative property-engineering of multiferroic domains.

DS 21.12 Wed 12:30 EB 107

**Anisotropy study of multiferroicity in the pyroxene NaFeGe<sub>2</sub>O<sub>6</sub>** — •LIONEL ANDERSEN<sup>1</sup>, THOMAS LORENZ<sup>1</sup>, MATTHIAS ACKERMANN<sup>2</sup>, LADISLAV BOHATY<sup>2</sup>, and PETRA BECKER<sup>2</sup> — <sup>1</sup>II. Physikalisches Institut - Universität zu Köln, Germany — <sup>2</sup>Institut für Kristallographie - Universität zu Köln, Germany

Since the mineral aegirine was found to be the first multiferroic member of the pyroxenes an intensive search for further related multiferroics was initiated [1]. In this contribution, we present a detailed study of the dielectric, magnetic and magnetoelastic properties of the pyroxene NaFeGe<sub>2</sub>O<sub>6</sub> with special respect to the anisotropy. Unlike other investigations on NaFeGe<sub>2</sub>O<sub>6</sub> [2] large single crystals were synthesized to examine pyroelectric currents, dielectric constants and magnetic susceptibilities as well as the thermal expansion and the magnetostriction. The spontaneous electric polarization detected below  $T_C \approx 11.6$  K in an antiferromagnetically ordered state ( $T_N \approx 13$  K) is mainly lying within the *ac* plane with a small component along *b*, indicating a triclinic symmetry of the multiferroic phase of NaFeGe<sub>2</sub>O<sub>6</sub>. The electric polarization can be strongly modified by applying magnetic fields along different directions. We derive detailed magnetic-field versus temperature phase diagrams and identify three multiferroic low-temperature phases, which are separated by a non-ferroelectric, antiferromagnetically ordered state from the paramagnetic high-temperature phase [3].

[1] S. Jodlauk *et al.* J. Phys.: Condens. Matter **19** (2007)  
 [2] I. Kim *et al.* J. Phys.: Condens. Matter **24** (2012)  
 [3] M. Ackermann *et al.* New J. Phys. (submitted, arXiv:1408.6772)

DS 21.13 Wed 12:45 EB 107

**Ab Initio analysis of ferroelectric and magnetic properties of potentially multiferroic aurivillius phases** — •AXIEL YAEL BIRENBAUM, JAN VAN DEN BROEK, and CLAUDE EDERER — Materials Theory, ETH Zürich

A promising class of high temperature polar magnetic multiferroic materials are the Aurivillius family of layered-perovskites related compounds. They combine high temperature ferroelectric properties with a layered structure that allows for systematic introduction of magnetic ions. The simplest of such cases to have been studied is Bi<sub>5</sub>FeTi<sub>3</sub>O<sub>15</sub>. However, no well-established value exists for its spontaneous electric polarization, and contradictory reports as to its magnetic states.

We perform Density Functional Theory calculations on Bi<sub>5</sub>FeTi<sub>3</sub>O<sub>15</sub>, and conclude on a high spontaneous electric polarization. To better understand the mechanism for ferroelectricity, we examine 9 systems, based on SrBi<sub>2</sub>Ta<sub>2</sub>O<sub>9</sub> as reference. We find a high spontaneous polarization even in the case of with no nominally ferroelectrically-active cations. We discuss these results in light of the tri-linear coupling between soft and hard modes demonstrated for SrBi<sub>2</sub>Ta<sub>2</sub>O<sub>9</sub> and the general concept of “hybrid improper ferroelectricity”. To clarify the range of temperatures expected for magnetic long range order despite a low concentration of magnetic ions and the short range of superexchange interactions, we perform Monte Carlo simulations. We discuss possible strategies to increase magnetic ordering temperatures.

## DS 22: Interfaces and Thin Films III (joint session with CPP)

Time: Wednesday 9:30–13:00

Location: C 243

DS 22.1 Wed 9:30 C 243

**Patterned Diblock co-polymer Thin Films as Templates for Advanced Anisotropic Metal Nanostructures** — ●STEPHAN V. ROTH<sup>1</sup>, GONZALO SANTORO<sup>1</sup>, JOHANNES F.H. RISCH<sup>1</sup>, SHUN YU<sup>2</sup>, MATTHIAS SCHWARTZKOPF<sup>1</sup>, PENG ZHANG<sup>1</sup>, SARATHLAL KOYILOTH VAYALIL<sup>1</sup>, MICHAEL A. RÜBHAUSEN<sup>3</sup>, NICK J. TERRILL<sup>4</sup>, PAUL STANIEC<sup>4</sup>, YUAN YAO<sup>5</sup>, EZZELDIN METWALLI<sup>5</sup>, and PETER MÜLLER-BUSCHBAUM<sup>5</sup> — <sup>1</sup>DESY, Notkestr. 85, 22607 Hamburg — <sup>2</sup>KTH, Teknikringen 56-58, 10044 Stockholm — <sup>3</sup>Inst. f. Nanostruktur- und Festkörperforschung, CFEL, APOG, Univ. Hamburg, Luruper Chaussee 149, 22761 Hamburg — <sup>4</sup>DLS, Harwell Sci. & Innov. Campus, Didcot, Oxfordshire OX11 0QX — <sup>5</sup>LS funkt. Mat., Physik-Department, TU München, James-Franck-Str. 1, 85748 Garching

The tailoring of the metal-polymer interface in hybrid materials plays a crucial role in modern advanced material science. Using glancing angle deposition of gold on a nanostructured diblock copolymer thin film (PS-*b*-PMMA), we are able to fabricate directional hierarchical structures. This approach exploits the selective wetting of Au on the PS block. We prove the asymmetric, localized growth of the gold nanoparticles and are able to extract the different growth laws by in situ scattering methods as well as imaging methods. The optical anisotropy of these hierarchical hybrid materials is probed by angular resolved spectroscopic methods and is correlated to the nanostructure. This approach offers the possibility to tailor functional hierarchical thin films for plasmonics and metamaterials, as nanoantennae arrays, in organic photovoltaics and sensor electronics.

DS 22.2 Wed 9:45 C 243

**Transparent aluminium oxide coatings on polymer substrate** — ●SAMANTHA MICCIULLA<sup>1</sup>, XIAOFEI DUAN<sup>2</sup>, ROBERT N. LAMB<sup>2</sup>, and REGINE VON KLITZING<sup>1</sup> — <sup>1</sup>Technische Universität Berlin — <sup>2</sup>The University of Melbourne

Smart coatings are highly versatile systems, applicable to diverse purposes and finely tunable by proper external stimuli. Polymers are mostly used to create responsive films, however they suffer hard conditions like high temperatures, aggressive chemicals, high mechanical stress, with consequent degradation or irreversible modifications. Therefore the use of a thin inorganic coating enriching the system of high mechanical and chemical stability may be the solution to this limitation. A good candidate to this purpose is aluminium oxide (Al<sub>2</sub>O<sub>3</sub>), which presents anti-corrosion properties, high wear resistance, and high biocompatibility. Moreover, the transparency of alumina ceramics in the UV-Vis range makes it suitable to optical applications. A synthetic route to prepare Al<sub>2</sub>O<sub>3</sub> was developed to reduce the risk of degradation of the underneath polymer, using low temperatures and mild chemicals. The composition of alumina/polymer coatings was studied by X-Rays Photoelectron Spectroscopy and the surface morphology by Scanning Electron Microscopy. The latter showed the achievement of a smooth, cracks-free coating upon hydrothermal treatment (105°C, 38 atm). Our studies focused on the preparation of alumina coatings on polymer substrates having different surface hydrophilicity, charge and structure, and revealed that the wetting properties of the polymer surface play the dominant role for the quality of the coating.

DS 22.3 Wed 10:00 C 243

**Tailoring the mechanics of ultrathin carbon nanomembranes by molecular design** — ●XIANGHUI ZHANG, CHRISTOF NEUMANN, POLINA ANGELOVA, ANDRÉ BEYER, and ARMIN GÖLZHÄUSER — Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld, Germany

Freestanding carbon nanomembranes (CNMs) with a thickness between 0.6 nm and 1.7 nm were prepared from self-assembled monolayers (SAMs) of diverse polyaromatic precursors via low energy electron induced cross-linking. The mechanical properties of CNMs were investigated by applying a pressure difference between the two sides of the membrane and by measuring the resulting deflection with atomic force microscopy. We found a correlation between the rigidity of the precursor molecules and the macroscopic mechanical stiffness of CNMs. While CNMs from rigid and condensed precursors like naphthalene and pyrene thiols prove to exhibit higher Young's moduli of 15–19 GPa, CNMs from non-fused oligophenyls possess lower Young's moduli of ~10 GPa. For CNMs from less densely packed SAMs, the presence of defects and nanopores plays an important role in determining their me-

chanical properties. The finite element method (FEM) was applied to examine the deformation profiles and simulate the pressure-deflection relationships.

DS 22.4 Wed 10:15 C 243

**Covalent modification of large area monolayer graphene towards biosensing.** — ●FELIX RÖSICKE<sup>1</sup>, MARC GLUBA<sup>1</sup>, GUOQUANG SUN<sup>2</sup>, KARSTEN HINRICHS<sup>2</sup>, JÖRG RAPPICH<sup>1</sup>, and NORBERT NICKEL<sup>1</sup> — <sup>1</sup>Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — <sup>2</sup>Leibniz - Institut für Analytische Wissenschaften - ISAS - e.V., Department Berlin, Berlin, Germany

We investigated the electrochemical grafting of para-N-maleimidophenyl (pMP) onto graphene from the respective diazonium salt (p-(N-Maleimido)benzenediazonium tetrafluoroborate, pMPDT) by electrochemical quartz crystal microbalance (EQCM), Raman- and infrared spectroscopies.

The p-MP is well known to react with any SH-group present in solution and is therefore a possible candidate to build up bio-sensing devices which, in combination with graphene, are very stable and conductive systems that can be transferred to any substrate. The sample preparation was performed by a transfer of CVD grown large area graphene [1] to an isolating layer of SiN<sub>x</sub> on Au-coated QCM chips. Using graphene as working electrode, the current behavior and the change in the resonant frequency of the EQCM reflect the electrochemical reduction of the diazonium compound. Raman and infrared spectroscopies reveal the binding of pMP onto the graphene layer. The charge used for the reduction of pMPDT correlates to the amount of grafted pMP and the observed defect density of graphene. Finally the pMP functionalized graphene surface was tested by reaction with 4-Nitrobenzenethiol.

DS 22.5 Wed 10:30 C 243

**Light absorption of Ultrathin Gallium Layers during Oxidation** — ●FRANK LAWRENZ<sup>1</sup>, CHRISTIAN A. HELM<sup>1</sup>, and STEPHAN BLOCK<sup>2</sup> — <sup>1</sup>Physik, Uni Greifswald, 17487 Greifswald, Germany — <sup>2</sup>Chalmers University of Technology, 412 96 Göteborg, Sweden

The fabrication of ultrathin metal oxide layers is important for many technological applications. Here we describe a simple method for the formation of 3 nm thick gallium oxide layers which extend up to 1 cm<sup>2</sup>. Liquid gallium is applied onto silica surfaces, leaving thin layers that are immediately oxidized at their surface under ambient conditions, followed by slower oxidation of the remaining layer. This is quantified using UV-Vis absorption measurements, indicating that the oxidation of the entire layer is completed after two weeks. A rate model is developed to describe the oxidation of ultrathin Ga layers.

DS 22.6 Wed 10:45 C 243

**Ambiguous Copolymer Surfaces from Light-Mediated Radical Polymerization** — ●CHRISTIAN W. PESTER<sup>1,2</sup>, JUSTIN E. POELMA<sup>2</sup>, CRAIG J. HAWKER<sup>2</sup>, and EDWARD J. KRAMER<sup>1</sup> — <sup>1</sup>UC Santa Barbara, Department of Materials, Department of Chemical Engineering — <sup>2</sup>Department of Chemistry and Biochemistry, Materials Research Laboratory, Santa Barbara, CA, 93106

We describe the use of visible-light-mediated living radical polymerization of methacrylate-based, anti-fouling relevant monomers, i.e., poly(trifluoroethyl methacrylate) (TFEMA) and poly(ethylene glycol methacrylate) (PEGMA). Resulting ambiguous surfaces are expected to show promising features for marine anti-fouling applications. Light-catalysis affords facile lithographic patterning. In this PEGMA-*b*-TFEMA case study we patterned these diblocks to give topographically and chemically well-defined ambiguous surfaces which combine hydrophilic and hydrophobic properties on the micron length scale. XPS, dynamic secondary ion mass spectroscopy, and scanning x-ray transmission microscopy, allowed us to precisely determine chemical surface composition, whereas AFM afforded precise analysis of topographical features inherent to patterning. The light-activated polymerization method we use was readily coupled to well-established ATRP techniques and afforded expansion of this case study to advanced monomers, e.g. highly fluorinated compounds and zwitterionic acrylates. Polymer backbone functionalization combined with lithography allowed spatial control over brush architecture, adding to the wide chemical and conformational accessible parameter space.

15 min. break

DS 22.7 Wed 11:15 C 243

**Light-Controlled Molecular Zippers based on Azobenzene Main Chain Polymers** — ●CHRISTOPHER WEBER<sup>1</sup>, TOBIAS LIEBIG<sup>1</sup>, ANTON ZYKOV<sup>1</sup>, LINUS PITHAN<sup>1</sup>, SEBASTIAN BOMMEL<sup>1,2</sup>, DAVID BLÉGER<sup>3</sup>, and STEFAN KOWARIK<sup>1</sup> — <sup>1</sup>Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin — <sup>2</sup>Deutsches Elektronen-Synchrotron, 22607 Hamburg — <sup>3</sup>Institut für Chemie, Humboldt-Universität zu Berlin, 12489 Berlin

We report that thin films of azobenzene main chain polymers with interdigitating dodecyl side chains (molecular zippers) can be switched reversibly with light between a semicrystalline and an amorphous state, corresponding to a closed and open state of the molecular zippers. Simultaneous time-resolved x-ray diffraction and optical spectroscopy measurements show that the kinetics of the amorphization of the crystalline domains is about 12 times slower than the photoisomerization of the azobenzene chromophores. Our findings suggest that the amorphization is triggered by *E-Z* isomerization of a small amount of azobenzene chromophores within the polymer film and that the slower kinetics of the photoinduced amorphization is determined by structural and topological constraints and not by a different isomerization mechanism in crystalline domains.

DS 22.8 Wed 11:30 C 243

**Monte Carlo Simulations for Switchable Model Molecules** — ●RAFFAELE TAVARONE<sup>1</sup>, PATRICK CHARBONNEAU<sup>2</sup>, and HOLGER STARK<sup>1</sup> — <sup>1</sup>Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin, Germany — <sup>2</sup>Departments of Chemistry and Physics, Duke University, Durham, North Carolina 27708, USA

Light-switchable molecules are chemical compounds that can undergo a light-induced, reversible *trans-cis* isomerization. They can be used to build functional monolayers with, for example, switchable wetting properties. A typical example of a light-driven *trans-cis* transition is the azobenzene isomerization.

Inspired by the conformational changes of the azobenzene compound, we build a model in which a *trans* isomer is regarded as a straight needle while a *cis* isomer is regarded as a bent needle. First, we determine the phase behavior of such molecules on a planar surface using Monte Carlo simulations. The resulting phase diagram (density versus molecular shape) shows several liquid-crystal mesophases.

Second, we build a kinetic model for a glassy monolayer inspired by a recent experiment [1]. They showed that the spontaneous algebraic relaxation of orientational order, inscribed in the sample with linearly polarized light, is strongly enhanced by illumination with circularly polarized light. In our simulations we allow molecules to switch between the *trans* and *cis* isomers due to the interaction with light. We are able to trace the influence of neighbors hindrance and other microscopic processes on the kinetic of the relaxation reported in the experiment.

[1] Fang, G. J., et al., Nature communications 4, 1521 (2013).

DS 22.9 Wed 11:45 C 243

**Effect of Binary Polymer Mixtures on the Growth of Polyelectrolyte Multilayers** — ●MALTE PASSVOGEL, PETER NESTLER, and CHRISTIANE A. HELM — Physik, Uni Greifswald, 17487 Greifswald, Germany

The buildup of polyelectrolyte multilayers (PEMs) is investigated in solution with multiple angle null-ellipsometry. Polyanion poly(styrenesulfonate) (PSS) and polycation polydiallyldimethylammonium (PDADMAC) are adsorbed sequentially from 0.1 NaCl solution. After  $N_{trans}$  deposited PDADMAC/PSS layer pairs a transition from parabolic to linear growth occurs, then the thickness per layer pair  $d_{BL}$  is constant.  $d_{BL}$  is 12.3 nm, if the molecular weight ( $M_w$ ) exceed threshold values which are specific for each polymer (25 kDa for PSS and 80 kDa for PDADMAC). If either the PDADMAC or the PSS molecular weight is decreased below the threshold values,  $d_{BL}$  either falls (for PDADMAC) or rises (for PSS) suggesting very different growth modes. Binary mixtures of PDADMAC and PSS with  $M_w$  below and above the threshold value are used, while  $M_w$  of the complementary polyanion is kept above the threshold.  $d_{BL}$  depends linearly on the mole fraction of the low-molecular-weight PDADMAC. However,  $d_{BL}$  is only influenced by low-molecular-weight PSS, if its molar fraction exceeds 90%. Always, the same linear relationship between  $N_{trans}$  and  $d_{BL}$  is found. These observations can be explained with an asymmetric growth model of polyelectrolyte multilayers.

DS 22.10 Wed 12:00 C 243

**The Swelling Behaviour of Voids inside Polyelectrolyte Multilayers** — ●MAXIMILIAN ZERBALL<sup>1</sup>, RALF KÖHLER<sup>2</sup>, OLAF SOLTWEDEL<sup>3</sup>, and REGINE VON KLITZING<sup>1</sup> — <sup>1</sup>Institut für Chemie, Technische Universität Berlin, Str. 17.Juni 124, 10623 Berlin — <sup>2</sup>Institut für Weiche Materie und funktionelle Materialien, Helmholtz-Zentrum Berlin, Hahn-Meitner-Platz 1, 14109 Berlin — <sup>3</sup>Max-Planck-Institut für Festkörperforschung, Lichtenbergstr. 1, 85747 Garching

Polyelectrolyte Multilayer (PEM) are organic films built up via subsequent adsorption of oppositely charged polyions. PEMs are highly sensitive to external parameter like the relative humidity (r.h.) of the ambient atmosphere. This ability makes them to ideal candidates for sensoric applications. In order to use these films as sensors it is important to understand and to control the swelling behavior. The uptaken water of swollen PEMs are subdividable into two contributions; the swelling water, which influences thickness and optical properties, and the void water, which only affects the optical properties of the PEM.

The swelling behavior of voids, i.e. the separated amount of uptaken water inside voids in comparison to the uptaken amount of water inside the PEM with increasing r.h., is rarely researched. For the purpose to understand the swelling behavior of voids more in detail, in this study the void water and swelling water of PEMs in dependence of the relative humidity was investigated by neutron reflectivity. The results suggest that the strongest increase of voidwater proceeds between 0% r.h. and 6% r.h. while beyond, the swelling water dominates the amount of water.

DS 22.11 Wed 12:15 C 243

**Influence of Barrier Layers on Interdiffusion in Polyelectrolyte Multilayers** — ●PETER NESTLER<sup>1</sup>, MALTE PASSVOGEL<sup>1</sup>, OLAF SOLTWEDEL<sup>2</sup>, RALF KÖHLER<sup>3</sup>, and CHRISTIANE A. HELM<sup>1</sup> — <sup>1</sup>Physik, Uni Greifswald, 17487 Greifswald, Germany — <sup>2</sup>MPI FKP 70569 Stuttgart, Germany — <sup>3</sup>Helmholtz-Zentrum Berlin, 14109 Berlin, Germany

Polyelectrolyte multilayers are made from poly(diallyldimethylammonium) (PDADMA), poly(styrenesulfonate) (PSS). Using selective PSS deuteration each film consists of a protonated and a deuterated compartment.

During annealing in 1 M NaCl solution the internal interface between these two compartments broadens due to interdiffusion. The PSS diffusion coefficient  $D_{PSS}$  inside the multilayer film is quantified via neutron reflectivity. Eventually the annealing leads to a uniform distribution of protonated and deuterated PSS inside the film. If one polycation layer in the film centre is branched poly(ethyleneimine) (PEI), then PEI serves as a diffusion barrier. In this case the barrier is impenetrable for up to 70% of PSS molecules. The diffusion behaviour of the remaining 30% can be described using a position-dependent distribution of DPSS inside the multilayer film. The effective PSS diffusion coefficient is reduced by one to two orders of magnitude.

DS 22.12 Wed 12:30 C 243

**Improved Electrolyte-Additive Induced Performance of Graphite Anodes for Lithium-Ion Batteries – Electrochemical and Electrode Surface Studies** — ●ANNA DIMITROVA<sup>1</sup>, ANDRE MÜLLER<sup>2</sup>, SVETLOZAR IVANOV<sup>2</sup>, MARCEL HIMMERLICH<sup>1</sup>, ANJA EISENHARDT<sup>1</sup>, ANDREAS BUND<sup>2</sup>, and STEFAN KRISCHOK<sup>1</sup> — <sup>1</sup>Technische Universität Ilmenau, Institut für Physik und Institut für Mikro- und Nanotechnologien, Germany — <sup>2</sup>Technische Universität Ilmenau, Fachgebiet Elektrochemie und Galvanotechnik, Germany

The electrolyte decomposition is a crucial stage in the formation cycle of Li-ion batteries. It results in the formation of a protective passivation layer on the graphite electrode surface, called *solid electrolyte interphase* (SEI). SEI formation competes with Li ion intercalation and its chemical composition and structure determines the battery cell life time. To control this process we designed a phosphorous enriched electrolyte, which enhances the rate performance and the capacity retention of the Li-ion battery compared to a non-modified electrolyte. In order to study charge-discharge cycles in the batteries and to analyze the SEI composition, we combined electrochemical studies with X-ray Photoelectron Spectroscopy (XPS). In this work the influence of the electrolyte on the SEI composition was investigated and a correlation between chemical structure and electrochemical characteristics of the Li-ion battery will be discussed.

DS 22.13 Wed 12:45 C 243

**Deposition of copper multilayers on Au(111) in sulphuric acid solution: An electrochemical scanning tunneling mi-**

**croscopy study** — ●BARTOSZ MADRY<sup>1</sup>, KLAUS WANDEL<sup>1,2</sup>, and MAREK NOWICKI<sup>1</sup> — <sup>1</sup>Institute of Experimental Physics, University of Wrocław, pl. M. Borna 9, 50-204 Wrocław, Poland. — <sup>2</sup>Institute of Physical and Theoretical Chemistry, University of Bonn, Wegelerstr. 12, 53115 Bonn, Germany.

The co-adsorption of submono-, mono- and multi-layers of Cu with sulfate anions on a Au(111) electrode surface was investigated in electrochemical environment (0.1 mM CuSO<sub>4</sub> + 0.1 M H<sub>2</sub>SO<sub>4</sub>) by cyclic voltammetry (CV) and in-situ scanning tunneling microscopy (STM).

Correlated with the STM investigations the CV measurements indicate co-adsorption/-desorption processes of Cu of submono-, mono- and multi-layer coverages with sulfuric acid species on Au(111). The formation of a quasi-hexagonal Moiré superstructure on terraces of copper multilayers was observed in situ by STM. In detail the observed Moiré-structure is similar but not identical to the one observed on the (111) surface of bulk copper. High resolution STM images show the formation of a ( $\sqrt{3} \times \sqrt{7}$ )-like sulfate structure on all multilayer copper terraces.

## DS 23: Topological insulators: Theory (HL with DS/MA/O/TT)

Time: Wednesday 9:30–11:30

Location: ER 270

DS 23.1 Wed 9:30 ER 270

**Weyl and Dirac semimetals: A platform for new interface phenomena** — ●ADOLFO G. GRUSHIN<sup>1</sup>, JORN W. F. VENDERBOS<sup>2</sup>, and JENS H. BARDARSON<sup>3</sup> — <sup>1</sup>Max Planck Institute for the physics of Complex Systems, Dresden, Germany — <sup>2</sup>Massachusetts Institute of Technology, Cambridge, MA, USA — <sup>3</sup>Max Planck Institute for the physics of Complex Systems, Dresden, Germany

The Weyl semimetal (WSM) state is sometimes loosely referred to as the three-dimensional cousin of graphene since its low energy theory is described by an even number of copies of the Weyl Hamiltonian. Closely related to WSM, the Dirac semimetals hosts the Weyl nodes at the same point in the Brillouin Zone and it is realised in Cd<sub>3</sub>As<sub>2</sub> and Na<sub>3</sub>Bi compounds. In this talk I will explore the rich surface state physics that these states can host and how can it be probed, including coexistence of Dirac and Fermi arc states at the topological insulator-weyl semimetal interfaces as well as signatures of the chiral anomaly.

DS 23.2 Wed 9:45 ER 270

**Spin chirality tuning and Weyl semimetal in strained HgS<sub>1-x</sub>Te<sub>x</sub>** — ●TOMÁŠ RAUCH<sup>1</sup>, STEVEN ACHILLES<sup>1</sup>, JÜRGEN HENK<sup>1</sup>, and INGRID MERTIG<sup>1,2</sup> — <sup>1</sup>Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle (Saale), Germany — <sup>2</sup>Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle (Saale), Germany

We have theoretically investigated the phase diagram of HgS<sub>1-x</sub>Te<sub>x</sub>. The parameters which have been varied are the concentration  $x$  and the in-plane strain, which could be applied by an appropriate substrate in an experiment. In the topological phase diagram we found a normal metallic phase, two topological insulator phases with different spin chiralities of the surface states and a Weyl semi-metal phase. The phases have been probed by calculating topological invariants and the dispersion of the surface states for both crystal terminations of the (001) surface by an *ab-initio* based tight-binding model.

DS 23.3 Wed 10:00 ER 270

**Topological phases in (interfacial) phase-change materials** — ●PETER SCHMITZ, WEI ZHANG, and RICCARDO MAZZARELLO — Institute for Theoretical Solid State Physics, RWTH Aachen University

We investigate the topological, spectral and structural properties of [Sb<sub>2</sub>Te<sub>3</sub>]<sub>x</sub>[GeTe]<sub>y</sub> (GST) compounds, some of which are interfacial phase change materials (IPCMs), as a function of strain and stacking sequence by performing a DFT study of bulk and slab models and discuss the relevance of a 3D (topological) Dirac semimetal phase ((T)DSM), eg. to GST225.

IPCMs can perform fast reversible transitions, induced by electric fields or heat, between crystalline states of different stacking. Since they also possess strong spin-orbit coupling and a strong topological insulator (STI) + normal insulator(NI) layering, they are a promising platform to investigate nontrivial interface states and direct applications to data storage in terms of switching topological phases. Until now they were shown to exhibit STIs and *unstable* DSM-like critical states corresponding to STI/Ni transitions [1]. Then recently [2] a *robust* TDSM phase was predicted for crystals having certain rotational symmetries: The STI/Ni transition point can be extended to a line and 2 Dirac points appear in the bulk spectrum.

Analyzing whether such phases can be obtained in GST compounds is also interesting since the problem of a TDSM in a multilayer structure has not yet been discussed.

[1] J. Tominaga et al, Adv. Mat. Inter. 1 (2014);

[2] B. Yang and N. Nagaosa, Nature Commun. 5, 4898 (2014)

DS 23.4 Wed 10:15 ER 270

**Effect of Bi bilayers on the topological states of Bi<sub>2</sub>Se<sub>3</sub>: A first-principles study** — KIRSTEN GOVAERTS<sup>1</sup>, KYUNGWHA PARK<sup>2</sup>, CHRISTOPHE DE BEULE<sup>1</sup>, DIRK LAMOEN<sup>1</sup>, and ●BART PARTOENS<sup>1</sup> — <sup>1</sup>CMT-group and EMAT, University of Antwerp, Belgium — <sup>2</sup>Virginia Tech, Department of Physics, USA

Bi<sub>2</sub>Se<sub>3</sub> and vice versa, has not been explored much. Bi bilayers are often present between the quintuple layers of Bi<sub>2</sub>Se<sub>3</sub>, since (Bi<sub>2</sub>)<sub>n</sub>(Bi<sub>2</sub>Se<sub>3</sub>)<sub>m</sub> form stable ground-state structures. Moreover, Bi<sub>2</sub>Se<sub>3</sub> is a good substrate for growing ultrathin Bi bilayers. By first-principles techniques, we first show that there is no preferable surface termination by either Bi or Se. Next, we investigate the electronic structure of Bi bilayers on top of, or inside a Bi<sub>2</sub>Se<sub>3</sub> slab. If the Bi bilayers are on top, we observe a charge transfer to the quintuple layers that increases the binding energy of the surface Dirac cones. The extra states, originating from the Bi bilayers, were declared to form a topological Dirac cone, but here we show that these are ordinary Rashba-split states. This result, together with the appearance of a new Dirac cone that is localized slightly deeper, might necessitate the reinterpretation of several experimental results. When the Bi bilayers are located inside the Bi<sub>2</sub>Se<sub>3</sub> slab, they tend to split the slab into two topological insulators with clear surface states. Interface states can also be observed, but an energy gap persists because of strong coupling between the neighboring quintuple layers and the Bi bilayers.

DS 23.5 Wed 10:30 ER 270

**Topological states in  $\alpha$ -Sn and HgTe quantum wells: a comparison of *ab-initio* results** — ●SEBASTIAN KÜFNER and FRIEDHELM BECHSTEDT — Friedrich Schiller Universität Jena

Quantum well (QW) structures based on HgTe are theoretically predicted and experimentally verified to exhibit the quantum-spin Hall phase. Despite the similarities of the bulk band structures, studies of  $\alpha$ -Sn QW structures are missing. We compare the properties of QW structures made by the different zero-gap semiconductors  $\alpha$ -Sn and HgTe, but both sandwiched in nearly lattice-matched CdTe barriers by means of first-principles calculations including quasiparticle corrections and spin-orbit interaction. The two well materials possess different space groups O<sub>h</sub><sup>7</sup> (diamond structure) and T<sub>d</sub><sup>2</sup> (zinc-blende structure). The spin-orbit interaction, in particular that in the  $p$ -derived valence states, is different due to the contribution of both atoms in the unit cell ( $\alpha$ -Sn) and mainly the anion (HgTe) to the states at the top of the valence bands, and the different local electrostatic properties due to the different bonding character in the QW layers and their interfaces with the CdTe barrier material. We investigate the similarities and differences of the two embedded zero-gap semiconductors on the formation of quantum-well, edge and interface states in detail.

DS 23.6 Wed 10:45 ER 270

**Quasiparticle band structure of the topological insulator Bi<sub>2</sub>Se<sub>3</sub>** — ●TOBIAS FÖRSTER, PETER KRÜGER, and MICHAEL ROHLFING — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

Bi<sub>2</sub>Se<sub>3</sub> is a prototype topological insulator. Its simple surface band structure with only one Dirac point makes it an ideal system for exploring the properties of topological surface states. Up to now, the vast majority of theoretical investigations of the electronic structure of Bi<sub>2</sub>Se<sub>3</sub> has utilized DFT calculations. In Bi<sub>2</sub>Se<sub>3</sub> and related compounds, however, many body perturbation theory in the *GW* approx-

imation yields both quantitative and qualitative quasiparticle corrections of the DFT bulk band structures [1].

Here we discuss results for bulk  $\text{Bi}_2\text{Se}_3$  from *GW* calculations employing a localized basis as well as from a perturbative *LDA+GdW* approach [2]. The latter provides a numerically very efficient method for the calculation of quasiparticle corrections with only slightly reduced precision compared to *GW*. The applicability of the *LDA+GdW* formalism to the  $\text{Bi}_2\text{Se}_3$  surface with the Dirac state will also be addressed.

[1] I. Aguilera *et al.*, Phys. Rev. B **88**, 045206 (2013)

[2] M. Rohlfing, Phys. Rev. B **82**, 205127 (2010)

DS 23.7 Wed 11:00 ER 270

### Calculation of topological invariants from a maximally localized Wannier functions derived model Hamiltonian

— ●PATRICK M. BUHL, CHENGWANG NIU, YURIY MOKROUSOV, DANIEL WORTMANN, GUSTAV BIHLMAYER, and STEFAN BLÜGEL — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Using density-functional methods it is possible to provide an accurate description of topological phases in complex materials. We demonstrate how topological characterization can be performed in a unified manner based on Wannier functions generated from the full-potential linearized augmented plane-wave method as implemented in the FLEUR code [1]. Taking as examples bcc Fe,  $\text{Na}_3\text{Bi}$  and  $\text{PbTe}$  we compute various topological invariants and identify topologically non-trivial points in the electronic structure of these materials in bulk and their close relation to the surface electronic structure. In particular, we focus on the Weyl semimetallic phase as a transitional phase between various topological phases in the same material and on the role of the Weyl

points in the electronic structure for topological properties. Financial support by the HGF-YIG Programme VH-NG-513 and SPP 1666 of the DFG is gratefully acknowledged.

[1] F. Freimuth *et al.*, Phys. Rev. B **78**, 035120 (2008)

DS 23.8 Wed 11:15 ER 270

### Functionalized Bismuth Films: Giant Gap Quantum Spin Hall and Valley-Polarized Quantum Anomalous Hall States

— ●CHENGWANG NIU, GUSTAV BIHLMAYER, HONGBIN ZHANG, DANIEL WORTMANN, STEFAN BLÜGEL, and YURIY MOKROUSOV — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The search for new large band gap quantum spin Hall (QSH) and quantum anomalous Hall (QAH) insulators is critical for their realistic applications at room temperature [1,2]. Here we predict, based on first principles calculations, that the band gap of QSH and QAH states can be as large as 1.01 eV and 0.35 eV in an H-decorated  $\text{Bi}(111)$  film [3]. The origin of this giant band gap lies both in the large spin-orbit interaction of Bi and the H-mediated exceptional electronic and structural properties. Moreover, we find that the QAH state also possesses the properties of quantum valley Hall state, thus intrinsically realizing the so-called valley-polarized QAH effect. We further investigate the realization of large gap QSH and QAH states in an H-decorated  $\text{Bi}(110)$  film and X-decorated (X=F, Cl, Br, and I)  $\text{Bi}(111)$  films.

This work was supported by the Priority Program 1666 of the DFG and project VH-NG-513 of the HGF.

[1] M. Hasan and C. Kane, Rev. Mod. Phys. **82**, 3045 (2010).

[2] X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. **83**, 1057 (2011).

[3] Chengwang Niu, Gustav Bihlmayer, Hongbin Zhang, Daniel Wortmann, Stefan Blügel, and Yuriy Mokrousov, submitted.

## DS 24: Metal substrates: Structure, epitaxy and growth (joint session with O)

Time: Wednesday 10:30–12:45

Location: MA 042

DS 24.1 Wed 10:30 MA 042

**Investigation of nanocluster formation far from equilibrium in heteroepitaxial system: Co/Cu(111)** — ●QUANG HUY VU, SEBASTIAN KUNZE, and KARINA MORGENSTERN — Physical Chemistry I, Ruhr-Universität Bochum, Universitätsstr. 150,44801 Bochum, Germany

Lattice mismatch plays an important role in heteroepitaxial systems. Here we present such a system, Co adsorbed on  $\text{Cu}(111)$ . Why is so important to study this system? The small lattice mismatch between cobalt and copper of 1.9% makes it attractive to investigate its structural characteristics and study its effect onto submonolayer adsorption. The growth mechanism of cobalt was measured by means of fast-scanning tunneling microscopy within the range of surface temperatures from 100 K to 300 K and for different deposition rates. At very low coverage, cobalt forms nanoclusters on  $\text{Cu}(111)$ . These clusters adsorb favorably at step edges on  $\text{Cu}(111)$  at 115 K. In contrast at higher coverage, cobalt forms islands of fractal shapes with 1 ML height at 165K. Furthermore, the nucleation of 2 ML island height is studied at 165 K not only on the terraces but also on the step edges. Finally, the etching of Cu is observed at room temperature indicates growth of intermixed nanoclusters. In this presentation the atomic processes of the island formation will be discussed

DS 24.2 Wed 10:45 MA 042

**Surface induced stabilization of the metallic Sn phases in Sn nanoparticles.** — ●NICOLAS G. HÖRMANN<sup>1</sup> and AXEL GROSS<sup>1,2</sup> — <sup>1</sup>Helmholtz Institute Ulm (HIU) Electrochemical Energy Storage, Helmholtzstr. 11, 89069 Ulm — <sup>2</sup>Universität Ulm, Institut für Theoretische Chemie, Albert-Einstein-Allee 11, 89069 Ulm

Sn is a widely used element and besides new applications in optoelectronics [1] it is also a promising electrode material for established and future battery systems ( $\text{Li}^+$ ,  $\text{Na}^+$  and  $\text{F}^-$  batteries [2,3]). Yet, not many detailed ab-initio studies have been reported so far.

In the presentation we will report results of DFT calculations of bulk and surface structures and energies of elemental Sn. By combining this with vibrational free energy data we derive the Gibbs free energy of Sn nanostructures and show that the phase stability diagram of Sn is significantly altered, which has significant impact on the expected performance of Sn nanostructures in real-world application. Furthermore

we discuss briefly the initial steps of battery charging which occurs via atomic adsorption processes.

[1] S. Küfner *et al.*, *Nanotechnology* **24**, 405702 (2013). [2] H. Zhu *et al.*, *Nano Lett.* **13**, 3093–3100 (2013). [3] M. Anji Reddy *et al.* *J. Mater. Chem.* **21**, 17059–17062 (2011).

DS 24.3 Wed 11:00 MA 042

**Intermixing of Pt and Cu atoms in PtCu/Ru(0001) surface alloys** — ●LUIS MANCERA<sup>1</sup>, AXEL GROSS<sup>1</sup>, ALBERT ENGSTFELD<sup>2</sup>, ANDREAS BENSCH<sup>2</sup>, and R. JÜRGEN BEHM<sup>2</sup> — <sup>1</sup>Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm, Germany — <sup>2</sup>Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

In this contribution, we report on a joint theoretical and experimental study addressing model surface catalysts consisting of bimetallic PtCu surface alloys formed on a  $\text{Ru}(0001)$  substrate. The  $\text{PtCu}/\text{Ru}(0001)$  surface is obtained by deposition of Pt onto a previously prepared monolayer of Cu on  $\text{Ru}(0001)$  surface. In spite of the high stability of  $\text{Ru}(0001)$  that prevents exchange of Cu or Pt atoms with the substrate,  $\text{Ru}(0001)$  can still induce strain on the deposited Cu layer, due to the different lattice parameter, and thus modulate the formation of the PtCu alloy. Using STM imaging, it has been observed that the surface alloy is formed following a specific nucleation behavior that shows an atypical island density increase with growing Pt coverage. Here we apply periodic density functional theory (DFT) calculations to study various situations for atom diffusion on different surface alloy configurations in order to elucidate the origin of those nucleation patterns. We determine the stability of PtCu surface alloys and address the diffusion of Pt and Cu atoms on  $\text{PtCu}/\text{Ru}(0001)$  as well as Pt-Cu atom-exchange processes that lead to the formation of these alloys. Based on these findings, the effect of Pt substitutional atoms in the nucleation is discussed.

DS 24.4 Wed 11:15 MA 042

### Alloying and dealloying of Mg on the Ag(100) surface

— ●MARINA SCHULER, PASCAL FERSTL, LUTZ HAMMER, and M.ALEXANDER SCHNEIDER — Lst. für Festkörperphysik, FAU Erlangen-Nürnberg

Ultrathin oxide films on metal substrates play an important role in basic surface research and technological applications. Since these ox-

ide films are often prepared via postoxidation of pre-deposited metal films, their structural properties may strongly influence the quality of the growing oxide. In this study we investigate the structures developing during Mg deposition on Ag(100) prior to oxidation to MgO by means of quantitative LEED and STM.

Submonolayers of Magnesium adsorbed at 90 K on top of the plain Ag(100) surface form an ordered  $(\sqrt{5} \times \sqrt{5})R \arctan 0.5$  phase. Annealing to 150 K leads to an atomic reorganisation at the surface and a  $c(2 \times 2)$  phase appears, which has been reported already [1]. The crystallographic structure of this  $c(2 \times 2)$  phase is shown to be a bimetallic surface alloy by means of a quantitative LEED analysis: every second Ag atom of the top layer is substituted by Mg, which relaxes outward by 0.13 Å. The Mg/Ag- $c(2 \times 2)$  structure persists further Mg deposition at elevated temperatures dissolving surplus Mg atoms into the underlying substrate layers. By offering  $1 \cdot 10^{-7}$  mbar oxygen at 400 K the dissolved Mg is driven at the surface of the crystal again, forming MgO films of the corresponding thickness.

[1] C. Tegenkamp Appl. Surf. Sci. 151 40 (1999)

DS 24.5 Wed 11:30 MA 042

**Comparative study of the carbide-modified surfaces C/Mo(110) and C/Mo(100) using high resolution x-ray photoelectron spectroscopy** — ●CHRISTOPH GLEICHWEIT, UDO BAUER, MAX AMENDE, STEFAN SCHERNICH, OLIVER HÖFERT, JÖRG LIBUDA, HANS-PETER STEINRÜCK, and CHRISTIAN PAPP — Lehrstuhl f. Physikal. Chemie II

We present a comparative study of the carbide-modified surfaces C/Mo(100) and C/Mo(110) using synchrotron-based high-resolution x-ray photoelectron spectroscopy (HR-XPS), with the objective of elucidating the differences and similarities of the two crystal facets depending on the C/Mo ratio. We are interested in changes at the surface due to exposure to carbon and oxygen right at the temperature sufficient to drive carbon into the interstitial sites of the Mo lattice. Carburization by dosing ethylene, i.e. carbide preparation, and subsequent oxidative carbon removal by dosing O<sub>2</sub> at 1200 K is followed in great detail through careful analysis of the C 1s, Mo 3d and O 1s core levels. We show that the thin carbide overlayers show spectroscopic differences compared to the thick carbides obtained at high carbon dose. Furthermore we show that the carbide thickness on Mo(110) influences the adsorption properties towards H<sub>2</sub> and CO, pointing towards the importance of the surface structure for reactivity.

DS 24.6 Wed 11:45 MA 042

**Surface self-diffusion of the battery anode materials lithium, sodium and magnesium studied using DFT** — ●MARKUS JÄCKLE<sup>1,2</sup> and AXEL GROSS<sup>1,2</sup> — <sup>1</sup>Helmholtz Institut Ulm - Elektrochemische Energiespeicherung, 89069 Ulm, Germany — <sup>2</sup>Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany

Lithium, sodium and magnesium represent rather interesting anode materials for next-generation batteries. These metals vary in their tendency to form dendrites which represent a hazard as their formation can lead to short-circuits during battery operation. As metal growth processes are intimately linked to diffusion, we have studied the self-diffusion properties of the metals in order to understand the differences in their tendency towards dendrite formation.

According to our calculations, self-diffusion of Mg is much faster than the one of Li or Na on the energetically most stable surface terminations [1]. These results can be connected to the fact that Mg is an hcp metal, whereas Li and Na are bcc metals. In addition, we have determined the interaction between adatoms of these metals. We will discuss the relevance of our findings for the understanding of the dendrite growth on battery anodes. Furthermore, we will address first attempts to assess the influence of the electrochemical environment on metal diffusion properties.

[1] M. Jäckle and A. Groß, J. Chem. Phys. **141**, 174710 (2014).

DS 24.7 Wed 12:00 MA 042

**Ultra-thin stepped iron oxide films on high index Pt surfaces** — ●ELIN GRÄNÄS<sup>1,2</sup>, NICLAS JOHANSSON<sup>1</sup>, MOHAMMAD A. ARMAN<sup>1</sup>,

JACEK OSIECKI<sup>3</sup>, KARINA THÄNEL<sup>3</sup>, JESPER N. ANDERSEN<sup>1,3</sup>, JOACHIM SCHNADT<sup>1</sup>, and JAN KNUDSEN<sup>1,3</sup> — <sup>1</sup>Division of Synchrotron Radiation Research, Lund University, Sweden — <sup>2</sup>Deutsches Elektronen Synchrotron (DESY), Hamburg, Germany — <sup>3</sup>MAX IV Laboratory, Lund University, Sweden

Iron oxide films grown on metal surfaces show high catalytic activity for reactions such as CO oxidation and the water-gas shift, and it has been suggested that the high activity is due to under-coordinated Fe atoms at the edge of FeO islands[1]. Whether the metal substrate is essential for the activity of the edge sites remain an open question and the few and heterogeneous edge sites present on FeO islands make it difficult to characterize them with chemically sensitive techniques like X-ray photoelectron spectroscopy (XPS).

We have grown FeO films on Pt(322), producing films with a very high density of homogenous FeO-FeO edge sites. Scanning tunneling microscopy show that approx. 20 % of the sites are edge sites. In water adsorption studies on the stepped FeO film we observe an enhanced ability to split water compared to planar FeO. As the Pt(322) substrate is fully covered by stepped FeO we assign the high water splitting ability to the pure FeO-FeO step site.

[1] L. Xu, Z. Wu *et al.*, J. Phys. Chem. C **115**, 14290 (2011)

DS 24.8 Wed 12:15 MA 042

**MD study of gold growth on MnAs** — ●ANDREAS RÜHL and CHRISTIAN HEILIGER — I. Physikalisches Institut, Justus Liebig Universität Giessen, D-35392 Giessen, Germany

We present the results of our Molecular Dynamics (MD) study concerning the atomic deposition of gold atoms on different MnAs surfaces. Those growth simulations show a 'layer-plus-island growth', also known as the Stranski-Krastanov (SK) growth. Our research is motivated by the experimental work on ferromagnetic MnAs nanoclusters, which can be easily tuned in different shapes and sizes. Taking two of those clusters and connect them via a non-magnetic metal, for example gold, leads to a GMR-like structure (Giant magnetoresistance).

In order to analyze the structure of the deposited gold atoms, needed for later calculation of the electric transport, we created an EAM potential for the MnAsAu system in the scope of Force Matching by fitting the potential model to ab initio data. The resulting potential is validated by different tests, including the comparison of bulk and surface energies to the corresponding ab initio data. We then carried out growth simulations for different MnAs surfaces and different substrate temperatures. The observed SK-growth exhibits a critical layer thickness at which the island growth starts and by using Bond-Angle analysis we see the gold atoms mainly relaxing to fcc phases.

DS 24.9 Wed 12:30 MA 042

**Development and testing of a plasma coating apparatus** — ●CORNELIA KUNZ<sup>1</sup>, SEBASTIAN DAHLE<sup>1,2</sup>, and WOLFGANG MAUS-FRIEDRICHS<sup>1,2</sup> — <sup>1</sup>Institut für Energieforschung und Physikalische Technologien, Technische Universität Clausthal, Leibnizstraße 4, D-38678 Clausthal-Zellerfeld, Germany — <sup>2</sup>Clausthaler Zentrum für Materialtechnik, Technische Universität Clausthal, Agricolastraße 2, D-38678 Clausthal-Zellerfeld, Germany

Thin coatings on metal surfaces have known advantages in many applications, e.g. passivation or corrosion protection. In this work, a plasma coating apparatus was constructed and tested to develop uniform, particle-free coatings on titanium surfaces. A primary Si<sub>3</sub>N-coating was achieved via plasma ignition in nitrogen diluted silane at atmospheric pressure. A procedure was devised to control the growth mechanisms yielding particle-free coatings. In order to minimize particle formation, nucleation and agglomeration of radicals formed in the plasma have to be inhibited. The critical parameter leading to a silicon radical controlled growth mode and thus to minimized nucleation was found to be the excitation frequency. In a secondary step, these Si<sub>3</sub>N-coatings were treated with air plasma, leading to oxidation and clean silicon dioxide coatings. Surface topography was analysed using atomic force microscopy (AFM) in order to determine a growth mode suppressing particle formation mode. In a following step, surface stoichiometry was determined via X-ray photoelectron spectroscopy (XPS).

## DS 25: GAEDE-PREIS 2015

Time: Wednesday 13:15–13:45

Location: HE 101

## Invited Talk

DS 25.1 Wed 13:15 HE 101

**Porphyrin molecules at interfaces** — ●WILLI AUWÄRTER — Physik Department E20, Technische Universität München, Germany

Porphyrins and related tetrapyrrole molecules possess an impressive variety of functional properties - including axial ligation, electron transfer, light harvesting and catalytic transformations - that have been exploited in natural and artificial systems. From a surface science perspective, porphyrins are thus ideally suited as building blocks for surface-anchored functional nanostructures [1-3]. We will review recent scanning tunneling microscopy and spectroscopy results, complemented by space-averaging techniques and computational modeling based on density functional theory, addressing such porphyrin systems with sub-molecular resolution. Key aspects include molecular

switching, conformation, axial ligation, metalation and self-assembly protocols. Particular emphasis is put on on-surface dehydrogenation reactions yielding novel porphyrin species on Ag(111), including covalently linked dimers and longer oligomers. Furthermore, the formation of metal-organic coordination networks and porphyrin arrays on atomically thin boron nitride (BN) layers grown on Cu(111) is discussed [4]. The BN template dictates the electronic level alignment of the porphyrin nanostructures and supports distinct coordination motifs.

[1] W. Auwärter et al., *Nature Chem.*, DOI: 10.1038/NCHEM.2159 (2015)

[2] K. Seufert et al., *Nature Chem.* 3, 114 (2011)

[3] W. Auwärter et al., *Nature Nanotech.* 7, 41 (2012)

[4] S. Joshi et al., *ACS Nano* 8, 430 (2014)

## DS 26: Layer Properties: Electrical, Optical, and Mechanical Properties

Time: Wednesday 15:00–19:00

Location: H 2032

DS 26.1 Wed 15:00 H 2032

**Tunable Ion Bombardment Induced by Altering Plasma Confinement in Magnetron Sputtering** — ●MATHIS TRANT, MARIA FISCHER, KERSTIN THORWARTH, HANS JOSEF HUG, and JÖRG PATSCHEIDER — Empa, Laboratory for Nanoscale Materials Science, Überlandstr. 129, CH-8600 Dübendorf, Switzerland

Ion bombardment is known to influence deposition processes and is widely used to control thin film growth. It offers a variety of possibilities including growth of non-equilibrium phases, changes in residual stress and defect densities. In the case of magnetron sputtering this topic is of special interest, since there is an intrinsic bombardment of particles with typically low kinetic energy.

In this contribution a variety of approaches for altering the ion bombardment are re-viewed by making use of additional plasma confinement. The implementation of an additional magnetic field from an electromagnetic coil in a reactive magnetron co-sputtering process is presented, showing the potential of this method. Among other improvements, an increase of the ion saturation current by a factor of 7 has been achieved. The influence on film properties of different magnetic configurations are discussed on the basis of aluminum sputter deposition in reactive and non-reactive atmospheres.

DS 26.2 Wed 15:15 H 2032

**Challenges in Depositing Aluminum Oxynitride Films by Reactive DC Magnetron Sputtering** — ●MARIA FISCHER, MATHIS TRANT, KERSTIN THORWARTH, HANS JOSEF HUG, and JÖRG PATSCHEIDER — Empa, Laboratory for Nanoscale Materials Science, Überlandstr. 129, CH-8600 Dübendorf, Switzerland

Thin, transparent coatings of aluminum oxynitride with different oxygen contents were prepared by reactive direct current (DC) magnetron sputtering from a pure aluminum target. The simultaneous use of the two reactive gases O<sub>2</sub> and N<sub>2</sub> poses challenges due to their different chemical behavior towards metallic targets. Various experimental parameters, including the position of the O<sub>2</sub> gas inlet inside the deposition chamber, have a strong influence on film properties and reproducibility. This applies also to the target poisoning and erosion state; experiments conducted at otherwise equal conditions yielded deposition rates varying by a factor of 2.5.

The setup in a conventional sputter deposition system was altered to improve the controllability of deposition processes conducted with an O<sub>2</sub>/N<sub>2</sub> gas mixture. The influences of the different experimental configurations on resulting films were investigated in terms of reproducibility, deposition rate, crystallinity, morphology, biaxial stress and hardness.

DS 26.3 Wed 15:30 H 2032

**Mechanische Spannungen in Cr-dotierten  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>-Schichten** — ●SEBASTIAN SCHIPPOREIT<sup>1</sup>, ALI HALIGÜR<sup>1</sup>, MARKUS NEUBERT<sup>1,2</sup> und VOLKER BUCK<sup>1</sup> — <sup>1</sup>Arbeitsgruppe Dünnschichttechnologie, Fakultät für Physik, Universität Duisburg-Essen und CENIDE, 47057 Duisburg — <sup>2</sup>Eifeler Werkzeuge GmbH, Duderstädter Str. 14, 40595 Düsseldorf

Oberflächentemperaturen sind ein entscheidender Parameter bei der Herstellung dünner Schichten. Insbesondere in stark leuchtenden Medien stößt die Temperaturbestimmung mit Hilfe der thermischen Emission an ihr Grenzen. Daher sind in dieser Arbeit die Erzeugung und der Einsatz von Cr-dotierten Al<sub>2</sub>O<sub>3</sub>-Schichten als thermographische Phosphore mittels HF-ICP/CCP-PECVD untersucht worden.

In dieser Arbeit ist es gelungen mit dem Einsatz eines induktiv gekoppelten Plasmas, die Temperaturen zur Erzeugung Cr-dotierter  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>-Schichten auf 780 °C bei Si-Substraten herabzusetzen. Die Experimente fanden in einer Niederdruck-Ar-Atmosphäre, bzw. Ar-O<sub>2</sub>-Atmosphäre statt, wobei das Gas je einen Tiegel mit den pulverförmigen Precursoren Al(acac)<sub>3</sub> und Cr(acac)<sub>3</sub> überströmte.

Die hergestellten Cr-dotierten Al<sub>2</sub>O<sub>3</sub>-Schichten weisen die R1 und R2 Emissionen der Rubin-Fluoreszenz auf. Die Intensität der Phosphore ist vom angeregten Volumen abhängig, daher sollten möglichst dicke Schichten hergestellt werden. Mit zunehmender Schichtdicke nimmt jedoch die Schichthaftung auf Grund innerer Spannungen in der Schicht ab. Daher ist hier die Schichtspannung in Abhängigkeit verschiedener Beschichtungsparameter und Schichtdicken untersucht worden.

DS 26.4 Wed 15:45 H 2032

**Solution Processed Deposition of Large-Size MoS<sub>2</sub> Nanoflakes** — ●XAOLING ZENG, MARLIS ORTEL, and VEIT WAGNER — Jacobs University Bremen, 28759 Bremen, Germany

The gap in understanding MoS<sub>2</sub> deposition processes needs to be closed in order to utilize all its excellent properties in nano-electronics. In this work, deposition of MoS<sub>2</sub>-flakes from precursor solution by dip-coating on Si-substrates was investigated. Ammonium tetrathiomolybdate (ATTM) dissolved in deionized water was used as precursor solution. The MoS<sub>2</sub>-flakes obtained from the precursor solutions were analyzed by atomic force and optical microscopy, PL, UV-Vis and Raman spectroscopy.

The deposition process of the flakes was found to obey Landau-Levich mechanism with respect to the relationship between the withdraw speed and film size and thickness. By optimization of deposition parameters, MoS<sub>2</sub> flakes exceeding 150 micro meter in lateral size were obtained. The thickness in the range of 2-5ML was confirmed by AFM and Raman measurements. Raman and PL measurements indicate that the quality of the film strongly depends on the post thermal treatment and its atmospheric composition. This low-cost solution-based deposition method is simple and non-toxic, which is also suitable for preparation of large transition metal dichalcogenides nanoflakes for various applications.

DS 26.5 Wed 16:00 H 2032

**Structural and electrical characterization of the ferrocristals [(SnSe)<sub>1+ $\delta$ ]<sub>m</sub>(NbSe<sub>2</sub>)<sub>1</sub></sub>** — ●CORINNA GROSSE<sup>1</sup>, MATTI ALEMAYEHU<sup>2</sup>, OLIVIO CHIATTI<sup>1</sup>, ANNA MOGILATENKO<sup>1,3</sup>, DAVID C. JOHNSON<sup>2</sup>, and SASKIA F. FISCHER<sup>1</sup> — <sup>1</sup>Novel Materials, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — <sup>2</sup>Department of Chemistry, University of Oregon, Eugene, OR, 97401, USA — <sup>3</sup>Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztech-

nik, 12489 Berlin, Germany

Ferrecrystals are layered intergrowth compounds consisting of few-atomic-layers thin transition metal dichalcogenide (TMDC) layers alternately stacked with monochalcogenide layers. TMDCs exhibit interesting electrical properties such as charge density waves, superconductivity or an ultralow thermal conductivity. In contrast to conventional misfit layer compounds, ferrecrystals show a turbostratic disorder and have a freely tunable stacking sequence.

In this work, we investigate the structural and electrical properties of  $[(\text{SnSe})_{1+\delta}]_m(\text{NbSe}_2)_1$  ferrecrystals as a function of the thickness of the SnSe layers separating single NbSe<sub>2</sub> layers. The atomic structure of the thin films was visualized using scanning transmission electron microscopy. In-plane resistivity, Hall coefficient and magnetoresistance were measured for temperatures down to 300 mK. The magnetoresistance measurements were analyzed using a two-band model. A superconducting transition is observed and the in-plane and cross-plane coherence lengths of superconductivity were determined. The influence of the ferrecrystal structure on the electrical properties is discussed.

DS 26.6 Wed 16:15 H 2032

**Weak antilocalization and disorder induced electron-electron interaction in DC-magnetron-sputtered Sb<sub>2</sub>Te<sub>3</sub> and Bi<sub>2</sub>Te<sub>3</sub> thin films** — •TOBIAS SCHÄFER<sup>1</sup>, HANNO VOLKER<sup>1</sup>, and MATTHIAS WUTTIG<sup>1,2</sup> — <sup>1</sup>I. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen, Germany — <sup>2</sup>JARA FIT, RWTH Aachen

Recently Sb<sub>2</sub>Te<sub>3</sub> and Bi<sub>2</sub>Te<sub>3</sub> have raised notable interest as topological insulators (TIs). A usual deposition technique for TI specimen is molecular beam epitaxy (MBE) as it ensures the required high crystalline and surface quality. Besides ARPES, low temperature magnetotransport measurements have become common techniques for characterization of Sb<sub>2</sub>Te<sub>3</sub> and Bi<sub>2</sub>Te<sub>3</sub> TI samples<sup>[1]</sup>.

Apart from that, the materials are also interesting as phase change materials (PCM). Particularly Sb<sub>2</sub>Te<sub>3</sub> is known for its fast and reversible switching between an amorphous and a crystalline phase<sup>[2]</sup>. In this context DC-magnetron sputtering followed by subsequent annealing is the commonly used deposition technique, which leads to more disordered films that do not suit the needs of TI surface states.

Here we present a magneto-transport study on highly disordered Sb<sub>2</sub>Te<sub>3</sub> and Bi<sub>2</sub>Te<sub>3</sub> thin films. The thicknesses are chosen to be smaller than the inelastic mean free path in order to achieve a quasi 2d behavior. The measurements are analyzed in the framework of HLN-theory<sup>[3]</sup> and compared to literature on MBE grown TI samples.

<sup>[1]</sup> e.g. Takagaki et al, Phys. Rev. B 86, 125137, (2012)

<sup>[2]</sup> Yamada et al, Jpn. J. Appl. Phys. 26 61, (1987)

<sup>[3]</sup> Hikami et al, Prog. Theor. Phys. 63 (2), (1980)

DS 26.7 Wed 16:30 H 2032

**Tip-enhanced Raman spectroscopy (TERS) on La<sub>2</sub>CoMnO<sub>6</sub> thin films: Field enhancement and polarisation effects** — •CHRISTOPH MEYER, SEBASTIAN MERTEN, SEBASTIAN HÜHN, MARKUS JUNGBAUER, VASILY MOSHNYAGA, BERND DAMASCHKE, and KONRAD SAMWER — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

B-site ordered La<sub>2</sub>CoMnO<sub>6</sub> (LCMO) with monoclinic P12<sub>1</sub>/n<sub>1</sub> structure can be derived from a perovskite ABO<sub>3</sub> by alternating layers of Co<sup>2+</sup> and Mn<sup>4+</sup> on the B-site. It is a promising material for spintronic applications due to ferromagnetic ordering, magnetodielectric coupling and multiferroic behavior. Since the performance of LCMO is strongly affected by the degree of B-site ordering, we applied Raman spectroscopy to correlate phonon spectra with the ordering. A study of the far-field Raman and tip-enhanced Raman spectroscopy (TERS) of LCMO thin films on SrTiO<sub>3</sub>(100) and SrTiO<sub>3</sub>(111) substrates, grown by metalorganic aerosol deposition (MAD), was performed. Polarization dependent TERS was carried out to determine the contributions for enhancement due to surface plasmon polariton (SPP) excitation and depolarization. Due to B-site cation ordering, the spectra exhibit a strong A<sub>g</sub> mode at 645 cm<sup>-1</sup>, generated by octahedral (Co/Mn)O<sub>6</sub> stretching vibrations with largest TERS contrast of ~ 60 – 100 in the crossed polarization configuration. A tip-induced depolarization effect and a significant enhancement due to general field amplification were observed. Financial support by the DFG via project SFB 1073/B04 is gratefully acknowledged.

15 min. break.

DS 26.8 Wed 17:00 H 2032

**Nitrogen concentration dependence of the stiffness of silicon nitride layers formed by low-dose N<sup>+</sup> ion implantation** — •MARINA SARMAANOVA<sup>1</sup>, HELMUT KARL<sup>2</sup>, STEPHAN MÄNDL<sup>1</sup>, DIETMAR HIRSCH<sup>1</sup>, STEFAN G. MAYR<sup>1,3</sup>, and BERND RAUSCHENBACH<sup>1,3</sup> — <sup>1</sup>Leibniz Institute of Surface Modification, D-04318 Leipzig, Germany — <sup>2</sup>University Augsburg, Institute of Physics, D-86135 Augsburg, Germany — <sup>3</sup>University Leipzig, Institute for Experimental Physics II, D-04103 Leipzig, Germany

Si wafer material was implanted at room temperature with 100 keV N<sup>+</sup> ions at fluences between  $1 \cdot 10^{15}$  and  $1 \cdot 10^{17}$  cm<sup>-2</sup>. Substoichiometric SiN<sub>x</sub> layers were formed in the near-surface region. Subsequent thermal annealing was performed at 800°C in three half-hour steps. Elastic properties of implanted layers were measured nanometer-resolved by contact resonance atomic force microscopy (CR-AFM) as function of ion fluence after each annealing step. Strong correlation between the nitrogen content and the indentation moduli was observed while recovering defects caused by the implantation inside the material. The determined indentation moduli range between 100 and 180 GPa depending on the annealing duration and nitrogen content. Reduction of the indentation moduli of as-implanted samples is caused by the implantation induced amorphization. Long-term annealing led to the increase of the indentation moduli of the high-fluence implanted Si wafers over the value of indentation modulus for crystalline silicon material (165 GPa). The high indentation moduli can be explained by formation of Si-N bonds verified by X-ray photoelectron spectroscopy.

DS 26.9 Wed 17:15 H 2032

**Optical and transport properties of epitaxial Nd<sub>1.83</sub>Ce<sub>0.17</sub>CuO<sub>4</sub> thin films** — •ANITA GUARINO<sup>1</sup>, ADOLFO AVELLA<sup>1</sup>, CARMELA BONAVOLONTÀ<sup>2</sup>, MASSIMO VALENTINO<sup>2</sup>, CORRADO DI LISIO<sup>2</sup>, LOREDANA PARLATO<sup>2</sup>, ANTONIO LEO<sup>1</sup>, GAIA GRIMALDI<sup>1</sup>, SANDRO PACE<sup>1</sup>, GIAMPIERO PEPE<sup>2</sup>, ANTONIO VECCHIONE<sup>1</sup>, and ANGELA NIGRO<sup>1</sup> — <sup>1</sup>CNR-SPIN Salerno and Dipartimento di Fisica E R Caianiello, Università di Salerno, via Giovanni Paolo II, 132, Fisciano (SA), Italy — <sup>2</sup>CNR-SPIN Napoli and Dipartimento di Fisica Università Federico II di Napoli, via Cinthia, 80126 Napoli, Italy

Electrical transport measurements and transient optical pump-probe experiments have been performed on epitaxial films of the electron doped Nd<sub>1.83</sub>Ce<sub>0.17</sub>CuO<sub>4</sub> compound for studying the non-equilibrium carrier dynamics in this material. In particular, the value of the quasi-particle relaxation time has been estimated in order to investigate the possible use of this compound as base material for superconducting optical detectors. Samples have been grown on (001)-oriented SrTiO<sub>3</sub> substrates by dc sputtering in a mixed atmosphere of both Ar and O<sub>2</sub>. X-ray diffraction analysis and Scanning Electron Microscope equipped with a wavelength dispersive spectroscopy detector have been used to characterize the structure and the morphology and composition of the thin films. Time-solved femtosecond pump-and-probe spectroscopy has been also carried out on our samples in the temperature range 4.2K-300 K. The data demonstrate a clear correlation between electrical and optical features.

DS 26.10 Wed 17:30 H 2032

**Significant Band Gap Narrowing of ALD Deposited ZnO:Al by Correlated Spectroscopic Ellipsometry, Photoluminescence and Spectrophotometry** — •MICHAEL LATZEL<sup>1,2</sup>, MANUELA GÖBELT<sup>1</sup>, GERALD BRÖNSTRUP<sup>1,3</sup>, CORNEL VENZAGO<sup>4</sup>, SEBASTIAN W. SCHMITT<sup>1</sup>, and SILKE H. CHRISTIANSEN<sup>1,3</sup> — <sup>1</sup>Max Planck Institute for the Science of Light, Günther-Scharowsky-Str. 1/Bau 24, Erlangen, Germany — <sup>2</sup>Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Institute of Optics, Information and Photonics, Staudtstr. 7/B2, Erlangen, Germany — <sup>3</sup>Helmholtz Center Berlin for Energy and Materials, Hahn-Meitner-Platz 1, Berlin, Germany — <sup>4</sup>AQura GmbH, Rodenbacher Chaussee 4, Hanau-Wolfgang, Germany

Knowing the dielectric function of a material for optoelectronic applications is essential for efficient device design and simulation. We investigated the contributions of different optical transitions in aluminum doped zinc oxide deposited by atomic layer deposition to a model dielectric function (MDF) over a wide range of photon energy. We found strong evidence for band gap narrowing due to aluminum doping and intrinsic defects and impurities. The derived MDF strongly depends on the actual band structure and therefore describes the dielectric properties very accurately. The presented MDF is solely based on physical parameters, in contrast to empirical models like e.g. widely used Sellmeier equation. This allows determining key electronic parameters like

the band gap or even charge carrier lifetimes.

DS 26.11 Wed 17:45 H 2032

**Detection of photoexcited hot charge carriers at the edges of metal nano films** — ●MARC THOMAS<sup>1,2</sup>, STEFFEN FRANZKA<sup>2</sup>, NILS HARTMANN<sup>2</sup>, DETLEF DIESING<sup>1</sup>, MATTHIAS HENSEN<sup>3</sup>, DOMINIK DIFFERT<sup>3</sup>, and WALTER PFEIFFER<sup>3</sup> — <sup>1</sup>Institut für Physikalische Chemie, Universität Duisburg Essen — <sup>2</sup>Interdisciplinary Center for Analytics on the Nanoscale, Universität Duisburg Essen — <sup>3</sup>Institut für Experimentalphysik, Universität Bielefeld

Metallic nanostructures differ from metallic bulk materials concerning their electrical, optical and chemical properties. Structured nano films produced by evaporation through shadow masks exhibit thickness wedges at the edge of the nanostructure. A home-built microscope setup allows the laterally resolved scanning of the nanofilm's reflectivity with a lateral resolution of  $3\mu\text{m}$ . Experimentally observed reflectivity maps at the edge of the nanostructure are compared with calculated reflectivity maps derived by optical multi layer models taking into account the interference phenomena in nanostructures. When the structured metallic nano film is deposited on a metal-insulator sandwich, one can monitor photo excited hot charge carriers in the top nano film as a current in the backside metal under the oxide. This photocurrent is characterised with respect to the energy of the excited carriers by applying a bias voltage between the top metal nano film and the backside metal when scanning the edge of the metal nano structure by coupling a cw 532 nm laser to the microscope setup. Future applications of this technique as the spectral characterisation of localised optical excitations are addressed.

DS 26.12 Wed 18:00 H 2032

**Optical and electrical properties of silicon nanocrystals based on a SiH<sub>4</sub>-O<sub>2</sub> PECVD process** — ●JAN LAUBE, SEBASTIAN GUTSCH, DANIEL HILLER, and MARGIT ZACHARIAS — Laboratory for Nanotechnology, Department of Microsystems Engineering - IMTEK, University of Freiburg, Georges-Koehler-Allee 103, 79110 Freiburg im Breisgau, Germany

A monosilane (SiH<sub>4</sub>) and oxygen (O<sub>2</sub>) based plasma-enhanced chemical vapor deposition process (PECVD) for the growth of silicon-rich oxide / silicon dioxide superlattices was developed.[1,2] In contrast to the conventional nitrous oxide (N<sub>2</sub>O) based oxynitride-process,[3] we achieved thereby PECVD-grown size-controlled silicon nanocrystals in pure, N-free silicon dioxide matrix.

We present a detailed study based on optical (PL), electrical (C-V, I-V) and structural (TEM) measurements that reveal the different properties of nominally identical Si nanocrystals in oxynitride and N-free oxide matrix. Most strikingly we find negligible differences in the optical performance (PL quantum yield), whereas substantial differences in the current transport and transient charging behaviour persist. The role of the pure oxide vs. oxynitride matrix on the properties of Si quantum dots is discussed in the context of potential applications in photovoltaics and optoelectronics.

[1] M. Zacharias et al., APL 80, 2002

[2] J. Laube et al., JAP 116, 2014

[3] A.M. Hartel et al., TSF 520, 2011

[4] S. Gutsch et al., JAP 113, 2013

DS 26.13 Wed 18:15 H 2032

**Comparison of Al<sub>2</sub>O<sub>3</sub> passivation layers by RF magnetron sputtering and ALD deposition** — ●FRANZ P. G. FENGLER<sup>1</sup>, DANIEL K. SIMON<sup>1</sup>, PAUL M. JORDAN<sup>1</sup>, THOMAS MIKOLAJICK<sup>1,2</sup>, and INGO DIRNSTORFER<sup>1</sup> — <sup>1</sup>NaMLab gGmbH, 01187 Dresden, Germany — <sup>2</sup>Lehrstuhl für Nanoelektronische Materialien, TU Dresden, 01187 Dresden, Germany

Decreasing wafer thicknesses of latest high efficient solar cells cause an increasing demand for superior surface passivations. Due to a high content of negative fixed charges Al<sub>2</sub>O<sub>3</sub> became the material of choice for p-type silicon. Today it is mainly deposited by atomic layer deposition

(ALD) and plasma enhanced chemical vapour deposition. Both processes are rather slow and require toxic gases e.g. Trimethylaluminum. An alternative is the physical vapor deposition (PVD) by means of magnetron sputtering. However, silicon passivated with PVD-films typically do not achieve lifetimes in the millisecond range. This study will investigate the reasons for the low performance by using structural, lifetime and capacitance-voltage measurements to analyze the difference of PVD- and ALD-layers. It will be shown that the content of oxygen and the distribution of hydrogen in the as-grown layers are crucial for the passivation performance. ALD and PVD layers significantly differ in density, which influences the hydrogen transport within the layer during the post deposition anneal. As a consequence, a PVD process with a low percentage of oxygen is needed in combination with an anneal in hydrogen containing atmosphere.

DS 26.14 Wed 18:30 H 2032

**Real-time monitoring of crystals \*breathing\* upon humidity guest loading** — ●THEODOROS BAIMPOS, BUDDHA RATNA SHRESTHA, and MARKUS VALTNER — Department for Interface Chemistry and Surface Engineering, Max Planck Institut für Eisenforschung GmbH, D-40237, Dusseldorf, Germany

Porous Metal-organic frameworks (MOFs) are 3D crystalline coordination polymers consisting of metal ions linked each other by organic ligands. One of their main applications is as membranes for gas mixtures separation/purification where the MOF crystal act as internal molecular sieve by permitting only in the smaller molecules to pass their pore and get adsorbed in the available adsorption sites, excluding the bigger ones. If the adsorption affects the size of the crystal (expansion or shrinkage) then the performance of the membrane is significantly affected. In this study we examine with with Surface Force Apparatus (SFA) and its high time resolution (500 msec) the effect of humidity adsorption on the size of HKUST-1 crystals. With SFA, even complicated series of swelling phenomena may be visible, real time, even with naked eye, monitored and recorded on a TV screen by watching the motion of the fringes of equal chromatic order (FECO). In particular for the case of HKUST-1 and the loading/unloading with humidity vapors, a complex deformation behavior (contraction-expansion-contraction-expansion) is noticed for first time, upon humidity loading which is attributed to the gradual filling of the 4 different kinds of adsorption sites found in the unit cell of the crystal.

DS 26.15 Wed 18:45 H 2032

**Damping of metallized bilayer nanomechanical resonators at room temperature** — ●MAXIMILIAN SEITNER, KATRIN GAJO, and EVA WEIG — Universität Konstanz, Fachbereich Physik, Konstanz, Germany

Nanoelectromechanical systems (NEMS) enable both the study of fundamental physical effects and future applications as integrated devices in ultra sensitive sensor technology. As an important representative, freely suspended nanomechanical string resonators are exploited for their remarkable mechanical properties, providing high quality factors even at room temperature. Hybrid nanostructures frequently rely on metallization films, providing functionalization for coupling mechanical resonators to other degrees of freedom. For those purposes, it is inevitable to acquire a deeper understanding of the metal's impact on the damping of the system as well as its influence on elastic parameters, especially at room temperature. We investigate the influence of gold thin-films subsequently deposited on a set of initially bare, doubly clamped, high-stress silicon nitride string resonators at room temperature. Providing analytical expressions for resonance frequency, quality factor and damping for both in- and out-of-plane flexural modes of the bilayer system we find the inverse quality factor to scale linearly with the gold film thickness, indicating that the overall damping is governed by losses in the metal. We extract mechanical quality factors of the gold film for both flexural modes and show that they can be enhanced by complete deposition of the metal in a single step, suggesting that surface and interface losses play a vital role in metal thin-films.

## DS 27: Micro- and Nanopatterning

Time: Wednesday 15:00–16:15

Location: H 0111

DS 27.1 Wed 15:00 H 0111

**Reactive sputter deposition of vertically oriented metal nitride nanopillar arrays** — ●THILO RICHTER and ZOE H. BARBER — University of Cambridge, Cambridge, United Kingdom

We have developed a method for fabricating porous, nano-columnar metal nitride thin film structures. Reactive DC magnetron sputtering from elemental targets is used with parameters which promote the formation of inter-grain voids by minimising the energy of sputtered species. The resulting structures have a wide range of applications. Conductive titanium nitride films can be used as electrodes in batteries and fuel cells. Similar TiN nanopillar arrays have been heat treated to form titanium oxynitrides and ultimately semiconducting oxides. Photocatalytic pollutant degradation under visible light has been demonstrated as one possible application of such oxides. Furthermore, electrochemical deposition within the inter-grain voids can result in extremely anisotropic structures.

DS 27.2 Wed 15:15 H 0111

**Pattern Guided Assembly and Inversion of Synthetic Opals** — ●MARTIN WALECZEK<sup>1</sup>, JEFFERSON JEAN DO ROSARIO<sup>2</sup>, JOSEP M. MONTERO MORENO<sup>1</sup>, ROBERT ZIEROLD<sup>1</sup>, SLAWA LANG<sup>3</sup>, ALEXANDER PETROV<sup>3</sup>, MANFRED EICH<sup>3</sup>, GEROLD SCHNEIDER<sup>2</sup>, and KORNELIUS NIELSCH<sup>1</sup> — <sup>1</sup>Institute of Nanostructure and Solid State Physics, Universität Hamburg, Hamburg, Germany — <sup>2</sup>Institute of Advanced Ceramics, Hamburg University of Technology, Hamburg, Germany — <sup>3</sup>Institute of Optical and Electronic Materials, Hamburg University of Technology, Hamburg, Germany

The influence of a patterned template on the crystallization of an opal structure fabricated by means of vertical convective self assembly is studied. Lines, cubic arrangements as well as hexagonal structures with periodicities in the range of 300 - 900 nm are chosen as patterns and introduced by one-step or two-step UV laser interference lithography on top of a simple glass substrate. The synthetic opals are fabricated by vertical convective self-assembly on these defined patterns. After infiltration of the structure with a ceramic layer by Atomic Layer Deposition (ALD), the spheres are removed and the remaining inverse opal structure can be optically characterized.

We utilized FFT of Scanning Electron Micrographs to determine the resulting structure and quantify the degree of order depending on various deposition parameters. In this presentation, the influence of variations of the pattern periodicity on the crystallization of opal structures is highlighted and the results are related to optical measurements on the respective inverted opal structures.

DS 27.3 Wed 15:30 H 0111

**Natural Curvature Induced Folding of an Elastic Film** — ●OCTAVIO ALBARRAN, ELENI KATIFORI, and LUCAS GOEHRING — Max Planck institute for dynamics and Self-Organization, Göttingen 37077, Germany

The wrinkling and folding transitions of elastic films have been extensively studied in the last decade. The exchange of energy from stretching to bending acts as a paradigm for a wide range of elastic instabilities, including the wrinkling of the gut, and the crinkling of

leaves. In two dimensions this type of problem is typically considered by the model of an elastica in compressive confinement. We show that, even without any external forces, an elastic surface supported by a fluid can bend and wrinkle when it acquires a non-zero natural curvature. Locally, we will demonstrate how a preferential curvature can be related to an effective compression, and hence a confining force that can vary spatially. This suggests a simple experimental setup, where we have characterised a variety of wrinkle patterns that can be generated for different mechanical properties and natural curvatures.

DS 27.4 Wed 15:45 H 0111

**Alternate Multi-Polymer Nano Droplet Array on Topographically Structured Surfaces** — NANDINI BHANDARU, ANUJA DAS, NAMRATA SALUNKE, and ●RABIBRATA MUKHERJEE — Indian Institute of Technology Kharagpur, Kharagpur, India

Submicron scale surface morphologies comprising of ordered multi-material domains find various applications in fabrication of multifunctional coatings, development of exotic metamaterials, high resolution microscopy etc., but these structures are still scientifically more challenging to fabricate. We have developed a novel method for creating alternate equi-sized binary polymer nano domains using sequential spin dewetting of polymethylmethacrylate (PMMA) and polystyrene (PS) solutions on topographically patterned substrates. Polymer solutions with concentrations as low as 0.1% (w/v) when spin coated over a non wettable substrate undergoes in-situ de-wetting during the coating process itself, by a phenomenon also known as Spin De-wetting. This phenomena, along with intermediate substrate silanization with octadecyl-trichloro-silane (OTS) results in a multi material droplet array. The formation takes place for range of solution concentration of both polymers and on a variety of substrate geometry leading to creation of a multifunctional surface.

DS 27.5 Wed 16:00 H 0111

**Phase Segregated Domains of Polymer Blend Thin Films: Effect of Molecular Weight, Surface Energy and Topographic Confinement** — ●NANDINI BHANDARU and RABIBRATA MUKHERJEE — Indian Institute of Technology Kharagpur, Kharagpur, India

The phenomenon of spontaneous phase segregation of an immiscible polymer blend system is a major area of research as these surfaces can be potentially leveraged in a wide variety of applications like as templates in tissue engineering, organic solar cells, etc. Spin cast films of these blends show a variety of random structures depending on the composition of the two polymers, the film thickness as well as the nature of the substrate. In this work, poly(styrene) (PS)-poly(methylmethacrylate) (PMMA) blend thin films of various concentrations and compositions were spin coated on flat as well as on different topographically patterned substrates and the phase segregated morphology all the cases are compared. Multiple parameters including the molecular weight of the polymers, the surface energy of flat and patterned substrates and nature of the topographic confinement were varied to obtain highly ordered multi-material nano structures. Also, the presence of patterns result in a certain reduction in the domain size for each of polymer component.

## DS 28: Multiferroics II (joint session with DF)

Time: Wednesday 15:00–18:50

Location: EB 107

## Invited Talk

DS 28.1 Wed 15:00 EB 107

**Low energy consumption spintronics using multiferroic heterostructures** — ●MORGAN TRASSIN — ETH Zurich, Zurich, Switzerland

Magnetization reversal in spintronics applications requires either an externally applied magnetic field or a large current density, which is accompanied by significant energy dissipation. A reversal of magnetization induced only by the application of an electric field would lead to low-power devices. Using multiferroics, previous approaches have seen limited success by only achieving rotations of the magnetization or a change in anisotropy by applying an electric field. To pave the way to new low-power devices, the more desirable electric-field driven magnetization reversal must be achieved and read out with a small current. In multiferroic heterostructures, ferromagnetic domains can be moved and switched using different charge states, strain configurations or magnetoelectric coupling. Ferroelectric domain engineering using epitaxial strain is critical towards the achievement of deterministic switchings. A combination of scanning probe microscopy and optical second harmonic generation were used to characterize multiferroic thin films strain state. Using electron microscopy and transport based techniques, a room temperature magnetization reversal of a CoFe thin layer solely induced by the application of a few volts to the heterostructure will be described.

DS 28.2 Wed 15:30 EB 107

**Probing ferroic order in thin film heterostructures with optical second harmonic generation** — ●GABRIELE DE LUCA, MANFRED FIEBIG, and MORGAN TRASSIN — ETH Zurich, Switzerland

The evidence of the electric field control on the antiferromagnetic ordering in multiferroic bismuth ferrite ( $\text{BiFeO}_3$ ) [1] increased interest in low energy consumption logic and memory devices. However, to exploit such functionality for devices it is essential to attain deterministic control of ferromagnetism at the single domain scale. Therefore a ferromagnet/multiferroic heterostructure has been designed based on the combination of magnetoelectric coupling in  $\text{BiFeO}_3$  (BFO) and exchange coupling between magnetic materials thus offering a new pathway for the electrical control of magnetism [2,3]. Here we show that second harmonic generation (SHG), can detect the distribution of ferroelectric domains in BFO thin films non-invasively and unimpeded by transport properties. We use epitaxial strain for engineering different types of BFO domain patterns that are characterized by SHG, showing a unique relation between the domain distribution and the film symmetry. We then manipulate the BFO film by voltage poling and demonstrate the sensitivity of the SHG process to this manipulation. The concept applied to BFO is transferable to other multiferroics compounds thus indicating the general feasibility of SHG as a characterization technique for heterostructures in which buried ferroelectricity plays a key role in the emergence of magnetoelectric coupling. 1.Zhao et al., Nat. Mat. 5, 823 (2006) 2.Heron et al., Phys. Rev. Lett. 107, 217202 (2011) 3.Trassin et al., Phys. Rev. B 87, 134426 (2013)

DS 28.3 Wed 15:45 EB 107

**Investigation of the antiferromagnetic coupling at  $\text{SrRuO}_3$  /  $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$  interfaces** — ●SUJIT DAS<sup>1,2</sup>, DIANA RATA<sup>1</sup>, ANDREAS HERKLOTZ<sup>3</sup>, ER JIA GUO<sup>4</sup>, ROBERT ROTH<sup>1</sup>, and KATHRIN DÖRR<sup>1,2</sup> — <sup>1</sup>Institute for Physics, MLU Halle-Wittenberg, 06099 Halle, Germany — <sup>2</sup>IFW Dresden, Postfach 270116, 01171 Dresden, Germany — <sup>3</sup>Oak Ridge National Lab., Oak Ridge, 37830 TN, USA — <sup>4</sup>Affiliation: Institute for Physics, Johannes-Gutenberg University Mainz, 55128 Mainz, Germany

$\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3/\text{SrRuO}_3$  superlattices grown on piezoelectric substrates show large antiferromagnetic coupling of the two ferromagnetic components and a significant strain effect on interfacial coupling [1]. Here we present a systematic investigation of the antiferromagnetic interface coupling in bilayers of  $\text{SrRuO}_3$  (SRO) and  $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$  (LSMO), grown by pulsed laser deposition (PLD) on (100)- oriented  $\text{SrTiO}_3$  substrates. Epitaxial and coherent growth of the bilayers was confirmed by in-situ RHEED and ex-situ x-ray diffraction (XRD). Magnetic characterization was performed by SQUID magnetometry. We observed a strong dependence of the AFM coupling on the layer sequence and the thickness of the individual layers. The bilayers exhibit exchange bias, with the magnitude and sign of the exchange field

strongly dependent on cooling field. Results of this study and ongoing work will be discussed. [1] Sujit Das et al, arXiv:1411.0411

DS 28.4 Wed 16:00 EB 107

**Massive magnetoelectric modulation of the magnetic anisotropy in an epitaxial  $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3/\text{PMN-PT}$  heterostructure** — ●MARTIN WAHLER<sup>1</sup>, SUJIT DAS<sup>1</sup>, KATHRIN DÖRR<sup>1</sup>, and GEORG SCHMIDT<sup>1,2</sup> — <sup>1</sup>Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany — <sup>2</sup>Interdisziplinäres Zentrum für Materialwissenschaften, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany

We use ferromagnetic resonance (FMR) to investigate the strain induced change of the in-plane magnetic anisotropy of an epitaxial ferromagnetic oxide layer on a piezoelectric substrate. The samples consist of 20 nm thick  $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$  layers on two different substrates, namely  $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})_{0.72}\text{Ti}_{0.28}\text{O}_3$  (PMN-PT) (001) and (110) single crystals. The two substrates induce either isotropic or anisotropic in-plane strain, respectively. For  $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$  on (001) PMN-PT substrate, it has already been demonstrated by SQUID magnetometry that the Curie-temperature and saturation magnetization can be changed by applying an electric field normal to the sample plane [1]. Here we show that for the same substrate orientation there is a small but significant change in FMR resonance fields along the directions of the magnetic easy axes. For the (110) substrate, however, a massive shift of the resonance fields is observed, resulting in a change of the uniaxial anisotropy of more than 0.5 kOe for an applied electric field of  $12 \text{ kV cm}^{-1}$ . All measurements are carried out at a temperature of 120 K.

[1] C. Thiele et al., Phys. Rev. B, **75** 054408 (2007)

DS 28.5 Wed 16:15 EB 107

**Inverse TMR effect in multiferroic tunnel junctions studied from first principles** — ●VLADISLAV BORISOV<sup>1,2</sup>, SERGEY OSTANIN<sup>2</sup>, and INGRID MERTIG<sup>1,2</sup> — <sup>1</sup>Institute of Physics, Martin Luther University Halle-Wittenberg — <sup>2</sup>Max Planck Institute of Microstructure Physics

The spin-polarized electronic transport in multiferroic tunnel junctions (MTJ): Co/PTO/Co and LSMO/PTO/Co was computed from first principles. We confirm that the so-called four-state tunnelling magnetoresistance (TMR) may be detected for each MTJ when its TMR and TER are controlled by the reversible barrier polarization as well as reversible magnetization of the leads. The *ab initio* based results are directly compared to the experimental features of the inverse TMR recently reported for LSMO/PZT/Co [1]. We show how the observed effect originates from the magnetoelectric coupling seen at both interfaces of the MTJ [2]. The role of half-metallic LSMO as well as the effect of Zr substitutes in PTO are analysed in the context of the inversion of the TMR signal [1]. Another important issue of TMR discussed here concerns the functional (insulating) barrier thickness, which is always less than the nominal thickness and which depends on the polarization direction. We found that the functional barrier thickness is systematically reduced when the polarization is directed toward the Co electrode due to charge transfer at the Co/PTO interface.

[1] D. Pantel et al., Nat. Mater. **11**, 289 (2012).[2] V. S. Borisov et al., Phys. Rev. B **89**, 054436 (2014).

DS 28.6 Wed 16:30 EB 107

**Origin of superstructures in (double) perovskite thin films** — ●VIKAS SHABADI, MARTON MAJOR, PHILIPP KOMISSINSKIY, ALDIN RADETINAC, MEHRAN VAFAEE, WOLFGANG DONNER, and LAMBERT ALFF — Institute of Materials Science, Technische Universität Darmstadt, Alarich-Weiss-Strasse 2, 64287 Darmstadt, Germany

We have investigated the origin of superstructure peaks as observed by X-ray diffraction of multiferroic  $\text{Bi}(\text{Fe}_{0.5}\text{Cr}_{0.5})\text{O}_3$  thin films grown by pulsed laser deposition on single crystal  $\text{SrTiO}_3$  substrates. The photon energy dependence of the contrast between the atomic scattering factors of Fe and Cr is used to rule out a chemically ordered double perovskite  $\text{Bi}_2\text{FeCrO}_6$  (BFCO). Structural calculations suggest that the experimentally observed superstructure occurs due to unequal cation displacements along the pseudo-cubic [111] direction that mimic the unit cell of the chemically ordered compound [1]. This result helps to clarify discrepancies in the correlations of structural and magnetic

order reported for  $\text{Bi}_2\text{FeCrO}_6$ . The observation of a superstructure in itself is not a sufficient proof of chemical order in double perovskites. [1] V. Shabadi, M. Major, P. Komissinskiy, M. Vafae, A. Radetinac, M. Baghaie Yazdi, W. Donner, and L. Alf, *J. Appl. Phys.* **116**, 114901 (2014).

DS 28.7 Wed 16:45 EB 107

**Using multiferroic systems as a spin filter - an ab initio study** — ●STEPHAN BOREK<sup>1</sup>, JÜRGEN BRAUN<sup>1</sup>, HUBERT EBERT<sup>1</sup>, ANGELIKA CHASSÉ<sup>2</sup>, GERD SCHÖNHENSE<sup>3</sup>, HANS-JOACHIM ELMERS<sup>3</sup>, DMYTRO KUTNYAKHOV<sup>3</sup>, and JÁN MINÁR<sup>1,4</sup> — <sup>1</sup>Ludwig-Maximilians-Universität München — <sup>2</sup>Martin-Luther-Universität Halle-Wittenberg — <sup>3</sup>Johannes-Gutenberg-Universität Mainz — <sup>4</sup>University of West Bohemia, Pilsen

Multiferroic heterostructures such as ultrathin  $\text{Fe}/\text{BaTiO}_3(001)$  films are of high interest for technical applications giving the opportunity to control the ferromagnetic state with an electric field or vice versa. In our theoretical study we investigated the effect of changing the electric polarization of the ferroelectric substrate  $\text{BaTiO}_3$  on the ferromagnetic state of Fe and Co thin films using the method of Spin Polarized Low Energy Electron Diffraction (SPLEED). This method has been shown to be an effective tool for the investigation of surface properties like the determination of surface magnetic moments and the local crystal structure. The possibility of an application of the multiferroic heterostructures  $\text{Fe}/\text{BTO}(001)$  and  $\text{Co}/\text{BTO}(001)$  as a spin filter is discussed. It will be shown that a change of the polarisation of the  $\text{BaTiO}_3$  results in a significant change of the exchange asymmetry giving the possibility to control the diffraction of electrons using the exchange interaction at the Fe (Co) surface. We focus on the systems of 1 ML, 2 ML and 3 ML Fe (Co) on  $\text{BaTiO}_3$  because their electronic and magnetic structure as well as the coupling mechanism between the ferroic phases have been intensively discussed in the literature.

## 20 min coffee break

DS 28.8 Wed 17:20 EB 107

**Optical investigation of ferroic domains beyond the resolution limit** — ●CHRISTOPH WETLI, VIKTOR WEGMAYR, THOMAS LOTTERMOSER, and MANFRED FIEBIG — Department of Materials, ETH Zurich, Zurich, Switzerland

In recent years optical second harmonic generation (SHG) has been shown to be a versatile, non-destructive tool to investigate the often complex domain structures of ferroic and multiferroic materials. Ferroic domains vary broadly in structure and size, depending on the nature of the ferroic ordering. So far, however SHG was restricted to domains larger than the optical resolution limit of  $1 \mu\text{m}$ . Here we present a method by applying a numerical model and simulation to overcome this limitation and to analyze ferroic domain structures some orders of magnitude smaller than the optical resolution limit. The method is based on the relation between the orientation of the ferroic order parameter and the phase of the nonlinear optical signal. It gives a relation between domain size and density, optical resolution and the intensity of the SHG signal. To show the reliability of the model, we applied it to several simulated domain structures. The simulation of the domain structures is based on an iterative geometrical algorithm, which allows us to generate complex domain patterns like the ferroelectric vortex structures or the irregular bubble like antiferromagnetic domains in hexagonal  $\text{YMnO}_3$ . The numerical calculations were compared with experimental data and found to be in excellent agreement.

DS 28.9 Wed 17:35 EB 107

**Multiferroicity in  $\text{DyMnO}_3$  thin films** — ●CHENGLIANG LU<sup>1,2</sup>, HAKAN DENIZ<sup>2</sup>, and JUN-MING LIU<sup>3</sup> — <sup>1</sup>School of Physics, Huazhong University of Science and Technology, Wuhan 430074, China — <sup>2</sup>Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle(Saale), Germany — <sup>3</sup>Laboratory of Solid State Microstructures, Nanjing University, Nanjing 210093, China

The mutual control of ferroelectricity and magnetism is stepping towards practical applications proposed for quite a few promising devices in which multiferroic thin films are involved. Although ferroelectricity stemming from specific spiral spin ordering has been reported in highly distorted bulk perovskite manganites, the existence of magnetically induced ferroelectricity in the corresponding thin films remains an unresolved issue, which unfortunately halts this step. Here we report magnetically induced electric polarization and its gigantic response to

magnetic field (an enhancement of 800% upon a field of 2 Tesla at 2 K) in  $\text{DyMnO}_3$  thin films grown on  $\text{Nb-SrTiO}_3$  substrates. Interestingly, we found a consecutive control of the polarization under a rotating magnetic field by detailed multiferroic response measurements. This is distinct to the standard polarization-flop process which results in a sudden change in polarization in multiferroics with spiral-spin-ordering state. The cooperative action of dual multiferroic mechanisms (the inverse Dzyaloshinskii-Moriya interaction among Mn moments and the exchange striction working between Dy and Mn moments) and phase coexistence associated with a twin-like structure was proposed as the origin of this phenomenon.

DS 28.10 Wed 17:50 EB 107

**Observation of direct and converse local magnetoelectric switching at room-temperature in modified single-phase bismuth ferrite** — ●LEONARD FREDERIC HENRICH<sup>1</sup>, OSCAR CESPEDÉS<sup>1</sup>, JAMES BENNETT<sup>1</sup>, JOACHIM LANDERS<sup>2</sup>, WOLFGANG KLEEMANN<sup>2</sup>, HEIKO WENDE<sup>2</sup>, DORU LUPASCU<sup>2</sup>, and ANDREW BELL<sup>1</sup> — <sup>1</sup>University of Leeds, Leeds, GB — <sup>2</sup>Universität Duisburg/Essen, Duisburg/Essen, Germany

Multiferroics are promising for applications in sensors and memory. However, no single-phase material with both ferroelectric and ferro- or ferrimagnetic order at room-temperature has been reported to date. Here, we observe very large local magnetoelectric coupling in the novel single-phase multiferroic  $(\text{BiFeCo}_{0.1}\text{O}_3)_{0.4}(\text{K}_{1/2}\text{Bi}_{1/2}\text{TiO}_3)_{0.6}$  at room-temperature. On ceramic samples, both direct and converse magnetoelectric switching was observed using piezoresponse force-microscopy and magnetic force-microscopy respectively. Areas where converse switching occurred, incorporate both a ferroelectric and magnetic domain-like cluster and thus appear to be (relaxor) ferroelectric and ferrimagnetic at room-temperature. The direct coupling-coefficient estimated from the experiments is  $1.0 \times 10^{-5} \text{ s/m}$ , and thus extremely large. The locally observed converse magnetoelectric effect has a similar of magnitude. We propose that the material can be interpreted as a pseudo-nanocomposite with an ideal strain-mediated coupling due to congruent polar and magnetic nanoregions which are related to the relaxor ferroelectric and superparamagnetic nature of the material.

DS 28.11 Wed 18:05 EB 107

**Tiny cause with large effects: the origin of the large magnetoelectric and magnetoelastic effect in  $\text{EuTiO}_3$**  — ●ANNETTE BUSSMANN-HOLDER — MPI-FKF, Heisenbergstr. 1, D-70569 Stuttgart, Germany

The magnetoelectric coupling in the perovskite  $\text{EuTiO}_3$  is analyzed within a spin-phonon coupled Hamiltonian. It is shown that the tiny magnetostriction which accompanies the onset of antiferromagnetic order at  $T_N = 5.7 \text{ K}$  induces a substantial hardening in the soft optic mode and a drop in the dielectric constant. The reduction of magnetostriction with increasing magnetic field reverses this behavior. While for small fields ferromagnetic order rapidly sets in accompanied by a volume expansion, this is destroyed with increasing fields and a strange paramagnetic state obtained. This exotic observation can be understood as stemming from the interplay between the enhanced oxygen  $p$  Ti  $d$  dynamical covalency which alters the crystal field at the Eu site and inhibits the virtual transition from  $4f7$  to  $4f65d$  responsible for ferromagnetic order.

DS 28.12 Wed 18:20 EB 107

**First principles calculations on the effect of inner cationic site disorder, single and multiple cation and anion doping on the magnetic properties of  $\text{GaFeO}_3$**  — ●JACQUELINE ATANELOV, WERNFRIED MAYR-SCHMÖLZER, and PETER MOHN — Institute of Applied Physics - Computational Materials Science, Vienna University of Technology, Austria

$\text{GaFeO}_3$  is a promising multiferroic suitable for a wide range of applications in electronic devices. Motivated by that we investigate the influence of single and multiple cation and anion doping on the electronic and magnetic properties of gallium ferrite. Further we consider the well known fact of inner cation site disorder in  $\text{GaFeO}_3$ . In terms of cation doping we replace Ga atoms by Fe atoms and vice versa so that in total a concentration range of  $0.9 \leq x \leq 2.0$  in  $\text{Ga}_{2-x}\text{Fe}_x\text{O}_3$  is investigated. In addition to that we substitute oxygen by B, C, N and S atoms. GFO is also known to show magnetic anisotropy for different crystallographic directions and sublattices. Beside changes in the total net magnetic moment induced by cation and anion doping, the magnetic anisotropy energy (MAE) can be affected as well. Doping

therefore can lead to an enhancement or reduction of the MAE. First principles density functional theory (DFT) calculations performed by the Vienna ab Initio Simulation Package (VASP) are used to predict and analyze the ground state electronic structure of the investigated systems.

DS 28.13 Wed 18:35 EB 107

**Mechanism of interfacial magnetoelectric coupling in composite multiferroics** — CHENGLONG JIA<sup>1</sup>, TONGLI WEI<sup>1</sup>, CHANGJUN JIANG<sup>1</sup>, DESHENG XUE<sup>1</sup>, ●ALEXANDER SUKHOV<sup>2</sup>, and JAMAL BERAKDAR<sup>2</sup> — <sup>1</sup>Key Laboratory for Magnetism and Magnetic Materials of MOE, Lanzhou University, Lanzhou 730000, China — <sup>2</sup>Institut für Physik, Martin-Luther-Universität, Halle-Wittenberg, 06099 Halle (Saale), Germany

We present a mechanism for the magnetoelectric coupling at ferroelectric/ferromagnetic interfaces based on screening via interfacial

spin-rearrangement [1]. We find an electric-polarization-driven, non-collinear spin region extending over the spin-diffusion length in the ferromagnet. The orbital motion of the carriers in the ferromagnet is affected by the gauge field associated with the non-collinear spin order and hence indirectly by the electric polarization. Changing the latter, e.g., via an electric field influences the interfacial magnetic order and hence the spin-orbital coupled motion of the carriers. This allows for tuning the interfacial spin-dependent transport via electric fields. The resulting coupling is robust at room temperature and can be well approximated by a linear polarization- magnetization coupling, whose strength estimate for the composite Co(40 nm)/(tetragonal)BaTiO<sub>3</sub> is in line with recent experiments [2].

[1] C.-L. Jia, T.-L. Wei, C.-J. Jiang, D.-S. Xue, A. Sukhov, J. Berakdar, Phys. Rev. B **90**, 054423 (2014). [2] N. Jedrecy, H.J. von Bardeleben, V. Badjcek, D. Demaille, D. Stanescu, H. Magnan, A. Barbier, Phys. Rev. B **88**, 121409(R) (2013).

## DS 29: Oxide and insulator surface: Structure, epitaxy and growth (joint session with O)

Time: Wednesday 15:00–18:15

Location: MA 042

DS 29.1 Wed 15:00 MA 042

**Surface phonons of BaTiO<sub>3</sub>(001) and BaTiO<sub>3</sub> ultrathin films on Pt(001) and Au(001)** — ●FLORIAN SCHUMANN<sup>1</sup>, KLAUS MEINEL<sup>1</sup>, ANDREAS TRÜTZSCHLER<sup>1</sup>, and WOLF WIDDRA<sup>1,2</sup> — <sup>1</sup>Institute of Physics, Martin-Luther-Universität Halle-Wittenberg — <sup>2</sup>Max-Planck- Institut für Mikrostrukturphysik, Halle

Phonons and their softening are key elements for the understanding of the long-range coupling in ferroelectric and multiferroic materials, which causes, e.g., the paraelectric to ferroelectric phase transition. In thin films, these ferroelectric properties are often controlled by strain from the underlying substrate or heterostructures. Here we study the surface phonons of BaTiO<sub>3</sub>(001) ultrathin films in comparison with a BaTiO<sub>3</sub> single-crystal with high-resolution electron energy loss spectroscopy (HREELS). For all BaTiO<sub>3</sub> structures, three well-developed phonon peaks at about 210, 460, and 670 cm<sup>-1</sup> dominate the HREELS spectra. Calculations of the energy loss spectra within a semi-classical approach identify the three phonons as the A(TO) surface phonon-polaritons (Fuchs-Kliewer modes) of BaTiO<sub>3</sub>(001). In comparison to the single crystal, the surface phonons of the thin films on Pt(001) and on Au(001) are shifted due to the lattice misfit of +2% and -2%, respectively. Furthermore, the surface phonons show a thickness dependent red shift in the thin films. Calculations identify this shift as phonon-polariton coupling to the metallic substrate.

DS 29.2 Wed 15:15 MA 042

**Preparation of Bi<sub>2</sub>Se<sub>3</sub>(0001) surface studied by scanning tunneling microscopy** — ●VASILII SEVRIUK, ALBERTO CAVALLIN, SAFIA OUAZI, DIRK SANDER, and JÜRGEN KIRSCHNER — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

Despite the fact that the Bi<sub>2</sub>Se<sub>3</sub>(0001) surface is relatively inert [1], carbon is a common surface contaminant. It is detected by Auger electron spectroscopy (AES) and in scanning tunneling microscopy (STM) it appears as protrusions. Here we report the preparation of Bi<sub>2</sub>Se<sub>3</sub>(0001) by Ar sputtering and annealing and by in vacuo cleavage. We find by STM that sputtering and annealing cycles lead to surface and sub-surface defects, which can be ascribed to Se vacancies [2] and Bi interstitials [3]. After several cycles of sputtering and annealing, a periodic spatial modulation on the length scale of 10–15 nm is observed in STM constant current maps, which we ascribe to a dislocation network [4]. Samples prepared by cleavage do not show this spatial modulation.

[1] V. A. Golyashov, K. A. Kokh, S. V. Makarenko, K. N. Romanyuk, I. P. Prosvirin et al. J. Appl. Phys. **112**, 113702 (2012).

[2] Y. S. Hor, A. Richardella, P. Roushan, Y. Xia, J. G. Checkelsky, A. Yazdani, M. Z. Hasan, N. P. Ong and R. J. Cava. Phys. Rev. B **79**, 195208 (2009).

[3] S. Urazhdin, D. Bilc, S. H. Tessmer, S. D. Mahanti, Theodora Kyratsi, and M. G. Kanatzidis, Phys. Rev. B **66**, 161306(R) (2002).

[4] M. Schmid, A. Biedermann, H. Stadler, and P. Varga. Phys. Rev. Lett. **69**, 925 (1992).

DS 29.3 Wed 15:30 MA 042

**Growth of cuprous oxide on Au(111) and Mo(001) - Role**

**of the support** — ●HANNA FEDDERWITZ, BORIS GROSS, HENDRIK STRÄTER, and NIKLAS NILIUS — Carl-von-Ossietzky Universität Oldenburg, Carl-von-Ossietzky-Str. 9 - 11, 26129 Oldenburg

Physical vapor deposition of Cu in an oxygen ambience is used to prepare Cu<sub>2</sub>O films on two single crystalline supports of different reactivity and lattice symmetry. While on Au(111), the oxide grows in a layer by layer fashion and develops atomically flat films, formation of nanoparticles is observed on a Mo(001) surface. The size and shape of the crystallites can be controlled by varying the temperature and O<sub>2</sub> partial pressure during oxide growth. Insight into the atomic configuration of the Cu<sub>2</sub>O facets is obtained from low-temperature STM measurements. Whereas Au-supported films expose the ideal (111) termination of cuprous oxide, modified only by a network of dislocation lines, a variety of low-index planes is discernable for deposits on the Mo support. The underlying growth mechanism is analyzed with the Wulff theory for nanoparticles in thermodynamic equilibrium. We discuss consequences of the different growth schemes on the two supports for possible applications of our cuprous-oxide samples in photocatalysis and photovoltaics.

DS 29.4 Wed 15:45 MA 042

**Atomic structure and electronic properties of Cu<sub>2</sub>O(111) films** — ●BORIS GROSS, HANNA FEDDERWITZ, HENDRIK STRÄTER, and NIKLAS NILIUS — Carl-von-Ossietzky Universität Oldenburg, Carl-von-Ossietzky Str. 9-11, 26129 Oldenburg

Atomically flat films of cuprous oxides were prepared by Cu deposition in oxygen onto an Au(111) surface, and analyzed by XPS, electron diffraction and STM. Depending on the preparation conditions, different surface reconstructions are obtained. Whereas the low-temperature structures have no analogy to respective bulk phases and are governed by interactions with the metal support, the high-temperature films have a similar atomic configuration as bulk-cut Cu<sub>2</sub>O(111). STM conductance spectroscopy reveals the pronounced 2.0 eV band gap of the oxide, in addition to an unoccupied surface state that occurs in the high-temperature phase. Field-emission resonances that govern the high-energy part of the STM spectra are used to monitor local variations in the work function of the system. Given their high crystallographic quality, our Cu<sub>2</sub>O films provide an ideal starting point to explore the defect landscape and optical properties for this reference material for photo-catalysis and photovoltaics.

DS 29.5 Wed 16:00 MA 042

**Growth of ultrathin Silica films on Ru(0001)** — ●HAGEN W. KLEMM, GINA PESCHEL, EWA MADEJ, ALEXANDER FUHRICH, MARTIN TIMM, THOMAS SCHMIDT, and HANS-JOACHIM FREUND — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Deutschland

The SiO<sub>2</sub> bilayer on Ru(0001) offers magnificent possibilities for understanding the transition from crystalline to vitreous phase[1], tuning of electronic structure, doping and catalysis[2]. In the thickness range of one to three monolayers we studied the growth of ultrathin Silica films by LEEM, LEED, XPS and XPEEM. We found that the oxidation temperature plays a crucial role for the quality of the resulting film, varying from incomplete oxidation to dewetting of the film. A

special focus of our investigation was the transition from crystalline to vitreous phase, as could be clearly seen in LEED. The influence of holes in the film and the morphology of the substrate will be discussed.

- [1] Lichtenstein, L. et. al., *Angew. Chem. Int. Ed.* 51, 404 (2012)  
 [2] Shaikhutdinov, S. et. al., *Chem. Phys. Chem.* 14, 71 (2013)

DS 29.6 Wed 16:15 MA 042

**Ultrathin Iron-Silicate films on Ru(0001)** — ●GINA PESCHEL, HAGEN KLEMM, THOMAS SCHMIDT, and HANS-JOACHIM FREUND — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Deutschland  
 Iron silicate can be seen as a model system for zeolites [1], which are important for catalysis and widely used in industry as desiccant, detergent or as molecular sieves. Of special interest is the relation between the specific structure and reactivity. In our case we studied the growth only of a one to two atomic layer thin film on a Ru(0001) support by LEEM, LEED, XPS and XPEEM measurements.

We found the formation of structural domains. The size of these domains increase with temperature and Fe/Si ratio. Furthermore, XPEEM measurements indicate that the domains contain iron and Silica, while in between the domains only Silica is found. The Si2p level shows a chemical shift between Silica bound to FeO and Silica on Ru(0001)only. Beside the (2x2) spots, typical for silica, LEED shows additional spots rotated by 30 ° and a Moiré structure. The unit cell of the new structure is about three percent larger than for ultra-thin silica films.

- [1] R. Włodarczyk, J. Sauer, X. Yu, J. Boscoboinik, B. Yang, S. Shaikhutdinov, H.-J. Freund, *J. Am. Chem. Soc.* 135 (2013), 19222-19228

DS 29.7 Wed 16:30 MA 042

**First-Principles Embedded Cluster Calculations of Surface Defects at TiO<sub>2</sub>(110)** — ●DANIEL BERGER, HARALD OBERHOFER, and KARSTEN REUTER — Technische Universität München

Bulk and surface defects critically determine many of the properties and functions that make TiO<sub>2</sub> such an interesting and widely studied material. Given this importance, it is both surprising and disconcerting to see how little is actually known especially about the surface defects of TiO<sub>2</sub>. For surface oxygen vacancies not even their thermodynamically favored charge state is unambiguously clear. We contribute to this context with first-principles embedded cluster calculations [1] of the rutile TiO<sub>2</sub>(110) surface. Our approach allows for a numerically particularly efficient application of hybrid density-functional theory inside the quantum mechanic (QM) cluster region. In the extended molecular mechanic (MM) embedding region specifically optimized interatomic potentials provide a quantitative account of the strong TiO<sub>2</sub> polarization response. We discuss the advantages of this QM/MM approach against more common periodic supercell calculations especially for charged O vacancies. Over a wide range of electrochemical potentials and oxygen partial pressures our calculations show the +2 state to be thermodynamically favored, which can be rationalized by the huge dielectric constant of TiO<sub>2</sub>.

- [1] D. Berger *et al.*, *J. Chem. Phys.* 141, 024105 (2014).

DS 29.8 Wed 16:45 MA 042

**Ordered Indium and Iron Adatoms on the Reduced In<sub>2</sub>O<sub>3</sub>(111) Surface** — ●MARGARETA WAGNER<sup>1</sup>, PETER LACKNER<sup>1</sup>, STEFFEN SEILER<sup>2</sup>, BERND MEYER<sup>2</sup>, LYNN A. BOATNER<sup>3</sup>, MICHAEL SCHMID<sup>1</sup>, and ULRIKE DIEBOLD<sup>1</sup> — <sup>1</sup>Institut für Angewandte Physik, Technische Universität Wien, Wiedner Hauptstrasse 8-10/134, 1040 Wien, Österreich — <sup>2</sup>Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center Friedrich-Alexander-Universität Erlangen-Nürnberg, Nögelsbachstrasse 25, 91052 Erlangen, Deutschland — <sup>3</sup>Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA

Indium oxide is one of the most important TCOs and commonly used as a contact material in many devices. Recently, In<sub>2</sub>O<sub>3</sub> single crystals, prerequisite for fundamental surface studies, have become available.

The In<sub>2</sub>O<sub>3</sub>(111) surface can be transformed from a bulk-terminated surface to one that is covered by single indium adatoms. The transformation and the intermediate stages were followed with Scanning Tunneling Microscopy (STM) and Density Functional Theory (DFT). DFT supports the formation of a stable array made of indium adatoms, which is favored over vacancy formation at the given oxygen chemical potential during reduction. The formation of an ordered adatom array is different from any known response of an oxide surface to chemical reduction. Also iron atoms deposited on the oxidized surface arrange as single adatoms in the same (1x1) superstructure. The adatom-covered

and oxidized In<sub>2</sub>O<sub>3</sub>(111) surfaces are expected to exhibit very different chemical and electronic properties.

DS 29.9 Wed 17:00 MA 042

**Infra-red and Raman frequencies of Co<sub>3</sub>O<sub>4</sub> – an *ab initio* study** — ANDRII TITOV<sup>1</sup>, ●DOMINIK LEGUT<sup>2,3</sup>, and LUCIE OBALOVA<sup>3</sup> — <sup>1</sup>Nanotechnology Centre — <sup>2</sup>IT4Innovations Centre — <sup>3</sup>Inst. Env. Techn., VSB–TU Ostrava, Ostrava, Czech Republic

Among well known catalyst for N<sub>2</sub>O decomposition belongs Co<sub>3</sub>O<sub>4</sub>. Since this reaction has oxidation-reduction mechanism, the electronic properties of Co<sub>3</sub>O<sub>4</sub> represent important feature. We have calculated electronic structure and lattice dynamics, i.e. atomic vibrations using first-principles calculations. We determined Raman and infra-red frequencies of the phonon modes. Our results were calculated using single electron framework within the density functional theory. For the electronic exchange correlation the general gradient approximation as parametrized by Perdew–Burke–Ernzerhof [1] was used. To obtain the correct description of the insulating behaviour the Hubbard U technique was used. The anti-ferromagnetic ordering and spin-orbit interaction were also considered. Lattice vibrations were calculated using Phonopy package [2]. The dependences of the band gap, infra-red and Raman frequencies on the Coulomb interaction (Hubbard U) were revealed and compared with experimental data measured at the VSB-TU Ostrava. The work was supported by the Grant Agency of the Czech Republic, project reg. No. 14-13750S.

#### References:

1. J.P. Perdew, K. Burke, M. Ernzerhof, *Phys. Rev. Lett.* 77, 3865 (1996).  
 2. A. Togo, F. Oba, I. Tanaka, *Phys. Rev. B* 78, 134106 (2008).

DS 29.10 Wed 17:15 MA 042

**Surface energy, structure and stability of crystalline corundum surfaces** — ●LILIT AMIRKHANYAN, TORSTEN WEISSBACH, and JENS KORTUS — Institute of Theoretical Physics, TU Bergakademie Freiberg, Leipziger Str. 23, D-09599 Freiberg, Germany

Using first-principles density function theory as implemented in Quantum-ESPRESSO we examined the surface energy of the stable  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> corundum phase. Corundum is very important for applications due to its outstanding hardness, high melting point, high thermal conductivity and low dielectric constant.

The [001], [100], [110], [112], [114], [113] and [223] crystal planes of  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> were studied. The surfaces have been modeled using slabs with periodic boundary conditions. We investigated the impact of different termination and the effect of relaxation on surface properties. Further, we discuss possible relations of surface properties to structural elements like number of broken bonds or missing oxygen atoms to complete the coordination.

DS 29.11 Wed 17:30 MA 042

**Surface Adsorbates and Defects on the Subsurface Cation Vacancy Stabilized Surface of Magnetite (001)** — ●EAMON MCDERMOTT<sup>1</sup>, ROLAND BLIEM<sup>2</sup>, GARETH PARKINSON<sup>2</sup>, ULRIKE DIEBOLD<sup>2</sup>, and PETER BLAHA<sup>1</sup> — <sup>1</sup>Institute for Material Chemistry, TU Wien, Vienna, Austria — <sup>2</sup>Institute of Applied Physics, TU Wien, Vienna, Austria

Having proposed a new surface reconstruction for the magnetite (001) surface which is stabilized by a subsurface cation vacancy, we are now studying the extended properties of this reconstruction, including its preferred adsorption sites for various metals, the properties of oxygen vacancies at the structure and the adsorption of CO and OH groups. The surface structure has interesting chemistry, due to the presence of an oxygen site with a +1 oxidation state. In particular, we are interested in understanding our database of known magnetite surface defects as observed by STM. Progress on several ongoing investigations will be reported.

DS 29.12 Wed 17:45 MA 042

**The Structure of Magnetite(100)-c(2x2) revisited** — ●LUTZ HAMMER<sup>1</sup>, PASCAL FERSTL<sup>1</sup>, M.ALEXANDER SCHNEIDER<sup>1</sup>, ROLAND BLIEM<sup>2</sup>, ULRIKE DIEBOLD<sup>2</sup>, and GARETH PARKINSON<sup>2</sup> — <sup>1</sup>Solid State Physics, FAU Erlangen-Nürnberg — <sup>2</sup>Inst. Appl. Physics, TU Wien

The widely accepted "Distorted-Bulk-Truncation" model [1,2] for the c(2x2) surface reconstruction of Fe<sub>3</sub>O<sub>4</sub>(100) fails to explain recent STM results for the adsorption and nucleation behaviour of metal adatoms on this surface [3,4]. We have therefore revisited the surface structure by means of a full-dynamical LEED intensity analysis.

We tested in particular a new model of subsurface cation vacancies and interstitials [5], which was not yet considered in a former LEED analysis [2]. This new model led to a remarkably better correspondence between experimental and calculated spot intensities expressed by a Pendry R-factor of 0.125 (compared to 0.34 of ref.[2]). The new analysis is based on a very large experimental data base of 11300 eV allowing a safe determination of as much as 59 structural parameters. The atomic coordinates derived from the LEED analysis are in excellent agreement with predictions from DFT for this structure [5]. This study also proves that there are no inherent problems in the LEED I-V methodology to properly determine the structure of oxide surfaces as frequently claimed in literature.

[1] R. Pentcheva et al., PRL 94, 126101 (2005); [2] R. Pentcheva et al., Surf. Sci. 602, 1299 (2008); [3] Z. Novotny et al., PRL 108, 216103 (2013); [4] G.S. Parkinson et al., Nat. Mater. 12, 724 (2013); [5] R. Bliem et al. Science, accepted

DS 29.13 Wed 18:00 MA 042

**Surface structure of Fe<sub>3</sub>O<sub>4</sub> under varying conditions studied by surface x-ray diffraction** — ●BJÖRN ARNDT<sup>1,2</sup>, ROLAND BLIEM<sup>3</sup>, HESHMAT NOEI<sup>1</sup>, OSCAR GAMBA<sup>3</sup>, JESSICA VAN DER HOVEN<sup>3</sup>, GARETH PARKINSON<sup>3</sup>, and ANDREAS STIERLE<sup>1,2</sup> —

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Magnetite (Fe<sub>3</sub>O<sub>4</sub>) exhibits interesting material properties which makes it attractive for industrial applications as a catalyst for the water-gas shift reaction. Therefore, it is important to understand its surface structure under different conditions. The (001) surface of magnetite shows a ( $\sqrt{2} \times \sqrt{2}$ )R45° reconstruction in UHV which gets lifted at around 450°C as well as upon water adsorption at room temperature. To clarify the recent controversy about the atomic structure of the reconstruction and to get insight into it at different conditions, we performed a surface x-ray diffraction experiment on a natural Fe<sub>3</sub>O<sub>4</sub> (001) single-crystal. The experiment was carried out at the ESRF ID03 beamline using an UHV-ambient pressure flow reaction chamber at 11 keV photon energy. Our data support the recently proposed surface model<sup>1</sup> with overstoichiometric oxygen concentration. Upon heating and upon water adsorption, the surface reconstruction vanishes.

[1] R. Bliem et al., submitted

## DS 30: Topological insulators: Structure and electronic structure (HL with DS/MA/O/TT)

Time: Wednesday 15:00–16:30

Location: ER 270

DS 30.1 Wed 15:00 ER 270

**New electron states at the Bi/InAs(111) interface** — K HRICOVINI<sup>1,2</sup>, J-M MARIOT<sup>3</sup>, ●L NICOLAI<sup>1,2,7</sup>, U DJUKIC<sup>1</sup>, M C RICHTER<sup>1,2</sup>, O HECKMANN<sup>1,2</sup>, T BALASUBRAMANIAN<sup>4</sup>, M LEANDERSSON<sup>4</sup>, J SADOWSKI<sup>4</sup>, J DENLINGER<sup>5</sup>, I VOBORNIK<sup>6</sup>, J BRAUN<sup>7</sup>, H EBERT<sup>7</sup>, and J MINÁR<sup>7,8</sup> — <sup>1</sup>LPMS, UCP,Cergy, France — <sup>2</sup>DSM-IRAMIS, SPEC, CEA-Saclay, France — <sup>3</sup>LCP-MR, UPMC Univ. Paris 06/CNRS, France — <sup>4</sup>MAX-lab, Lund Univ., Sweden — <sup>5</sup>ALS, Berkeley, USA — <sup>6</sup>EST, Trieste, Italy — <sup>7</sup>LMU Munich, Germany — <sup>8</sup>Univ. of West Bohemia, Plzeň, Czech Republic

The Bi(111) surface is a prototype system to study Rashba-split surface states. Theoretical studies [1] predicted non-trivial topological surface states appearing on a single bi-layer of Bi(111) and a more complex behaviour was suggested for a variable film thickness as a function of layer thickness [2]. This clearly indicates that the electronic properties of thin films of this material are far from being understood. Here we present combined theoretical and ARPES studies of the electronic structure of Bi(111) films grown on InAs(111). Bi growth is epitaxial and a monocrystal of very high quality is obtained after depositing several monolayers. The ARPES experiments on these samples show several new types of electronic states. It is shown that a part of these new states corresponds to novel bulk-like features. These features are well reproduced by the one-step model of photoemission as implemented in the SPR-KKR package [3]. [1] M. Wada et al., Phys. Rev. B 83, 121310 (2011). [2] Z. Liu et al., Phys. Rev. Lett. 107, 136805 (2011). [3] H. Ebert, D. Ködderitzsch, J. Minár, Rep. Prog. Phys. 74, 096501 (2011).

DS 30.2 Wed 15:15 ER 270

**Ultrafast currents at the surface of the topological insulator Bi<sub>2</sub>Se<sub>3</sub>** — ●LUKAS BRAUN<sup>1</sup>, LUCA PERFETTI<sup>2</sup>, GREGOR MUSSLER<sup>3</sup>, MARKUS MÜNZENBERG<sup>4</sup>, MARTIN WOLF<sup>1</sup>, and TOBIAS KAMPFRATH<sup>1</sup> — <sup>1</sup>Fritz-Haber-Institut Berlin (MPG) — <sup>2</sup>Ecole Polytechnique Palaiseau — <sup>3</sup>Forschungszentrum Jülich — <sup>4</sup>Universität Greifswald

Optical excitation of topological insulators (TIs) can launch electron currents along the TI surface whose direction can be controlled by varying the polarization of the driving light [J. W. McIver *et al.*, Nat. Nanotech. 7, 96]. So far, photocurrents have been detected with a time resolution from DC to picoseconds [C. W. Luo *et al.*, Adv. Opt. Mat. 1, 804]. Since electrons moving through a solid typically undergo scattering on a 100fs time scale, it is highly desirable to generate and detect TI photocurrents with femtosecond time resolution in a contact-free manner. For this purpose, we excite n-doped Bi<sub>2</sub>Se<sub>3</sub> (Fermi energy at 300meV) crystals with a femtosecond laser pulse (10fs, 1.55eV). The resulting photocurrent gives rise to the emission of a broadband terahertz (THz) electromagnetic pulse (1 to 20THz) whose transient electric field is detected by means of electro-optic sampling. We present

a method that allows us to extract the transient current  $j(t)$  from the measured field  $E(t)$ . The AC photocurrents are found to be dominated by shift currents along the surface and photo-Dember injection currents into the bulk. We finally discuss the origin of  $j(t)$  and implications for the dynamics of photoexcited TI electrons.

DS 30.3 Wed 15:30 ER 270

**Observation of the photon drag effect in epitaxially grown (Bi<sub>1-x</sub>Sb<sub>x</sub>)<sub>2</sub>Te<sub>3</sub> based topological insulators** — ●H. PLANK<sup>1</sup>, L. E. GOLUB<sup>2</sup>, P. OLBRICH<sup>1</sup>, T. HERRMANN<sup>1</sup>, S. BAUER<sup>1</sup>, V. V. BEL'KOV<sup>2</sup>, G. MUSSLER<sup>3</sup>, J. KAMPMEIER<sup>3</sup>, D. GRÜTZMACHER<sup>3</sup>, and S. D. GANICHEV<sup>1</sup> — <sup>1</sup>University of Regensburg, Regensburg, Germany — <sup>2</sup>Ioffe Institute, St. Petersburg, Russia — <sup>3</sup>Jülich Aachen Research Alliance (JARA-FIT), Jülich, Germany

We report on the observation of a terahertz (THz) radiation induced photon drag effect in epitaxially grown (Bi<sub>1-x</sub>Sb<sub>x</sub>)<sub>2</sub>Te<sub>3</sub> three-dimensional topological insulators. We demonstrate that the excitation with polarized radiation results in a dc electric photocurrent. While at normal incidence a current arises due to the photogalvanic effect in the surface states, caused by asymmetrical scattering of Dirac fermions [1], at oblique incidence it is outweighed by the trigonal photon drag effect. The currents are generated in *n*- and *p*-type (Bi<sub>1-x</sub>Sb<sub>x</sub>)<sub>2</sub>Te<sub>3</sub> samples with various composition applying linearly and circularly polarized THz radiation. Results are analysed in terms of phenomenological theory and microscopic model based on transfer of photon momentum to free carriers resulting in an asymmetric distribution of electrons (holes) in *k*-space. Our analysis describes well all experimental findings including e.g. variation of the angle of incidence, radiation polarization and frequency. The observed trigonal photon drag and photogalvanic effect provide an opto-electronic method to study high frequency transport of Dirac fermions even at room temperature.

[1] P. Olbrich *et al.*, Phys. Rev. Lett. 113, 096601(2014)

DS 30.4 Wed 15:45 ER 270

**Cyclotron Resonance Induced Spin Polarized Photocurrents in Surface States of a 3D Topological Insulator** — ●K.-M. DANTSCHER<sup>1</sup>, D.A. KOZLOV<sup>2</sup>, Z.D. KVON<sup>2</sup>, P. FALTERMEIER<sup>1</sup>, M. LINDNER<sup>1</sup>, P. OLBRICH<sup>1</sup>, C. ZOTH<sup>1</sup>, G.V. BUDKIN<sup>3</sup>, S.A. TARASENKO<sup>3</sup>, V.V. BEL'KOV<sup>3</sup>, N.N. MIKHAILOV<sup>2</sup>, S.A. DVORETSKI<sup>2</sup>, D. WEISS<sup>1</sup>, and S.D. GANICHEV<sup>1</sup> — <sup>1</sup>University of Regensburg, Regensburg, Germany — <sup>2</sup>Institute of Semiconductor Physics, Novosibirsk, Russia — <sup>3</sup>Ioffe Institute, St. Petersburg, Russia

We report on the observation of cyclotron resonance (CR) induced photocurrents excited by cw radiation, with frequencies of 2.54, 1.62 and 0.69 THz in a 3D topological insulator based on 80 nm strained HgTe films. To support the complex study, including optical, opto-electronic and electron transport experiments, various sample designs

have been used. The measurements were done in a wide range of temperatures (1.6 to 120 K). We demonstrate that the photocurrent is generated in the topologically protected surface states. Studying the resonance response in the gated samples we examined the behaviour of the photocurrent and Dirac fermions cyclotron mass upon variation of Fermi energy. For large gate voltages we also detected CR in the bulk HgTe with the mass about two times larger than that obtained for the surface states. Based on this data we develop a microscopic theory of the effects and show that the asymmetry of light-matter coupling in the system of Dirac fermions subjected to an external magnetic field causes the electric current to flow. We show that the current is spin polarized.

DS 30.5 Wed 16:00 ER 270

**Response of the topological surface state to surface disorder in TlBiSe<sub>2</sub>** — FLORIAN PIELMEIER<sup>1</sup>, ●ANDREAS EICH<sup>2</sup>, GABRIEL LANDOLT<sup>3,4</sup>, BARTOSZ SLOMSKI<sup>3,4</sup>, JULIAN BERWANGER<sup>1</sup>, ALEXANDER A. KHAJETOORIAN<sup>5</sup>, JENS WIEBE<sup>2</sup>, ROLAND WIESENDANGER<sup>2</sup>, JÜRIG OSTERWALDER<sup>3</sup>, FRANZ J. GIESSIBL<sup>1</sup>, and J. HUGO DIL<sup>3,4,6</sup> — <sup>1</sup>Institute of Experimental and Applied Physics, Universität Regensburg, D-93040 Regensburg, Germany — <sup>2</sup>Department of Physics, University of Hamburg, Jungiusstrasse 11, D-20355 Hamburg, Germany — <sup>3</sup>Physik-Institut, Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland — <sup>4</sup>Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen, Switzerland — <sup>5</sup>Institute of Molecules and Materials, Radboud University, 6500 GL Nijmegen, Netherlands — <sup>6</sup>Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

By a combination of experimental techniques we show that the top-most layer of the topological insulator TlBiSe<sub>2</sub> as prepared by cleavage is formed by irregularly shaped TI islands. No trivial surface states are

observed in photoemission, which suggests that these islands can not be regarded as a clear surface termination. The topological surface state is, however, clearly resolved in photoemission experiments. This is interpreted as a direct evidence of its topological self-protection and shows the robust nature of the Dirac cone like surface state.

DS 30.6 Wed 16:15 ER 270

**Wet etch process for HgTe nanostructure fabrication** — ●KALLE BENDIAS<sup>1</sup>, ERWANN BOCQUILLON<sup>1</sup>, ALEX HUGHES<sup>2</sup>, CHRISTOPH BRÜNE<sup>1</sup>, HARTMUT BUHMANN<sup>1</sup>, and LAURENS W. MOLENKAMP<sup>1</sup> — <sup>1</sup>EP3, Physikalisches Institut, Universität Würzburg — <sup>2</sup>Department of Physics, Stanford University

Topological insulators (TI) are a new class of material with outstanding spin properties. Grown in 2d quantum wells HgTe does not only host Quantum Spin Hall edge channels [1][2], but also a giant Rashba splitting [3]. Both could lead to numerous applications in spintronic devices. In order to perform experiments such as spininjection, -probing [3] or quantum point contact collimation [4] a high carrier mobility and i.e. a long ballistic mean free path is essential.

The conventional processing method using ion milling to define the structure strongly affects these surface properties on small microstructures. In this talk the development and results of an alternative lithography etch method using KI:I:HBr as wet etchant are presented. Measurements on microstructures will be shown, indicating comparable mobilities on big and small structures.

[1] Markus König et al., Journal of the Physical Society of Japan 77.3 (2008), S. 031007.

[2] C. Brüne et al., Nature Physics 6.6 (2010), S. 448-454.

[3] J. Hinz et al., Semiconductor science and Technology 21.4 (2006), S 501-506.

[4] L.W. Molenkamp et al., Phys. Rev. B 41, 1274 (1990)

## DS 31: Topological insulators: Transport (HL with DS/MA/O/TT)

Time: Wednesday 11:45–13:00

Location: ER 270

DS 31.1 Wed 11:45 ER 270

**Surface Transport on a Bulk Topological Insulator** — ●FREDERIK EDLER<sup>1</sup>, LISA KÜHNEMUND<sup>1</sup>, MARCO BIANCHI<sup>2</sup>, ELLEN M.J. HEDEGAARD<sup>3</sup>, MARTIN BREMHOLM<sup>3</sup>, BO B. IVERSEN<sup>3</sup>, PHILIP HOFMANN<sup>2</sup>, and CHRISTOPH TEGENKAMP<sup>1</sup> — <sup>1</sup>Inst. f. Festkörperphysik, Uni. Hannover — <sup>2</sup>Dep. of Physics and Astronomy, Uni. Aarhus — <sup>3</sup>CMC, Dep. of Chemistry and iNANO, Uni. Aarhus

Topological insulators are guaranteed to support metallic surface states on an insulating bulk, and one should thus expect that the electronic transport in these materials is dominated by the surface states. Alas, due to the high remaining bulk conductivity, surface contributions to transport have mainly only been singled out indirectly via quantum oscillations, or for devices based on gated and doped topological insulator thin films, a situation in which the surface carrier mobility could be limited by defect and interface scattering. This issue was first overcome for Bi<sub>2</sub>Te<sub>2</sub>Se where compensation of defects leads to low bulk conductivity and surface-dominated transport could directly be observed [1]. Here we present a direct measurement of surface-dominated conduction on atomically clean surfaces of Bi<sub>2</sub>Te<sub>3</sub>. Using a four tip STM for nano-scale four point transport measurements with variable contact distance we show that the transport at 30 K is again two-dimensional rather than three-dimensional. The sheet conductivity is  $7.9(3) \times 10^{-4} \Omega^{-1}$  corresponding to a mobility of 505 cm<sup>2</sup>/Vs. Besides, results regarding the temperature dependence of the conductivity and the influence of structural defects, e.g steps, present after cleavage will be discussed. [1] Barreto et al., Nano Lett. 14, 3755 (2014)

DS 31.2 Wed 12:00 ER 270

**Aharonov-Bohm oscillations in quantum wire of topological insulator** — ●LOUIS VEYRAT<sup>1</sup>, JOSEPH DUFOULEUR<sup>1</sup>, ROMAIN GIRAUD<sup>1</sup>, EMMANOUIL XYPAKIS<sup>2</sup>, JENS BARDARSON<sup>2</sup>, CHRISTIAN NOWKA<sup>1</sup>, SILKE HAMPEL<sup>1</sup>, and BERND BÜCHNER<sup>1</sup> — <sup>1</sup>IFW-Dresden — <sup>2</sup>MPIPKS

Studying Aharonov-Bohm (AB) effect in a nanowire of topological insulator is a convenient way to reveal the specific properties of the topological surface states (SS), which are spin-chiral Dirac fermions. In the short perimeter limit, we evidenced in a previous work the ballistic

transport of the SS in the perimeter of the nanowire, revealed by the temperature dependance of the phase coherence length [1] and showing the weak scattering effect of disorder on Dirac fermions. The quantum transverse confinement of SS is further revealed by the observation of non-universal conductance fluctuations. In the longer perimeter limit, we surprisingly find that the transport remains ballistic in the perimeter, despite the presence of disorder. The interaction with disorder is revealed by specific phase-jump of the AB oscillations under transverse magnetic field.

[1] Dufouleur et al., Phys. Rev. Lett. 110, 186806 (2013)

DS 31.3 Wed 12:15 ER 270

**The effect of strain on the two-dimensional topological insulator HgTe** — ●PHILIPP LEUBNER, ANDREAS BUDEWITZ, CHRISTOPH BRÜNE, HARTMUT BUHMANN, and LAURENS MOLENKAMP — Experimentelle Physik III, Fakultät für Physik, Universität Würzburg, Germany

In the past years, HgTe quantum wells have been used extensively to study the magnetotransport signature of two-dimensional topological insulators, namely the quantum spin Hall effect. It has been shown that the band structure of those systems strongly depends on the thickness of the quantum well, and that, in particular, the topology changes from trivial to nontrivial at a critical thickness of 6.3 nm.

As an additional degree of freedom, the influence of strain on the band structure is investigated in this work. By using different CdTe-ZnTe superlattices grown on GaAs as virtual substrates, we are able to tune the strain of the HgTe quantum well layer from tensile to compressive, and thus modify the shape of the valence band.

Depending on strain, temperature dependent transport measurements on nominally identical wells reveal either features of topological insulators or semimetals, with the obtained fitting parameters nicely agreeing with band structure calculations. Further experiments focus on the correlation between the magnitude of the inverted bandgap and stability of the quantum spin Hall edge states.

DS 31.4 Wed 12:30 ER 270

**Transport measurements on Mn-doped HgTe quantum wells** — ●ANDREAS BUDEWITZ, KALLE BENDIAS, PHILIPP LEUBNER, CHRISTOPH BRÜNE, HARTMUT BUHMANN, and LAURENS W.

MOLENKAMP — Universität Würzburg, Lehrstuhl für experimentelle Physik III

In 2007 HgTe quantum wells have been experimentally identified as a quantum spin Hall system [1]. One open question is how quantum spin Hall states interplay with magnetic impurities. Especially the formation of the anomalous quantum Hall effect raises a lot of interest [2, 3]. Since Mn-doped HgTe is a paramagnetic topological insulator it is important to investigate the onset of the  $\nu = -1$  plateau at low fields. Here we present transport measurements on Mn-doped HgTe quantum wells. Therefore we show results on different temperatures, magnetic fields, Mn concentration and quantum well width. We discuss our results in comparison to undoped HgTe quantum wells.

[1] M. König, S. Wiedmann, C. Brüne, A. Roth, H. Buhmann, L. W. Molenkamp, X.-L. Qi and S.-C. Zhang, *Science* 318, 766 (2007)

[2] Chao-Xing Liu, Xiao-Lang Qi, Xi Dang, Zhong Fang and Shou-Cheng Zhang, *PRL* 101, 14682 (2008)

[3] Hsiu-Chang Hsu, Xin Liu and Chao-Xing Liu, *Phys. Rev. B* 88, 085315 (2013)

DS 31.5 Wed 12:45 ER 270

**Quantum hall states equilibration in lateral heterojunctions on inverted HgTe quantum wells** — ●M. REYES CALVO<sup>1,2</sup>, CHRISTOPH BRÜNE<sup>3</sup>, CHRISTOPHER AMES<sup>3</sup>, PHILIPP LEUBNER<sup>3</sup>, HARTMUT BUHMANN<sup>3</sup>, LAURENS W. MOLENKAMP<sup>3</sup>, and DAVID GOLDBERGER-GORDON<sup>1</sup> — <sup>1</sup>Department of Physics, Stanford University, Stanford, U.S.A. — <sup>2</sup>C.I.C. Nanogune, San Sebastián, Spain — <sup>3</sup>Physikalisches Institut (EP3), Universität Würzburg, Würzburg, Germany

We study lateral heterojunctions on HgTe quantum wells with inverted band structure. At high densities and fields, we can explore the equilibration between Quantum Hall (QH) states with different filling factor. The resulting resistance plateaus are particularly clear in the n-n'-n quadrant and fit the expected values for a 2D electron gas heterojunction. The low density and moderate magnetic field regime is of more interest, since due to the inverted band structure of HgTe, Quantum Spin Hall (QSH) edge states could be present. In this regime, we observe unexpected features in the Hall resistance, which could be associated with the interplay between chiral QH edge modes and helical QSH edge modes.

## DS 32: Spins in organics

Time: Wednesday 16:30–18:45

Location: H 0111

DS 32.1 Wed 16:30 H 0111

**Organized nanoscale assemblies of metal-free organic magnets: Electronic structure and stability from ultra high vacuum to air exposure.** — ●FRANCESCA CICCULLO, REZA KAKAVANDI, and MARIA BENEDETTA CASU — Institute of Physical and Theoretical Chemistry, Tübingen, Germany

Metal-free organic-based magnets are relatively new materials with open-shell structure that may offer new opportunities for applications based on the presence of spatially delocalized unpaired electrons. Essential tools such as X-ray Photoelectron Spectroscopy (XPS) and Near Edge X-ray Absorption Fine structure (NEXAFS) Spectroscopy are used to study the electronic structure and the paramagnetic character of nitronyl nitroxide radicals. The molecule-substrate interface and the thin film properties are investigated, focusing on their impact on the magnetic character of the systems. Our work also identifies a quantitative correlation between the results obtained by the simultaneous use of X-ray photoemission and electron spin resonance spectroscopy. This result can be used as a standard diagnostic tool in order to link the (in-situ-measured) electronic structure with classical ex-situ paramagnetic investigations.

DS 32.2 Wed 16:45 H 0111

**Peculiar Transport Properties of Nanosized Vertical Organic Spin-Valves** — ●ROBERT GÖCKERITZ<sup>1</sup>, NICO HOMONNAY<sup>1</sup>, TIM RICHTER<sup>1</sup>, ALEXANDER MÜLLER<sup>1</sup>, BODO FUHRMANN<sup>2</sup>, and GEORG SCHMIDT<sup>1,2</sup> — <sup>1</sup>Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany — <sup>2</sup>Interdisziplinäres Zentrum für Materialwissenschaften, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany

Organic spin-valves are seen as promising candidates for future spintronic devices based on organic semiconductors. So far most publications report on devices with lateral dimensions of more than 100 micrometer. We present a fabrication process for vertical organic spin-valve devices which offers the possibility to continuously scale down organic spin-valves down to the 100 nm regime. The process uses oxide windows as lateral limitations of the devices and shadow masks during deposition of the active layers. Samples of a LSMO/Alq3/MgO/Co layer stack with lateral dimensions between 100 micrometer and 500 nm have been fabricated and characterized. Upon downscaling we observed a non-linear behavior of the resistance area product and furthermore for similar nanosized devices a large variation of the magnetoresistance between +90% and -170%. These results indicate that the transport is merely determined by pinholes with a certain statistical distribution and that transport and magnetoresistance are mainly dominated by tunneling at the pinhole sites where the organic layer is thin enough.

DS 32.3 Wed 17:00 H 0111

**TSCuPc/Au Hybrid Trench Devices: a Comparative Study of Solution Processed and Thermally Evaporated Molecu-**

**lar Channels** — ●SREETAMA BANERJEE<sup>1,2</sup>, DANIEL BÜLZ<sup>1</sup>, DANNY REUTER<sup>2,3</sup>, KARLA HILLER<sup>2</sup>, THOMAS GESSNER<sup>2,3</sup>, DIETRICH R. T. ZAHN<sup>1</sup>, and GEORGETA SALVAN<sup>1</sup> — <sup>1</sup>Semiconductor Physics, Technische Universität Chemnitz, Germany — <sup>2</sup>Zentrum für Mikrotechnologien, Technische Universität Chemnitz, Germany — <sup>3</sup>Fraunhofer ENAS, Chemnitz, Germany

Organic semiconductors have potential applications in the spintronics field due to the weak spin scattering mechanism in organic molecules, which implies that the spin polarization of the carriers can be maintained for a much longer time (in the range  $\mu$ s to ms) than in inorganic materials. Cost-efficient, wafer level fabrication of such devices is one of the main challenges in this field. Currently e-beam lithography is used for fabricating the required small electrode gap dimensions. Previously, we reported an alternative approach for fabricating laterally stacked organic trench devices using conventional optical lithography, where paramagnetic (CoPc, CuPc) and diamagnetic Alq<sub>3</sub> molecules were evaporated to form the organic channels. It was observed that the molecules form a membrane between the electrodes. In this work, solution processing of organic materials was tested by drop-coating of water-soluble 3,4',4'',4'''-copper(II) phthalocyanine-tetrasulfonic acid tetrasodium salt (TSCuPc). Using this approach it was possible to fill the trenches. A comparative study of a solution processed device and a device with evaporated channel material is presented.

DS 32.4 Wed 17:15 H 0111

**The Influence of a Magnetic Field on Organic Field Effect Transistors: Comparison between Metal-Free and Metal-Phthalocyanines** — ●DANIEL BÜLZ<sup>1</sup>, SREETAMA BANERJEE<sup>1,2</sup>, DIETRICH R. T. ZAHN<sup>1</sup>, and GEORGETA SALVAN<sup>1</sup> — <sup>1</sup>Semiconductor Physics, Technische Universität Chemnitz, Germany — <sup>2</sup>Zentrum für Mikrotechnologien, Technische Universität Chemnitz, Germany

Organic semiconductors are of great interest in today's electronics because of their tunable optical and electrical properties. Especially they are suitable for spintronics due to their weak spin scattering compared to inorganic materials, which results in longer spin lifetimes.

It was shown, that some of these materials respond to an external magnetic field with a change of resistivity. Furthermore, it is reported that organic field effect transistors (OFETs) are suitable to measure this dependence [1]. Therefore we here investigate OFETs made from different metal-free and metal-phthalocyanines in order to compare the influence of the metal center on the magnetic field dependence.

[1] T. Reichert, T. P. I. Saragi; *Organic Electronics* **13**, 377-383, 2012

DS 32.5 Wed 17:30 H 0111

**Computational scanning of phthalocyanine hetero-structures for molecular spintronic applications** — ●TOBIAS BIRNBAUM, TORSTEN HAHN, and JENS KORTUS — Institut für Theo. Physik, TU BA Freiberg, Leipziger Str. 23, 09599 Freiberg

The combination of different functionalized metal phthalocyanines was found to lead to new charge- and spin transfer compounds. The high degree of freedom in functionalization and/or metal center allows the controlled engineering of charge transfer and spin with respect to optimizing properties for possible application of these materials in molecular spintronic applications [1,2]. We will present an extensive computational study of metal phthalocyanines functionalized with electron donating and electron accepting side groups. The trends in frontier energy levels are analyzed and from the level alignment between individual molecules promising candidates for new hetero-structures can be selected. For selected examples we demonstrate that this simplified procedure is actually capable to deliver a correct forecast. A subsequent spatial sampling of a phthalocyanine dimer configuration space is studied in terms of a cost-benefit analysis. Although the method utilizes spin-resolved all-electron DFT calculations, the information on stability, possible spin groundstates, as well as coupling constants can be worth the effort. The detailed analysis is used as input to guide further experimental studies.

[1] R. Friedrich, S. Lindner, T. Hahn, C. Loose, S. Liebing, M. Knupfer, and J. Kortus, Phys. Rev. B 87, 115423 (2013). [2] R. Friedrich, B. Kersting, and J. Kortus, Phys. Rev. B 88, 155327 (2013).

DS 32.6 Wed 17:45 H 0111

**Energy level alignment at the ordered C<sub>60</sub>/Co(0001) hybrid interface** — •JOHANNES STÖCKL, MARTIN LAUX, NORMAN HAAG, JOHANNES SEIDEL, ROMAN FETZER, NICOLAS GROSSMANN, BENJAMIN STADTMÜLLER, MIRKO CINCHETTI, and MARTIN AESCHLIMANN — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schroedinger-Strasse 46, 67663 Kaiserslautern, Germany

The future success of organic semiconductors in spin memory devices depends strongly on our ability to tailor and control the structural properties and the energy level alignment at hybrid interfaces formed between the organic molecules and ferromagnetic surfaces. Hence, many studies focused on the electronic properties of prototype molecules like Alq<sub>3</sub> on Co(100) [1]. On this ferromagnetic substrate, however, the molecular films usually lack any long range order due to the strong molecule substrate interaction and the low thermal energy of the adsorbates. To overcome this limitation, we studied the growth of (sub)monolayer films of C<sub>60</sub> adsorbed on hcp Co(0001) using LEED, STM and spin resolved photoemission spectroscopy (SR-PES). For sub-monolayer coverage LEED and STM indicate that the C<sub>60</sub> molecules form long-range ordered islands after thermal activation. The size of these islands increases with increasing coverage. The SR-PES data show a significant reduction of the spin polarization in comparison to the clean Co(0001) surface which we correlate to the suppression of a Co-surface state by the molecular adsorbates.

[1] Steil et al., Nature Physics 9, 242 (2013)

DS 32.7 Wed 18:00 H 0111

**Spin pumping through C<sub>60</sub> thin films** — •TIM RICHTER<sup>1</sup>, MARTIN WAHLER<sup>1</sup>, MATTHIAS GRÜNEWALD<sup>1</sup>, ROBERT GÖCKERITZ<sup>1</sup>, and GEORG SCHMIDT<sup>1,2</sup> — <sup>1</sup>Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany — <sup>2</sup>Interdisziplinäres Zentrum für Materialwissenschaften, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany

Spin pumping and inverse spin-Hall effect (ISHE) are well established as methods for the creation and detection of pure spin currents [1]. Recently it has been shown that these methods can also be used to investigate pure spin currents in organic materials [2]. Here we use yttrium iron garnet (YIG) deposited by pulsed laser deposition as a source for spin pumping and sputtered platinum (Pt) for the detection via ISHE in order to investigate the propagation of spin currents in an organic material, namely C<sub>60</sub>. C<sub>60</sub> is a small molecule which can

be deposited by UHV evaporation. In our sample thin films of C<sub>60</sub> are sandwiched between YIG and Pt. The sample is then excited by ferromagnetic resonance (FMR) inducing a spin current from the YIG through the C<sub>60</sub> into the Pt where it is detected as a DC ISH-voltage. For layers of C<sub>60</sub> which have a thickness of less than 10 nm we observe the ISHE. These results indicate that we observe merely a tunnelling through the C<sub>60</sub> rather than spin diffusion which is also in agreement with typical transport in undoped C<sub>60</sub>.

[1] Saitoh et al., Appl. Phys. Lett. 88, 182509, (2006)  
[2] Watanabe et al., Nat. Phys. 10, 308, (2014)

DS 32.8 Wed 18:15 H 0111

**Transferring spin into an extended  $\pi$ -orbital of a large molecule** — •T. ESAT<sup>1</sup>, T. DEILMANN<sup>2</sup>, B. LECHTENBERG<sup>3</sup>, C. WAGNER<sup>1</sup>, P. KRÜGER<sup>2</sup>, R. TEMIROV<sup>1</sup>, F.B. ANDERS<sup>3</sup>, M. ROHLFING<sup>2</sup>, and F.S. TAUTZ<sup>1</sup> — <sup>1</sup>Peter Grünberg Institute (PGI-3), FZ Jülich, Germany — <sup>2</sup>Institut für Festkörpertheorie, Universität Münster, Germany — <sup>3</sup>Lehrstuhl für Theoretische Physik II, TU Dortmund, Germany

The electronic and magnetic properties of molecules can be tuned in a wide range by charge transfer from molecules[1] and metal surfaces[2-4] or by doping with atoms[5].

In this work we tune the electronic structure by doping archetypal organic molecules with single metal atoms. An on-surface chemical reaction leads to electron spin transfer into a  $\pi$ -orbital that extends over the whole molecule, unlike in common molecular magnets where the spin usually resides in a d- or f-orbital of a metal ion that is shielded by organic ligands. We show that this complex has an unpaired spin which interacts with electrons in the metallic substrate and forms a Kondo singlet state. The advantage of such a radical may lie in its propensity to interact magnetically with its neighbours, offering the potential to harness this coupling.

[1] I. Fernández-Torrente et al., Phys. Rev. Lett. 108, 036801 (2012)  
[2] R. Temirov et al., Nanotechnology 19 (6), 065401 (2008)  
[3] C. Toher et al., Phys. Rev. B 83, 155402 (2011)  
[4] A. Greuling et al., Phys. Stat. Sol.(b) 250, 2386 (2013)  
[5] C. Krull et al., Nature Materials 12, 337-343 (2013)

DS 32.9 Wed 18:30 H 0111

**Interface-assisted sign inversion of Magnetoresistance in Molecular Spin Valves based on Novel Lanthanide Quinolines** — •AMILCAR BEDOYA-PINTO<sup>1</sup>, SARA GOMEZ<sup>2</sup>, EUGENIO CORONADO<sup>2</sup>, and LUIS HUESO<sup>1</sup> — <sup>1</sup>CIC nanoGUNE, San Sebastián, Spain — <sup>2</sup>Instituto de Ciencia Molecular (ICMoL), Valencia, Spain

Molecules have recently emerged as promising materials for spintronics, owing to their weak spin relaxation mechanisms. However, the rules that govern spin injection and transport in molecules are not yet fully understood. In this work, combining advanced molecular synthesis and device engineering, we study how i) the magnetic nature of the molecule and ii) the ligand hybridization at the metal interface impacts the spin injection and transport in molecular spin-valve devices. We have synthesized novel [NaLn(5,7Clq)4] molecules with lanthanide ion centers exhibiting distinct magnetic behavior (diamagnetic Y/ single-ion magnet Dy), and assembled them in spin valve structures using Co and NiFe electrodes. While the magnetic nature of the molecule does not have any major effect on the spin injection and transport properties, the hybridization of metal and molecular ligand states is found to have a strong impact on the interface spin polarization. Spin valves featuring a Na[Ln(5,7Clq)4]/Co interface exhibit a positive magnetoresistance, typically found in other molecule/FM metal systems; whereas the interaction of Na[Ln(5,7Clq)4] with NiFe triggers a negative magnetoresistance, i.e., an inversion of the interface spin polarization. These results highlight the potential of molecules to tailor spin-dependent properties at the interface level.

## DS 33: Mitgliederversammlung

Time: Wednesday 19:00–20:00

Location: H 0111

DS Mitgliederversammlung

## DS 34: Focused Session: Oxide semiconductors I (joint session with HL)

Time: Thursday 9:30–12:45

Location: H 2032

## Invited Talk

DS 34.1 Thu 9:30 H 2032

**Growth, properties and devices of gallium-oxide-based wide-gap semiconductors** — ●SHIZUO FUJUTA — Kyoto University, Kyoto, Japan

Recently, high-power devices with orthorhombic  $\alpha$ -Ga<sub>2</sub>O<sub>3</sub> have attracted increasing interest supported by solution-grown highly-crystalline substrates. However, orthorhombic crystals are rare in semiconductor family, hence there hardly are other semiconductors of the same crystal structure for alloys or multilayer structures with  $\alpha$ -Ga<sub>2</sub>O<sub>3</sub>. On the other hand we have developed the growth of corundum-structured  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>,  $\alpha$ -Ga<sub>2</sub>O<sub>3</sub>,  $\alpha$ -In<sub>2</sub>O<sub>3</sub> and their alloys achieving the band gap engineering from 3.8 to 8.8 eV, overcoming metastable phases of  $\alpha$ -Ga<sub>2</sub>O<sub>3</sub> and  $\alpha$ -In<sub>2</sub>O<sub>3</sub>. For the growth we can apply a low-cost and environmental-friendly mist CVD method, which allowed highly-crystalline films as evidenced by FWHM of  $\omega$ -scan XRD curves as small as <50 arcsec for  $\alpha$ -Ga<sub>2</sub>O<sub>3</sub> and <500 arcsec for others. The author will report crystal qualities, electrical properties, doping and preliminary device performances with MOS structures at the conference. In addition, alloying with transition-metal oxides such as  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> or  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> achieves addition of magnetic properties to semiconductors, as evidenced by magnetization hysteresis at >300K. This can also develop new multifunctional materials and devices with function engineering.

DS 34.2 Thu 10:00 H 2032

**Growth-Kinetics Study and Doping the Group-III Sesquioxide  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>** — ●PATRICK VOGT and OLIVER BIERWAGEN — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5 - 7, 10117 Berlin, Germany

In the present talk, a comprehensive study of the growth-kinetics of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> (-201) on Al<sub>2</sub>O<sub>3</sub> (0001) is given. The growth was performed by plasma-assisted molecular beam epitaxy. Under ultra-high vacuum conditions atomic gallium and oxygen plasma were reacting amongst others to form  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>. Besides the growth-kinetics studies for undoped Ga<sub>2</sub>O<sub>3</sub> we also doped this material with tin. Under different growth conditions we investigated the carrier concentration depending on different growth parameters like growth temperature (T<sub>growth</sub>) and metal fluxes, Ga and Sn flux, respectively.

This study shows the variation of the growth-rate depending on various growth-parameter such as the gallium beam equivalent pressure, T<sub>growth</sub> and the oxygen flux. It turned out, that in the gallium-rich regime the formation of the volatile suboxide Ga<sub>2</sub>O reduce the growth-rate of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> and result in an etching of the film when no oxygen is supplied. In order to investigate the carrier concentration of the Ga<sub>2</sub>O<sub>3</sub> : Sn transport measurements were performed.

DS 34.3 Thu 10:15 H 2032

**Au-Schottky contact on In<sub>2</sub>O<sub>3</sub> single crystals** — ●MARYAM NAZARZADEHMOAFI<sup>1</sup>, CHRISTOPH JANOWITZ<sup>1</sup>, MATTIA MULAZZI<sup>1</sup>, STEPHAN MACHULIK<sup>1</sup>, ZBIGNIEW GALAZKA<sup>2</sup>, and RECARDO MANZKE<sup>1</sup> — <sup>1</sup>Institut für Physik, Humboldt Universität zu Berlin, Newtonstraße 15, 12489 Berlin, Germany — <sup>2</sup>Leibniz Institut für Kristallzüchtung, Max Born Str. 2, 12489 Berlin, Germany

Au contacts on melt-grown-In<sub>2</sub>O<sub>3</sub> (111) single crystals were studied using angle-resolved photoemission spectroscopy to monitor the band bending by core level and valence band spectra, with correction for the photovoltage effect. The measurement was performed through step-wise Au evaporation onto the (111) surface of In<sub>2</sub>O<sub>3</sub> at room temperature (RT) as well as low temperature (LT). A small Schottky barrier on RT-samples and a larger one on LT-samples were observed. The comparison of the experimental barrier height with the predicted one from the Schottky-Mott rule shows a discrepancy. It implies that the complexity of the atomic structure of the present metal-semiconductor interface is beyond the applicability of the Schottky-Mott rule. The results indicate that an explicit reference to the surface electron accumulation layer is not necessary when discussing the Schottky character of the Au/In<sub>2</sub>O<sub>3</sub> contact. In addition, the results reveal the epitaxial growth of Au on In<sub>2</sub>O<sub>3</sub> and also the chemical reaction and formation of an Au-In alloy at RT.

DS 34.4 Thu 10:30 H 2032

**Schottky contacts and pn-heterojunctions on heteroepitaxial**

**In<sub>2</sub>O<sub>3</sub> thin films grown by pulsed laser deposition** — ●DANIEL SPLITH, FLORIAN SCHMIDT, STEFFEN LANZINGER, STEFAN MÜLLER, HOLGER VON WENCKSTERN, and MARIUS GRUNDMANN — Universität Leipzig, Institut für Experimentelle Physik II, Leipzig, Germany

Oxide semiconductors like In<sub>2</sub>O<sub>3</sub> are promising materials for a new generation of transparent electronic devices. While the properties of highly tin-doped In<sub>2</sub>O<sub>3</sub> (ITO) for use as a transparent conductive oxide (TCO) are well investigated, interest in the semiconducting properties of In<sub>2</sub>O<sub>3</sub> for the investigation of material properties and application in devices arose recently. In order to create devices like diodes or field-effect transistors, the creation of a space charge region is required, which can be done either by a Schottky contact (SC) or a pn-junction.

In this contribution we discuss the fabrication of rectifying contacts based on SCs [1] and pn-heterojunctions with an amorphous *p*-type oxide like NiO or ZnCo<sub>2</sub>O<sub>4</sub> [2]. To optimize the performance of the rectifying contacts different approaches were used: By introducing a Mg-doped In<sub>2</sub>O<sub>3</sub> layer, the reverse current was decreased by several orders of magnitude since Mg acts as an acceptor in In<sub>2</sub>O<sub>3</sub> and therefore increases the width of the space charge region. Also, a tin doped back contact layer was employed in order to decrease the series resistance of the contacts. Further, different substrates were used to investigate the influence of the crystal quality on the rectifying properties.

[1] H. von Wenckstern *et al.*, APL Mat. 2, 046104 (2014)[2] F.-L. Schein *et al.*, Appl. Phys. Lett. 104, 022104 (2014)

DS 34.5 Thu 10:45 H 2032

**Temperature-dependent thermal conductivity in Mg-doped and undoped  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> bulk-crystals** — ●MARTIN HANDWERG<sup>1,2</sup>, RÜDIGER MITDANK<sup>1</sup>, ZBIGNIEW GALAZKA<sup>3</sup>, and AND SASKIA F. FISCHER<sup>1</sup> — <sup>1</sup>AG Neue Materialien, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — <sup>2</sup>Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — <sup>3</sup>Leibniz Institute for Crystal Growth, Max-Born-Strasse 2, 12489 Berlin, Germany

Transparent semiconducting insulators like Ga<sub>2</sub>O<sub>3</sub> are important materials for high power electronics and optoelectronics. For  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> only little information exist concerning the thermal properties, especially the thermal conductivity  $\lambda$ . Here, the thermal conductivity is measured by applying the electrical  $3\omega$ -method on Czochralski-grown  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> bulk crystals, which have a thickness of 200  $\mu$ m and 800  $\mu$ m. At room temperature the thermal conductivity along the [100]-direction in Mg-doped electrical insulating and undoped semiconducting  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> is confirmed as  $13 \pm 1 \text{ Wm}^{-1}\text{K}^{-1}$  for both crystals [1]. The phonon contribution of  $\lambda$  dominates over the electron contribution below room temperature. The observed function  $\lambda(T)$  is in accord with phonon-phonon-Umklapp scattering and the Debye-model for the specific heat at  $T \gtrsim 90 \text{ K}$  which is about 0.1 fold of the Debye-temperature  $\theta_D$ . Here a detailed discussion of the phonon-phonon-Umklapp scattering for  $T < \theta_D$  is carried out. The influence of point defect scattering is considered for  $T < 100 \text{ K}$ .

[1] Martin Handweg *et al.*, 2014, SST, accepted (arXiv 1407 4272)

## 30 min. break.

## Invited Talk

DS 34.6 Thu 11:30 H 2032

**BaSnO<sub>3</sub>; The next generation of transparent conducting oxide?** — ●DAVID SCANLON — Department of Chemistry, University College London, UK — Diamond Light Source Ltd., Harwell, UK.

La-doped cubic perovskite BaSnO<sub>3</sub> has been reported to possess electron mobilities as high as  $320 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$  for carrier concentrations of  $8 \times 10^{19} \text{ cm}^{-3}$ , comparable to the very best transparent conducting oxides (TCOs). In this presentation we will examine the electronic structure and defect chemistry of BaSnO<sub>3</sub>, and use this information to explain why La-doped BaSnO<sub>3</sub> possesses all the qualities needed to be the next generation *n*-type TCO.

DS 34.7 Thu 12:00 H 2032

**Nitrogen doping in tin dioxide thin film grown by chemical vapor deposition** — ●JIE JIANG, YINMEI LU, BENEDIKT KRAMM, and BRUNO K MEYER — I. Physics Institute, Justus-Liebig-University Giessen, Giessen, Germany

As a direct band gap semiconductor, tin dioxide (SnO<sub>2</sub>) is a promising

candidate for next generation ultraviolet light emitting diodes (LEDs) and photo detectors, due to its large band gap of 3.6 eV, and high carrier mobility of about 250 cm<sup>2</sup>/Vs at room temperature. An essential step to fabricate SnO<sub>2</sub>-based optoelectronic devices is to obtain high quality p-type SnO<sub>2</sub> films. Nitrogen could be an excellent p-type dopant in SnO<sub>2</sub> owing to its suitable electronegativity and ion size, high solubility limit, and non-toxicity. At the same time, only a few experimental investigations were performed on N-doped SnO<sub>2</sub>. For this reason, we deposit the N-doped SnO<sub>2</sub> thin films on c-sapphire substrates via chemical vapor deposition (CVD), using SnI<sub>2</sub> powder and O<sub>2</sub> and NH<sub>3</sub> gas as source materials. Both undoped and N-doped samples are annealed at different temperature for a short time using a rapid thermal processing. The crystal structure, electrical properties and optical properties of the films were measured and investigated by X-ray diffraction (XRD), Hall effect measurements, optical transmittance, secondary ion mass spectrometry (SIMS) and X-ray photoelectron spectroscopy (XPS), respectively. The effect of short-time annealing on structural, optical and electrical properties is also analyzed.

DS 34.8 Thu 12:15 H 2032

**Dopant clustering in p-type transparent semiconducting Cr<sub>2</sub>O<sub>3</sub>:Mg** — ●KARSTEN FLEISCHER, DAVID CAFFREY, LEO FARRELL, EMMA NORTON, DARAGH MULLARKEY, ELISABETTA ARCA, and IGOR V. SHVETS — School of physics and Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College Dublin, Dublin 2, Ireland

We present an analysis of the Raman spectra of p-type transparent conducting Cr<sub>2</sub>O<sub>3</sub>:Mg grown by various techniques including spray pyrolysis (SP), pulsed laser deposition (PLD), molecular beam epitaxy (MBE) and reactive magnetron sputtering (RMS). The best performing films show a distinct broad range Raman signature related to defect-induced vibrational modes not seen in stoichiometric, undoped material. Our comparative study demonstrates that Raman

spectroscopy can quantify unwanted dopant clustering in the material at high Mg concentrations, while also being sensitive to the Mg incorporation site. By correlating the Raman signature to the electrical properties of the films, growth processes can be optimised to give the best conducting films and the local defect structure for effective p-type doping can be studied.

DS 34.9 Thu 12:30 H 2032

**Annealing effects on electrical properties of room-temperature deposited zinc oxynitride thin films** — ●ANNA REINHARDT, HEIKO FRENZEL, HOLGER VON WENCKSTERN, and MARIUS GRUNDMANN — Universität Leipzig, Institut für Experimentelle Physik II, Semiconductor Physics Group

Amorphous oxide semiconductors have attracted much attention as channel material for thin-film transistors (TFT) due to their comparatively large electron mobility (> 10 cm<sup>2</sup>/Vs) achieved already by low-temperature fabrication. In order to further increase channel mobilities while maintaining the stability of oxide-based TFTs the alloying of ZnO by nitrogen was suggested [1].

We have investigated the electrical properties of semiconducting zinc oxynitride (ZnO<sub>x</sub>N<sub>y</sub>) thin films depending on annealing temperature and doping. Therefore we conducted annealing experiments in air and N<sub>2</sub> atmosphere up to 400°C. The ZnO<sub>x</sub>N<sub>y</sub> thin films were deposited on glass substrates by reactive radio-frequency magnetron sputtering of a metallic zinc target at room-temperature. Electrical properties were examined using the four-probe van der Pauw technique. The as-deposited films show n-type semiconducting behaviour with carrier concentrations of 1 × 10<sup>17</sup> – 3 × 10<sup>18</sup> cm<sup>-3</sup> and Hall mobilities ranging from 10 to 20 cm<sup>2</sup>/Vs. With increasing annealing temperature the resistivity decreases whereas the mobility increases. In addition, possible structural changes due to annealing were analyzed using x-ray diffraction.

[1] Y. Ye *et al.*, J. Appl. Phys., 106, 074512 (2009)

## DS 35: Graphen

Time: Thursday 9:30–13:00

Location: H 0111

DS 35.1 Thu 9:30 H 0111

**Graphene Growth and Isotope Engineering** — ●MICHAEL HILKE<sup>1,2</sup>, ERIC WHITEWAY<sup>1</sup>, WAYNE YANG<sup>1</sup>, and VICTOR YU<sup>1</sup> — <sup>1</sup>McGill University, Montreal, Kanada — <sup>2</sup>FU Berlin, Berlin, Deutschland

Graphene is grown by chemical vapor deposition (CVD) on copper using different relative concentrations of C12 and C13 isotopes. This allows us to measure the dynamics of the growth and extract important growth parameters, in particular in relation to regular and fractal graphene (graphlocons) growth. Further, the use of different isotopes, opens the door to new phonon properties such as phonon Anderson localization, phonon waveguides and more generally phonon engineering.

DS 35.2 Thu 9:45 H 0111

**Synthesis of long-range ordered crystalline Graphene by chemical vapor deposition over Iridium (111) films on Sapphire** — ●ARTI DANGWAL PANDEY and ANDREAS STIERLE — Deutsches Elektronen-Synchrotron, Hamburg, Germany

High-quality and large-area Graphene is in demand to exploit its unique physical properties for various applications, including future electronic devices and sensors. Large-area epitaxial graphene have been deposited successfully by CVD on transition metal single crystals. These substrates are of high quality, but very expensive. This drives the search for other alternatives to use cheaper substrates. Ir has low carbon solubility, and so Ir thin film is a good choice for growing Graphene on it. Only single article is published till date for preparing epitaxial graphene on single crystal Ir film. [1] We have synthesized long-range ordered crystalline Graphene over few nanometer thick Ir films deposited on sapphire. Ethylene is used as a carbon source for depositing graphene by CVD and Ir films are grown by physical vapor deposition. LEED reveals the long-range crystallinity of graphene and Ir films, and XPS measurements confirmed the high purity of Ir films. Influence of growth parameters on the quality of Ir film, and thus on Graphene, will be discussed in Detail.

[1] Chi Vo-Van *et al.* App. Phys. Lett. 98 (2011) 181903.

DS 35.3 Thu 10:00 H 0111

**Rotated domain network in graphene on cubic-SiC(001)** — ●VICTOR ARISTOV<sup>1,2,3</sup>, ALEXANDER CHAIKA<sup>1,4</sup>, OLGA MOLODTSOVA<sup>2</sup>, ALEXEI ZAKHAROV<sup>5</sup>, DMITRY MARCHENKO<sup>6</sup>, JAIME SÁNCHEZ-BARRIGA<sup>6</sup>, ANDREI VARYKHALOV<sup>6</sup>, SERGEY BABENKOV<sup>2</sup>, MARC PORTAIL<sup>7</sup>, MARCIN ZIELINSKI<sup>8</sup>, BARRY MURPHY<sup>4</sup>, SERGEY KRASNNIKOV<sup>4</sup>, OLAF LUEBBEN<sup>4</sup>, and IGOR SHVETS<sup>4</sup> — <sup>1</sup>ISSP RAS Chengolovka, Russia — <sup>2</sup>DESY Hamburg, Germany — <sup>3</sup>Uni Hamburg, Germany — <sup>4</sup>Trinity College Dublin, Ireland — <sup>5</sup>MAX-lab Lund, Sweden — <sup>6</sup>BESSY Berlin, Germany — <sup>7</sup>CNRS-CRHEA Valbonne, France — <sup>8</sup>NOVASiC Le Bourget du Lac, France

The atomic structure of the cubic-SiC(001) surface during UHV graphene synthesis has been studied using PES, STM and LEED. The studies prove the synthesis of a uniform, millimeter-scale graphene overlayer consisting of nanodomains rotated by \*13.5° relative to the <110>-directed boundaries. The preferential directions of the domain boundaries coincide with the directions of carbon atomic chains on the SiC(001)-c(2x2) reconstruction, fabricated prior to graphene synthesis. The presented data show the correlation between the atomic structures of the SiC(001)-c(2x2) surface and the graphene /SiC(001) rotated domain network and pave the way for optimizing large area graphene synthesis on low cost cubic SiC(001)/Si(001) wafers. Acknowledgments: This work was supported by the RAS, RFBR grants No 140200949 and 140201234, by the BMBF-Project No. 05K12GU2, PSP-Element No. U4606BMB1211, by a Marie Curie IIF grant No 12/IA/1264, by SPP 1459 of DFG.

DS 35.4 Thu 10:15 H 0111

**Investigation of atomic-scale strain variations in graphene as a function of applied strain** — ●STEFAN E. HUBER<sup>1</sup>, GERARD VERBIEST<sup>2</sup>, CHRISTOPH STAMPFER<sup>2</sup>, and KARSTEN REUTER<sup>1</sup> — <sup>1</sup>Technische Universität München — <sup>2</sup>RWTH Aachen

Graphene exhibits unique electronic and mechanical properties. The very high electron mobilities that can be reached in state-of-the-art

devices suggest this material to revolutionize present-day electronics. The demand for high mobilities raises the question what actually limits these in graphene. Recent experiments provide evidence that most likely nanometer-scale strain variations are the mechanism responsible for the limitation of the charge carrier mobility [1,2].

Homogeneously straining graphene is expected to reduce local strain fluctuations and thus to increase the electron mobility. We address this issue with atomistic simulations of two distinct mechanisms that may give rise to nanometer-scale strain variations in the presence of overall strain. Using (and comparing) a series of interatomic potentials to describe graphene, we study (i) the effect of surface defects in a hexagonal boron-nitride substrate deduced from first-principles DFT calculations as well as (ii) thermally induced fluctuations. In both respects, we discuss the effective suppression of out-of-plane distortions already at moderate global strains of a few per cent. In stark contrast, in-plane deformations are enhanced upon the application of global strain, a result clearly beyond the limitations of linear elasticity theory.

[1] N.J.G. Couto *et al.*, Phys. Rev. X 4, 041019 (2014)

[2] S. Engels *et al.*, Phys. Rev. Lett. 113, 126801 (2014)

DS 35.5 Thu 10:30 H 0111

### Uniformity of the pseudo-magnetic field in strained graphene

— ●GERARD VERBIEST, SASCHA BRINKER, and CHRISTOPH STAMPFER — JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany

Graphene is a very promising candidate as active material in future electronic applications. However, its electrical properties are very sensitive to mechanical disturbances, as graphene is only one atomic layer thick. This coupling theoretically gives rise to a so-called "pseudo-vector field", and consequently to a "pseudo-magnetic field".

The pseudo-magnetic field can, just as a real magnetic field, induce Landau levels in graphene, if the field is strong enough. In order to utilize, i.e. measure this effect, one needs (i) a high sample quality and (ii) a large uniformity of the pseudo-magnetic field.

Here we present numerical simulations of the pseudo-magnetic field in graphene with a hexagonal shape as a function of tri-axial strain. We defined a radius of uniformity, as the radius for which the standard deviation from the pseudo-magnetic field in the center reaches 1%. For a hexagon with sides of 100 nm and a strain of 10%, the pseudo-magnetic field strength is  $\sim 40$  T and is uniform within a diameter of 34 nm. For a hexagonal sample size with sides of 1 micron with a strain of 3.5%, the maximum pseudo-magnetic field is reduced to  $\sim 1.2$  T, but it is uniform within a diameter of 540 nm.

DS 35.6 Thu 10:45 H 0111

**Nanopores in Silicon Nitride Membranes, Graphene and CNM: Milling and Imaging Techniques at the Helium Ion Microscope** — ●DANIEL EMMRICH<sup>1</sup>, EMANUEL MARSCHEWSKI<sup>1</sup>, ACHIM NADZEYKA<sup>2</sup>, FRANK NOUVERTNE<sup>2</sup>, ARMIN GÖLZHÄUSER<sup>1</sup>, and ANDRÉ BEYER<sup>1</sup> — <sup>1</sup>Physics of Supramolecular Systems, Bielefeld University, 33615 Bielefeld, Germany — <sup>2</sup>Raith GmbH, Konrad Adenauer Allee 8, 44263 Dortmund, Germany

The Helium Ion Microscope (HIM) is a charged particle microscope employing Helium ions for probing the sample. In the low dose regime, the HIM operates as microscope, high doses enable material modification and sputtering. Compared to conventional focussed ion beams (FIB) using metal ions like Gallium, the HIM offers a very small focal spot size down to 0.35 nm and a strongly localized sputter interaction with the material. We employ the HIM for both milling nanopores in free standing membranes as well as for the inspection of pores. The He+ beam with its unique properties overcomes the resolution limit of conventional FIB tools as we show in a comparison with a high resolution Ga-FIB. We achieve smallest He-milled nanopores with a diameter of about 4 nm in all investigated membranes: 30 nm thick Silicon Nitride, Graphene and 1 nm thick carbon nanomembranes (CNM) made from aromatic self-assembled monolayers by electron-induced cross-linking. Different strategies for the characterization of pores with the HIM will be discussed. In particular, we compare the feasibility of the ion generated secondary electron signal to the He+ transmission signal.

DS 35.7 Thu 11:00 H 0111

**Doping of graphene on SiO<sub>2</sub> with N<sup>+</sup> and B<sup>+</sup> ions by low-energy ion irradiation.** — ●STEFFEN WEIKERT, JULIAN ALEXANDER AMANI, and HANS CHRISTIAN HOFSSÄSS — II. Physikalisches Institut, Georg-August-Universität Göttingen, Deutschland

Its unique electrical properties make graphene a promising candidate

for future electronic devices. An important milestone, especially for the industrial production of those devices, is the realization of a method for large-scale doping of graphene. A potential method for controlled doping of graphene, while minimizing the damage inflicted upon the sample, is low-energy ion irradiation.<sup>[1–3]</sup>

This work shows experiments on the irradiation of monolayer graphene on SiO<sub>2</sub> by N<sup>+</sup> and B<sup>+</sup> ions at 25 eV. For the experimental realization a mass-selected ion beam deposition system was used.<sup>[4]</sup> The irradiation was also simulated using the Monte Carlo program SDTrimSP. In addition to the irradiation of the graphene, I-V measurements were made before and after the irradiation.

[1] U. Bangert, W. Pierce, D. M. Kepaptsoglou, Q. Ramasse, R. Zan, M. H. Gass, J. A. Van den Berg, C. B. Boothroyd, J. Amani, and H. C. Hofssäss, Nano Lett. 2013, 13, 4902-4907.

[2] E. H. Åhlgren, J. Kotakoski, and A. V. Krashennnikov, Phys. Rev. B (2011), 83, 115424.

[3] Y. Xu, K. Zhang, C. Brüsewitz, X. Wu, and H. C. Hofssäss, AIP Advances (2013), 3, 072120.

[4] H. Hofssäss, H. Binder, T. Klumpp and E. Recknagel, Diam. Relat. Mater. (1994), 3, 137.

15 min. break.

DS 35.8 Thu 11:30 H 0111

### Field induced enhancement of refractive index and conductivity - a substrate effect in graphene

— ●MATTHIAS VAUPEL<sup>1</sup>, ANKE DUTSCHKE<sup>1</sup>, ULRICH WURSTBAUER<sup>2</sup>, and FRANK HITZEL<sup>3</sup> — <sup>1</sup>Carl Zeiss Microscopy GmbH, Königsallee 9-21, 37081 Göttingen, Germany — <sup>2</sup>Dept. of Physics, Columbia University New York, NY 10027, USA — <sup>3</sup>DME Nanotechnologie GmbH, D-38106 Braunschweig, Germany

We study the effect of different substrates, conductive Si vs. isolating SiO<sub>2</sub>, on the electro-optic properties of graphene layers. To this end phase profiles of graphene layers were recorded by total interference contrast (TIC) microscopy, while atomic force microscopy measured the topography of the layers [1]. An optical model consistent with the measured height and phase profile of graphene yields the refractive index  $N$  and conductivity of graphene. Extraordinary high  $N = 3.9 + 9.2i$  is obtained for the graphene on conductive substrate. The optical conductivity is 38 fold increased with respect to the reference value obtained on isolating substrate by TIC [1] and by ellipsometry [2]. These observations are mathematically consistent with the dielectric Drude function, which describes a damped harmonic electron oscillation with zero eigenfrequency and nonzero effective electron mass. The model applies for FETs and electro-optic devices made of graphene.

[1] M. Vaupel, A. Dutschke, U. Wurstbauer, F. Hitzel, A. Pasupathy, J.Appl.Phys. 114, (2013) 183107 [2] U. Wurstbauer, C. Röling, U. Wurstbauer, W. Wegscheider, M. Vaupel, P.H. Thiesen, D. Weiss, Appl. Phys. Lett. 97, (2010) 231901

DS 35.9 Thu 11:45 H 0111

### Charge and spin transport in graphene nanoribbons with adatoms and defects

— ●FLAVIANO JOSÉ DOS SANTOS<sup>1,2</sup>, FILIPE SOUZA MENDES GUIMARÃES<sup>1,2</sup>, and ROBERTO BECHARA MUNIZ<sup>1</sup> — <sup>1</sup>Institute of Physics, Universidade Federal Fluminense, Niterói, Brazil — <sup>2</sup>Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Several features of spintronic systems are related to the spin-orbit coupling (SOC). Since SOC is relatively small in carbon atoms, several studies have been conducted in order to obtain a way to increase SOC in graphene (e.g., via adsorption of impurities on the graphene surface), which would allow to employ graphene as a basic material for spintronic devices. We have studied the charge and spin transport in graphene nanoribbons, in the linear response regime, affected by the presence of defects (vacancies and edge constrictions) and adatoms. We used effective models for light and heavy adsorbed impurities, some of them inducing enhancement of the SOC [1]. The results are obtained through a combination of analytical and numerical derivations. We investigated the impact of impurity concentration on the establishment of topologically protected edge states giving rise to a spin polarized current flux through the sample. In addition to conductance, local densities of states and current distribution calculations, we also simulate maps of real space local conductance properties for dual-probe Scanning Tunneling Microscope [2] setups on these systems. [1] C. Week *et al.*, Phys. Rev. X 1, 021001 (2011). [2] M. Settnes *et al.*, Phys. Rev. Lett. 112, 096801 (2014). Funding: Capes and CNPq (Brazil).

DS 35.10 Thu 12:00 H 0111

**Electronic properties of Co atoms on Graphene / Ir(111) by photoelectron spectroscopy** — ●MICHAEL HEBER<sup>1</sup>, MARKUS SCHOLZ<sup>1</sup>, ADRIAN BENZ<sup>1</sup>, DENIZA CHEKRYGINA<sup>1</sup>, MICHAEL MARTINS<sup>1</sup>, and WILFRIED WURTH<sup>1,2</sup> — <sup>1</sup>Physics Department and Center for Free-Electron Laser Science, Univ. Hamburg, 22761 Hamburg, Germany — <sup>2</sup>DESY Photon Science, 22607 Hamburg, Germany

Despite of the enormous achievements in our understanding of the interaction of deposited metal atoms with the underlying substrates, they still bear a variety of unexplored features. Recently, Graphene grown on metal substrates has proven to be a versatile template to create ordered arrays of adsorbed metal atoms. It was shown, that the electronic properties of adsorbed transition metal atoms strongly depend on the hybridization between the transition metal d-orbitals and the graphene  $\pi$ -band. The graphene  $\pi$ -band itself can hybridize with the valence states of the metal substrates. This opens a gateway to manipulate the adsorbate-Graphene interface itself and thus the electronic properties. We present core and valence level photoemission measurements of Co atoms deposited on Graphene/Ir(111) to obtain a detailed picture of the hybridization effects on the electronic structure of the metal atoms. This work is supported by the SFB 668 "Magnetism from single atoms to nanostructures"

DS 35.11 Thu 12:15 H 0111

**hydration of bilayered graphene oxide** — ●BITA REZANIA<sup>1</sup>, NIKOLAI SEVERIN<sup>1</sup>, ALEXANDR V TALYZIN<sup>2</sup>, and JÜRGEN P RABE<sup>1</sup> — <sup>1</sup>Humboldt University, Berlin, Germany — <sup>2</sup>Umeå University, Umeå, Sweden

Recently, it has been shown that graphene oxide (GO) membranes show remarkable selectivity in permeation of water molecules. This was attributed to the hydration of the membranes - the key to understand the water permeation mechanism. We investigated the change of the interlayer distance in bilayer GO as function of humidity and in liquid water using SFM [1]. The increase of relative humidity from 2 to \*80% results in gradual expansion of interlayer distance by approximately 1 Å. The immersion into liquid water results in increase of the interlayer distance by another 3 Å. Our results are in good agreement with the averaged distance measured by X-ray diffraction on multilayered graphite oxides, which is commonly explained with an interstratification model. However, our experimental design excludes effects connected to interstratification. We find that the hydration is a continuous process of incorporation of water molecules into various sites within the GO layers, while liquid water inserts as a monolayer. The similarity of hydration for our bilayer and previously reported multilayered materials implies GO few and even bilayers to be suitable for selective water transport.

[1] Rezanian, B., et al. Nano Lett. 2014, 14, 3993.

DS 35.12 Thu 12:30 H 0111

**Humidity dependent oxygen transport through single layer graphene oxide** — ●MOHAMMAD FARDIN GHOLAMI, PHILLIP LANGE, NIKOLAI SEVERIN, and JÜRGEN P. RABE — Department of Physics and IRIS Adlershof, Humboldt-Universität zu Berlin, Newtonstr. 15, D-12489 Berlin, Germany

Graphene oxide (GO) is a strongly oxidized and nano-porous single sheet of graphene. Few layer thick GO membranes have been shown to exhibit molecular selective gas transport (H.W. Kim *et al.* and H. Li *et al.*, *Science*, 2013). The molecular selectivity is humidity dependent, which has been attributed to water molecules blocking either GO interlayers or pores. The latter would imply that also single layer GO may exhibit similar properties. Here we used the sensitivity of the fluorescence of thin films of a regioregular poly(3-hexylthiophene-2,5-diyl) to photo-oxidation in order to investigate the transport of oxygen through single layer GOs put on the polymer films by following its fluorescence decaying with time (P. Lange *et al.*, *J. Phys. Chem. C*, 2011). For samples exposed to humid mixtures of 80% nitrogen and 20% oxygen with 32% relative humidity we find that the fluorescence of the polymer covered by GO decays two times slower than the uncovered one. We did not observe any difference in the decay rates when the film was exposed to the corresponding dry gas mixture. We attribute the slower fluorescence decay of the polymer film covered by the humidified GO to slower permeation of oxygen molecules through GO pores clogged by the water molecules. This implies that even single layer GO can be used as a humidity dependent molecular sieve.

DS 35.13 Thu 12:45 H 0111

**In-situ Creation of Reduced Graphene Oxide Paper on Substrates** — PENG LI<sup>1</sup>, ●MATTHIAS M. L. ARRAS<sup>2</sup>, FUPING DONG<sup>2</sup>, XIN WANG<sup>1,2</sup>, and KLAUS D. JANDT<sup>2</sup> — <sup>1</sup>Department of Materials Science, Key Laboratory of Automobile Materials of MOE, Jilin University, Changchun, 130012, P. R. China — <sup>2</sup>Chair of Materials Science (CMS), Otto Schott Institute of Materials Research, Friedrich Schiller University Jena, Jena, Germany

Generally, the synthesis conditions of reduced graphene oxide paper (rGOP) require special substrates for its fabrication and, thus, it must often be transferred to application-suitable substrates, afterwards. Here, we tested the hypothesis that rGOP can be synthesized in-situ, e.g., on a polymer substrate, by using a mild step-by-step annealing of graphene oxide hydrosol. By applying the step-by-step annealing at 60, 100 and 160°C for 12 h, shiny and non-crimpling rGOP was created on polymer and glass substrates. The rGOP was characterized by Raman, infra red and X-ray photoelectron spectroscopy, as well as by optical and electron microscopy. Based on the results, a simple formation mechanism for the rGOP was proposed. The presented method will allow to equip surfaces with rGOP functionality directly and is also suitable for a patterned functionalization.

## DS 36: Poster Session I

Time: Thursday 9:30–12:00

Location: Poster A

DS 36.1 Thu 9:30 Poster A

**Sponge-like Si-SiO<sub>2</sub> nanocomposite as photovoltaic absorber: Synthesis by solid vs liquid state decomposition of SiO<sub>x</sub>** — ●ERIK SCHUMANN<sup>1</sup>, KARL-HEINZ HEINIG<sup>1</sup>, RENÉ HÜBNER<sup>1</sup>, VERÓNICA CARCELEN<sup>2</sup>, MATTHIAS KRAUSE<sup>1</sup>, and SIBYLLE GEMMING<sup>1</sup> — <sup>1</sup>Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstr. 400, 01328 Dresden, Germany — <sup>2</sup>Abengoa Research, Energía Solar 1, Palmas Altas 41014, Sevilla, Spain

Absorber layers consisting of nanostructured Si are candidates to improve the efficiency of thin film Si solar cells. Si-SiO<sub>2</sub> nanocomposites with sponge-like Si embedded in SiO<sub>2</sub> are promising materials due to a widened band gap and a maintained electrical interconnectivity. These structures can be formed upon isothermal or rapid thermal annealing of SiO<sub>x</sub> films ( $x < 1$ ), which leads to phase separation into a percolated network of Si nanowires embedded in SiO<sub>2</sub>, tentatively accompanied by crystallization of the Si. SiO<sub>x</sub> layers have been grown by ion beam sputter deposition as well as by reactive magnetron sputtering. Phase separation into Si-SiO<sub>2</sub> nanocomposites has been achieved by classical thermal oven treatment, which has been compared to a very rapid thermal processing by scanning a diode laser line source. Composi-

tional and structural characterization has been performed by Rutherford backscattering spectroscopy, energy filtered transmission electron microscopy, and Raman spectroscopy. The two sputter techniques of SiO<sub>x</sub> lead to distinct nanostructures during the classical thermal treatment throughout a phase separation in the solid state. In contrast, the decomposition with laser treatment occurs in the liquid state.

DS 36.2 Thu 9:30 Poster A

**Reflectometry as a non-destructive tool for CZTS-synthesis control** — ●STEPHAN VAN DUREN, SERGIU LEVCENCO, JUSTUS JUST, and THOMAS UNOLD — Helmholtz-Zentrum Berlin, Hahn-Meitner-Platz 1, 14109 Berlin

Kesterite (Cu<sub>2</sub>ZnSnS<sub>4</sub> or CZTS) is an attractive non-toxic, earth abundant material for thin film solar cells. Current challenges are absorber homogeneity and reproducibility. In this study, reflectometry has been used to gain better understanding of the secondary phases, impure absorbers and its potential for in-situ process control. Ex-situ reflection measurements were performed on CuS, ZnS and CZTS absorbers with different composition. An in-situ reflection setup has been designed and built to be used in conjunction with a vacuum chamber. Temperature dependent reflection measurements were carried out to study

CuS and ZnS in a range from 25°C to 550 °C. A characteristic dip in the reflection spectrum around 620 nm of CuS was identified, also during thermal treatment. A structural change of the CuS to Cu<sub>2</sub>-xS could be deduced from the irreversible change of the reflection spectrum during annealing to 550°C. For a ZnS thin film, a phase shift and reduction of the interference pattern amplitude was observed across the full spectral range (UV-VIS-NIR) after annealing at 500°C. From comparison with XRD measurements of samples before and after annealing we attribute these changes to an improved crystallinity of the layer and changes in the optical constants. Experimental results have been compared with several simulated configurations such as ZnS/CZTS/Mo, CuS/CZTS/Mo and CZTS/Mo.

DS 36.3 Thu 9:30 Poster A

**The maximum crystal growth velocity of phase-change materials** — PETER ZALDEN<sup>2</sup>, ●ALEXANDER VON HOEGEN<sup>1</sup>, AARON LINDENBERG<sup>2</sup>, and MATTHIAS WUTTIG<sup>1</sup> — <sup>1</sup>Physikalisches Institut (IA), RWTH Aachen University, 52066 Aachen, Germany — <sup>2</sup>Department of Materials Science and Engineering, Stanford University, Stanford, California, 94305, USA

The crystallization process is the time limiting step in the switching cycle of a phase-change memory device (PCRAM). We present a technique to determine crystal growth velocities of amorphous thin films over a wide temperature range. It is based on the repetitive excitation of the glass with femtosecond optical pulses and probing the transient optical reflectivity. Due to the fast cooling rate, this technique allows reaching the supercooled liquid state up to the melting point of the corresponding crystalline phase. For the phase-change material Ag<sub>4</sub>In<sub>3</sub>Sb<sub>67</sub>Te<sub>26</sub> (AIST) we obtain a maximum crystal growth velocity of more than 100 m/s and are able to probe it up to the melting temperature. The resulting data contains additional information about the glass transition and the kinetic fragility.

DS 36.4 Thu 9:30 Poster A

**Growth Study of the Ternary Compound Sn<sub>1</sub>Bi<sub>2</sub>Te<sub>4</sub> via UHV DC Magnetron Sputter Deposition** — ●JURI BANCHEWSKI<sup>1</sup>, FELIX R.L. LANGE<sup>1</sup>, TOBIAS SCHÄFER<sup>1</sup>, JONAS HUYENG<sup>1</sup>, STEFAN JAKOBS<sup>1</sup>, and MATTHIAS WUTTIG<sup>1,2</sup> — <sup>1</sup>Physikalisches Institut (IA), RWTH Aachen University, Germany — <sup>2</sup>JARA - Fundamentals of Information Technology, RWTH Aachen University, Germany

The development of high-speed optical data storage and non-volatile memory has gained increasing attention in the last decades. Allowing a switching mechanism between structural phases on a nanosecond timescale, Phase Change Materials (PCM) are some of the most promising materials for future data storage applications [1]. Stoichiometric compounds like the pseudo-binary Ge<sub>1</sub>Sb<sub>2</sub>Te<sub>4</sub> with an additive Sn<sub>1</sub>Bi<sub>2</sub>Te<sub>4</sub> alloy have already been tested and proved to show enhanced crystallization kinetics [2]. Both constituents exhibit an amorphous, a metastable cubic and a stable hexagonal phase dependent on growth parameters and post-treatment. In terms of optimizing device parameters, full control of structural ordering is essential.

Here, we have performed a growth study of Sn<sub>1</sub>Bi<sub>2</sub>Te<sub>4</sub> on mica and silicon by DC magnetron sputter deposition under UHV conditions. The growth was carried out at elevated substrate temperature in order to investigate the structural and morphological evolution of the alloy.

[1] Matthias Wuttig and Noboru Yamada. *Nature Materials* 6, 824-832 (2007)

[2] Tae-Yon Lee and Ki-Bum Kim. *Appl. Phys. Lett.* 80, 3313 (2002)

DS 36.5 Thu 9:30 Poster A

**Photoelectron Spectroscopy Study of Disorder Controlled Ge<sub>1</sub>Sb<sub>2</sub>Te<sub>4</sub>** — ●MATTHIAS M. DÜCK<sup>1</sup>, FELIX R. L. LANGE<sup>1</sup>, TOBIAS SCHÄFER<sup>1</sup>, SEBASTIAN MÄDER<sup>1</sup>, HANNO VOLKER<sup>1</sup>, and MATTHIAS WUTTIG<sup>1,2</sup> — <sup>1</sup>Physikalisches Institut (IA), RWTH Aachen University, D-52056 Aachen, Germany — <sup>2</sup>JARA - Fundamentals of Information Technology, RWTH Aachen University, 52056 Aachen, Germany

Phase Change Materials (PCM) display a significant contrast in optical reflectivity and electrical resistivity upon crystallization, which is attributed to the formation of resonant bonding in the crystalline state. Due to the long-term stability of the phases as well as the ability to switch between the states reversibly on a nanosecond time scale, PCM are well suitable for fast non-volatile solid state memory devices.

In 2011, Siegrist et al. identified structural disorder to cause an Anderson-like insulator-to-metal transition in most phase-change materials along the line between GeTe and Sb<sub>2</sub>Te<sub>3</sub> [1]. In these materials Te atoms form an anion sublattice while the second site is randomly

occupied by Ge, Sb and a stoichiometric amount of vacancies. Via annealing these cation sites can be ordered, which finally triggers the transition from insulating to metallic behavior. Here we investigate this transition by means of photoelectron spectroscopy supported by Hall- and four-point resistivity as well as X-ray diffractometry measurements.

[1] Siegrist et.al. Disorder-induced localization in crystalline phase-change materials. *Nature Mater.* 10, 202-208 (2011)

DS 36.6 Thu 9:30 Poster A

**Investigation of the crystallization kinetics in the amorphous phase change material GeTe** — ●JULIAN PRIES<sup>1</sup>, JULIA BENKE<sup>1</sup>, MANUEL BORNHÖFFT<sup>2</sup>, JOACHIM MAYER<sup>2,3,4</sup>, and MATTHIAS WUTTIG<sup>1,3</sup> — <sup>1</sup>Physikalisches Institut IA, RWTH Aachen University, 52074 Aachen, Germany — <sup>2</sup>GFE, RWTH Aachen University, 52074 Aachen, Germany — <sup>3</sup>JARA-FIT, RWTH Aachen University, 52056 Aachen, Germany — <sup>4</sup>ER-C, FZJ, 52425 Jülich, Germany

Phase change materials are a group of materials which are able to be switched between the amorphous high resistive, low reflective state and the crystalline low resistive, high reflective state rapidly. This makes them potential candidates for memory applications such as non-volatile RAM. The amorphization can be done on a very short timescale compared to the more time consuming recrystallization. In order to speed up the data writing and erasing rate in a memory device, a better understanding of the recrystallization speed is essential.

Therefore, thin film GeTe samples were prepared and heated in order to induce crystal grains. After heating, the samples were investigated by a Transmission Electron Microscope (TEM) to measure the size of crystalline grains. From alternating heating and TEM measurements, we could determine crystal growth velocities.

DS 36.7 Thu 9:30 Poster A

**Electrical Properties of Textured Thin Films of the Phase Change Material GeSb<sub>2</sub>Te<sub>4</sub>** — ●ENNO BRÖRING<sup>1</sup>, TOBIAS SCHÄFER<sup>1</sup>, FELIX R. L. LANGE<sup>1</sup>, HANNO VOLKER<sup>1</sup>, and MATTHIAS WUTTIG<sup>1,2</sup> — <sup>1</sup>Physikalisches Institut (IA), RWTH Aachen University, Germany — <sup>2</sup>JARA - FIT, RWTH Aachen, Germany

Phase change materials (PCM) are an interesting sub-class of chalcogenides with unique properties. The material can be switched between the amorphous und crystalline state within nanoseconds. Both phases are stable at ambient conditions and differ in their optical and electrical properties. Therefore the materials are of big interest for data storage (e.g. solid state memories). The amorphous state shows an insulating behaviour with a high resistance while the resistance of the crystalline state is orders of magnitude smaller. The crystalline state shows unique features like resonant bonding and disorder induced localization (Anderson localization). Former studies have shown a metallic as well als insulating behaviour for the crystalline state. These measurements were focused on highly disordered polycrystalline films.

Here we present the electrical properties of textured GeSb<sub>2</sub>Te<sub>4</sub> phase change films. The material is sputter deposited on different heated substrates to achieve a close to epitaxial growth leading to lower disorder. The quality of the textured films is measured by x-ray diffractometry. The influence of texture on the electrical properties is determined via low temperature transport measurements.

DS 36.8 Thu 9:30 Poster A

**Chalcogenide Superlattices (CSL) for Energy Efficient Data Storage by Magnetron Sputtering** — ●FELIX LANGE<sup>1</sup>, JAMO MOMAND<sup>2</sup>, HENNING HOLLERMANN<sup>1</sup>, JURI BANCHEWSKI<sup>1</sup>, STEFAN JAKOBS<sup>1</sup>, ANDREA REDAELLI<sup>3</sup>, ENRICO VARES<sup>3</sup>, BART J. KOOI<sup>2</sup>, and MATTHIAS WUTTIG<sup>1,4</sup> — <sup>1</sup>Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen, Germany — <sup>2</sup>Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands — <sup>3</sup>Micron Semiconductor Italia, Process R&D, Agrate Brianza, Italy — <sup>4</sup>JARA - Fundamentals of Information Technology, RWTH Aachen University, 52056 Aachen, Germany

Phase change materials (PCM), as a sub-group of the chalcogenides, have already been extensively used in rewritable optical data storage (e.g. CD-RW). Since they combine scalability and fast switching speed with low power consumption, they are nowadays traded as promising candidates for next-generation memory, most suitable for mobile applications. Only recently it has been proposed, that the performance could be even enhanced, by using superlattices of GeTe and Sb<sub>2</sub>Te<sub>3</sub> instead of just bulk (Sb<sub>2</sub>Te<sub>3</sub>)<sub>x</sub>(GeTe)<sub>y</sub> (GST). It is argued that in this case, the change in electrical resistivity would be realized by a change

in atomic coordination of Germanium at the interfaces only. Here we explore the feasibility to grow highly textured thin alternating layers of GeTe and Sb<sub>2</sub>Te<sub>3</sub> using DC magnetron sputter deposition by using X-ray diffraction and transmission electron microscopy (TEM) techniques.

DS 36.9 Thu 9:30 Poster A

**Characterization of laser irradiated Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub> films by Cs-corrected STEM** — ●ANDRIY LOTNYK, XINXING SUN, SABINE BERNÜTZ, MARTIN EHRHARDT, and BERND RAUSCHENBACH — Leibniz Institute of Surface Modification, Permoserstr. 15, D-04318, Leipzig, Germany

Phase change materials become more and more important for data storage application due to their technologically eminent optical and electronic properties. In particular, Te-based Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub> (GST) material is of high interest because of its outstanding switching times and thermal stability. In this study, we have investigated the microstructure of amorphous and metastable GST thin films grown onto SiO<sub>2</sub>/Si substrates by using aberration-corrected scanning transmission electron microscope (STEM). Amorphous GST thin films were deposited by pulsed laser deposition at a room temperature. Crystallisation of the amorphous GST films was induced by using fs- and ns-laser pulses. The specimens for STEM studies were prepared by a combination of focused Ga ion beam and focused low-energy Ar ion beam techniques. X-ray spectroscopy data showed a homogeneous composition of GST thin films with a slight local variation in Ge, Sb and Te content. However, the grain size and morphology in the crystallized GST films varied with the applied laser pulse duration. The results on local atomic structure supported by image simulations will be also presented and discussed.

DS 36.10 Thu 9:30 Poster A

**Epitaxial Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub> thin films on Silicon Substrate by Pulsed Laser Deposition** — ●ISOM HILMI, ERIK THELANDER, JÜRGEN GERLACH, PHILIPP SCHUMACHER, DIETMAR HIRSCH, and BERND RAUSCHENBACH — Leibniz-Institut für Oberflächenmodifizierung e. V., 04318 Leipzig

Ge-Sb-Te based material is one of the most widely investigated phase change materials (PCM) for the data storage application. Recently, the more oriented crystalline state of GST-based PCM storage device has been shown having lower switching energy. Further result showed that epitaxial Ge-Sb-Te films in highly ordered atomic arrangement has been achieved using MBE, although there is a severe limitation regarding the deposition rate. Pulsed Laser Deposition (PLD) offers high rate deposition, and has been successfully employed for deposition Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub> (GST), which is interesting for industrial point of view.

Thin films of Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub> (GST) have been deposited on single crystal Si(111) substrate by means of PLD, over a substrate temperature range from room temperature to ~300°C. The crystallinity and epitaxial content of the films were then analyzed using x-ray diffraction based methods and their surface topographies were studied using AFM. At low substrate temperatures strongly textured hexagonal (0001) oriented polycrystalline films are obtained. At higher substrate temperatures epitaxial films forms. At temperatures in the near of 300°C, loss of Ge and Te was also found which resulted in a shift in composition from Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub> to Ge<sub>1</sub>Sb<sub>2</sub>Te<sub>4</sub>. In conclusion, PLD can be used to deposit high quality epitaxial Ge-Sb-Te layers on Si(111) substrates.

DS 36.11 Thu 9:30 Poster A

**Resistive Switching Properties of Chemically Synthesized TiO<sub>2</sub> Nanoparticles and Sb<sub>2</sub>Te<sub>3</sub> Hexagonal Platelets** — ●TOBIAS SALTZMANN<sup>1</sup>, DIRK OLIVER SCHMIDT<sup>1</sup>, HEHE ZHANG<sup>2</sup>, MANUEL BORNHÖFFT<sup>3</sup>, MICHAEL NOYONG<sup>1</sup>, SUSANNE HOFFMANN-EIFERT<sup>2</sup>, JOACHIM MAYER<sup>3</sup>, and ULRICH SIMON<sup>1</sup> — <sup>1</sup>IAC, RWTH Aachen University and JARA - FIT, 52074 Aachen, Germany — <sup>2</sup>Forschungszentrum Juelich GmbH, PGI 7 and JARA - FIT, 52425 Juelich, Germany — <sup>3</sup>GFE, RWTH Aachen University, Aachen, 52074, Germany

We chemically synthesized TiO<sub>2</sub> nanoparticles (NPs) and Sb<sub>2</sub>Te<sub>3</sub> hexagonal platelets (HPs) as resistively switching nanostructures and electrically characterized these structures in situ in a SEM by means of a nanomanipulator setup. As a model material for phase change switching, we synthesized single crystalline Sb<sub>2</sub>Te<sub>3</sub> HPs via a solvothermal reaction route. We identified four characteristic reaction intermediates and monitored their evolution by means of nanodiffraction in a STEM. The single HPs were electrically addressed and we monitored phase change switching. As model valence change material

we synthesized spherical TiO<sub>2</sub> NPs which were subsequently calcined or vacuum-annealed, respectively. For vacuum-annealed NPs we report I-V curves exhibiting forming-free bipolar as well as complementary resistive switching, whereas as synthesized or calcined NPs showed no I-V hysteresis. The properties of the individual NPs were compared with TiO<sub>x</sub> thin films grown by atomic layer deposition, from which comparable results were obtained.

DS 36.12 Thu 9:30 Poster A

**Suppressing a Charge Density Wave by Changing Dimensionality in the Ferecrystalline Compounds ([SnSe]<sub>1.15</sub>)<sub>1</sub>(VSe<sub>2</sub>)<sub>n</sub> with n = 1, 2, 3, 4** — ●ANDREAS FIEDLER<sup>1</sup>, MATTHIAS FALMBIGL<sup>2</sup>, DAVID C. JOHNSON<sup>2</sup>, and SASKIA F. FISCHER<sup>1</sup> — <sup>1</sup>Novel Materials, Department of Physics, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — <sup>2</sup>Department of Chemistry, University of Oregon, Eugene OR 97401-3753, USA

The compounds, ([SnSe]<sub>1.15</sub>)<sub>1</sub>(VSe<sub>2</sub>)<sub>n</sub> with n = 1, 2, 3, and 4, were prepared using designed precursors in order to investigate the influence of the thickness of the VSe<sub>2</sub> constituent on the charge density wave transition found in [1]. The structure of each of the compounds was confirmed by X-ray diffraction and scanning-transmission electron microscopy. The charge density wave transition observed in the resistivity of ([SnSe]<sub>1.15</sub>)<sub>1</sub>(VSe<sub>2</sub>)<sub>1</sub> was confirmed and is suppressed as the layer thickness of the VSe<sub>2</sub> constituent is increased beyond a single layer. The temperature of the resistivity minimum systematically increases from 118 K (n = 1) to 172 K (n = 3). For n = 1 this temperature correlates with the charge density wave transition temperature. The Hall-coefficient also changes sign when n is greater than 1, reflecting the abrupt difference in electronic properties on increasing the thickness of the VSe<sub>2</sub> layer beyond a single layer.

[1] Atkins, R. *et al.*: *Chem. Mater.*, **26** (9), 2862–2872, (2014).

DS 36.13 Thu 9:30 Poster A

**Setup and characterization of an optical tester for in-situ experiments on the switching behavior of phase-change materials** — ●CHRISTOPH PERSCH, JULIA BENKE, and MATTHIAS WUTTIG — 1.Physikalisches Institut IA, RWTH Aachen University, 52074 Aachen, Germany

Phase-change materials constitute a class of materials characterized by a pronounced difference in physical properties between the crystalline and the amorphous phase. The crystalline state usually features a low electric resistance and a high reflectivity while the amorphous state features a high electric resistance and a low reflectivity. As phase transitions are inherently fast, phase-change materials are of great interest for non-volatile memory applications, such as solid state PC-RAM or optical storage media.

To investigate the switching behavior of phase-change materials, a measurement setup comprised of a pulse-probe laser system and a detection unit has been established. To induce phase transition by thermal activation, the high-power pulse laser (405nm) generates flat-top nanosecond pulses. The change in reflectivity is measured simultaneously with a bandwidth of 1.2 GHz, using the probe laser (445nm) and the detection unit. In addition, the measurement setup is thoroughly analyzed regarding its performance characteristics to allow for precise and reliable experiments.

DS 36.14 Thu 9:30 Poster A

**Preparation and Characterization of H<sub>2</sub>S-Sensors based on Cu<sub>2</sub>O deposited by RF-sputtering** — ●CHRISTIAN KANDZIA<sup>1</sup>, PHILIPP HERING<sup>1</sup>, JÖRG HENEMANN<sup>2</sup>, ANGELIKA POLITY<sup>1</sup>, BRUNO MEYER<sup>1</sup>, and BREND SMARSLY<sup>2</sup> — <sup>1</sup>1.Physikalisches Institut, Justus Liebig Universität Gießen, Heinrich-Buff-Ring 16 — <sup>2</sup>Physikalisch-Chemisches Institut, Justus-Liebig Universität Gießen, Heinrich-Buff-Ring 58

Cuprite (Cu<sub>2</sub>O) is an oxide-semiconductor with a direct band gap of 2.1 eV. It can be used for example as a sensor element for H<sub>2</sub>S-Gas exposure. For this purpose, thin films were deposited by RF-sputtering on c-sapphire and quartz-glass heated at 650 °C to provide good film-quality. During the sputtering process different amounts of hydrogen were added, which have effects on the morphology. These sensors were aerated with a gasmixture of synthetic air and H<sub>2</sub>S. After exposure the material reacts to Cu<sub>x</sub>S which has a significantly higher conductivity. It is found that the conductivity increase is due to percolation paths on the surface. This switching threshold is investigated dependent on the surface-morphology. Beside the samples were investigated by XRD-, SEM-, transmission- and Hall-measurements.

DS 36.15 Thu 9:30 Poster A

**Frequency dependent measurements of Ta<sub>2</sub>O<sub>5</sub> and BaTiO<sub>3</sub>-based memristors** — ●LAURITZ SCHNATMANN, NORMAN SHEPHEARD, STEFAN NIEHÖRSTER, SAVIO FABRETTI, and ANDY THOMAS — Center for Spinelectronic Materials and Devices, Physics Department, Bielefeld University, Germany

Memristors can be used to develop new computer components and increase the efficiency of computers. With this new component computers might be able to learn even without complex programming.

We investigated thin memristive tunneling barriers of BaTiO<sub>3</sub> and Ta<sub>2</sub>O<sub>5</sub>. Beside a conventional i-v transport measurements, we carried out the frequency dependent measurements. Further, we varied the amplitude and investigated the different switching behaviors of our tunneling systems. For our measurements we chose frequencies from 0.006 mHz up to 2 mHz and amplitudes from 150 mV up to 325 mV.

Chua et al. [1] predict the switching behavior in 1976. He described the change of the switching behavior with frequency variation.

Another point of view gives the theory by Pershin and Di Ventra [2]. Memristors can be distinguished in two different types. The two types show different behaviors at the 0V point in the hysteresis loops, which is found for Ta<sub>2</sub>O<sub>5</sub> and BaTiO<sub>3</sub>, respectively.

[1] Chua et al. 'memristive devices and systems', Proceedings of the IEEE, 64, 209-223, 1976

[2] Yuriy V Pershin and Massimiliano Di Ventra 'Memory effects in complex materials and nanoscale systems', Advances in Physics, 60, 145-227, 2011

DS 36.16 Thu 9:30 Poster A

**TaO-based Memristive Tunnel Junctions and their Integration to neuromorphic Circuits** — ●STEFAN NIEHÖRSTER<sup>1</sup>, SAVIO FABRETTI<sup>1</sup>, LAURITZ SCHNATMANN<sup>1</sup>, ALESSIA NIESEN<sup>1</sup>, MARKUS SCHÄFFERS<sup>1</sup>, KARSTEN ROTT<sup>1</sup>, ANDY THOMAS<sup>1</sup>, and ELISABETTA CHICCA<sup>2</sup> — <sup>1</sup>Center for Spinelectronic Materials and Devices, Physics Department, Bielefeld University, Germany — <sup>2</sup>Neuromorphic Behaving Systems, CITEC, Bielefeld University, Germany

We produced memristive tunnel junctions by magnetron sputtering. They consist of a 2/3nm TaO barrier between a noble Pd electrode and an ignoble Ta electrode to generate two different interfaces. The barrier was fabricated by reactive sputtering of a Ta target in an atmosphere of 1:3 argon and oxygen. This improved the memristive switching to a value of more than 200% compared to 120% in former series with a plasma oxidized thin Ta film as barrier. These devices also can change their resistance continuously, so we are able to generate more than just two states, which is a fundamental condition for a synaptical behavior.

We succeeded in placing our working memristive devices on stated electrodes of a neuromorphic chip to take over the part of artificial synapses. To contact the devices to the chip, we had to overcome several obstacles like a 2μm thick protection layer and a large roughness, which results from the focused ion beam etching.

DS 36.17 Thu 9:30 Poster A

**Combined threshold and memory resistive switching in Pt/Nb<sub>2</sub>O<sub>5</sub>/Ti/Pt crossbar structures obtained from amorphous Nb<sub>2</sub>O<sub>5</sub> thin films** — ●CARSTEN FUNCK, NABEEL ASLAM, STEPHAN MENZEL, EIKE LINN, and SUSANNE HOFFMANN-EIFERT — Peter Grünberg Institut (PGI-7) and JARA-FIT, Forschungszentrum Jülich, 52425 Jülich, Germany

Redox-based resistive switching memory cells (ReRAM) are intensively studied due to their potential to fulfill the increasing demands of future information technology. ReRAM can be realized in passive crossbar arrays, representing the highest integration density. Unfortunately, the leakage current through unselected cells limits the selectivity and the maximum size of the array. Therefore, selector elements are required to overcome this "sneak path" problem. ReRAM cells based on niobium oxide allow the integration of selector and memory element in one cell. Nb<sub>2</sub>O<sub>5</sub> is an insulator allowing for VCM-type resistive switching while NbO<sub>2</sub> shows a temperature induced metal-insulator transition resulting in a negative differential resistance. The corresponding threshold switching behavior is a volatile resistance change which can be used as a highly non-linear selector. Pt/Nb<sub>2</sub>O<sub>5</sub>/Ti/Pt crossbar structures are fabricated from amorphous Nb<sub>2</sub>O<sub>5</sub> layers grown by atomic layer deposition. Tuning of the electrical stimuli during electroforming and resistive switching enables a control of the fraction of volatile threshold and non-volatile memory switching. An empirical model of the switching behavior is presented and first results from a finite element

simulation of the threshold behavior.

DS 36.18 Thu 9:30 Poster A

**Growth of VO<sub>2</sub> thin films by low-oxygen MAD: influence of O<sub>2</sub>-background** — ●SVEN ESSER, VICTOR PFAHL, SEBASTIAN HÜHN, MARKUS MICHELMANN, and VASILY MOSHNYAGA — 1. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

A possible candidate for a fast optical switch (FOS) is VO<sub>2</sub> with structural phase transition at 340 K and coupled metal insulator transition (MIT) with a resistivity change by 3-4 orders of magnitude [1,2]. MIT can also be driven quasi optically, which opens the possibility for application as FOS [3].

Due to several possible oxidation states of vanadium, different vanadium oxides (VO, V<sub>2</sub>O<sub>3</sub>, VO<sub>2</sub>, V<sub>2</sub>O<sub>5</sub>, ... [4]) can be prepared. For high quality films of definite composition a precise control of the oxygen background during preparation is necessary.

We report the growth of epitaxial VO<sub>2</sub> and V<sub>2</sub>O<sub>3</sub> thin films on Al<sub>2</sub>O<sub>3</sub> substrates by controlling the chamber pressure with LO-MAD technique. The thin films were characterized by x-ray diffraction and by scanning tunneling microscopy. Resistivity measurements reflect the influence of the O<sub>2</sub>-background on the shape and position of the MIT.

This work is supported by the German Science Foundation through SFB 1073, TP B04.

[1] V. Eyert, Ann. Phys. (Leipzig) **11**, 650-702 (2002)

[2] H.S. Choi *et al.*, Phys. Rev. B **54**, 4621 (1996)

[3] S. Chen *et al.*, Infra. Phys. & Techn. **45**, 239-242 (2004)

[4] A. Stork, Dissertation, TU Berlin (2011)

DS 36.19 Thu 9:30 Poster A

**Growth and Modification of single-crystalline VO<sub>2</sub> Nanostructures** — ●ALEXANDER TILLE, TIM BARTH, JURA RENSBERG, and CARSTEN RONNING — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Unstrained single-crystalline Vanadium dioxide (VO<sub>2</sub>) nanostructures show an extremely sharp metal-insulator phase transition (MIT) at a critical temperature of 68 °C. Phase pure VO<sub>2</sub> has a narrow existence region in the V-O-phase diagram, thus mixed vanadium oxides (VO<sub>x</sub>) are easily obtained by thermal annealing of VO<sub>2</sub> in either reducing or oxidizing environment. In this work free-standing, single-crystalline VO<sub>2</sub> nanowires were grown on SiO<sub>2</sub> substrates using an evaporation method. After transfer to a clean insulating substrate, NWs were annealed up to 600 °C in both ambient atmosphere and high vacuum. In both cases, temperature dependent electrical measurements show a shift of the critical temperature to lower values. Furthermore, temperature dependent Raman spectroscopy reveals a correlation between this shift and the structural properties of the NWs. Thus, we gained a deeper insight in the relationship between the structure and the critical temperature of the MIT.

DS 36.20 Thu 9:30 Poster A

**Investigation of oxygen vacancies in HfO<sub>2</sub> from density functional theory** — ●MARTA GIBERTINI, DANIEL WORTMANN, ANDREA NOBILE, and STEFAN BLÜGEL — Peter Grünberg Institute (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich GmbH and JARA, Jülich, Germany

Study of point defects in materials is important to understand the role that they play in electronic devices such as the resistive random access memory (ReRAMs). The exact mechanism of switching of a ReRAMs between two states: low and high resistance, is unknown, but the movement of oxygen vacancies in an oxide, under applied electrical field is an important ingredient.

In this poster we present a density functional theory study of oxygen vacancies in HfO<sub>2</sub> employing the electronic structure code juRS, a real-space finite-difference implementation of the projector augmented wave (PAW) method. First the optimized lattice parameters, band structures and band gaps are calculated for the three different crystalline phases of HfO<sub>2</sub> and compared with experimental results from literature. Then, the nature and stability of defects in different positions is studied in a monoclinic crystal supercell. Furthermore, we will present the energy barrier for defect migration on different paths using the nudged elastic band (NEB) method.

– Work is supported by SFB 917 (Nanoswitches).

DS 36.21 Thu 9:30 Poster A

**Resistive switching behavior of HfO<sub>2</sub> thin films grown by plasma-assisted atomic layer deposition** — ●ALEXANDER HARDTDEGEN and SUSANNE HOFFMANN-EIFERT — Peter Grünberg Institut (PGI-7) and JARA-FIT, Forschungszentrum Jülich, 52425 Jülich, Germany

Thin films of HfO<sub>2</sub> utilized in resistive switching memory (ReRAM) devices are usually grown by sputtering or thermal atomic layer deposition (ALD) using water or ozone as oxygen sources. Another interesting technique is plasma-assisted ALD, where the oxygen source is supplied by an oxygen-plasma. Advantages of this method are higher growth rates and extension of the ALD regime to lower deposition temperatures.

In this study we investigate the potential of plasma assisted ALD HfO<sub>2</sub> films for application in resistive switching memory cells. Thin HfO<sub>2</sub> films are grown by plasma assisted ALD from tetrakis[ethylmethylamino]hafnium (TEMAH) and oxygen plasma as the co-reactant. The effect of variations in the growth conditions on the thin films properties is analyzed. Thin film characterization with respect to the thickness, density, roughness, and chemical composition is performed by a variety of analytical methods.

Further, different HfO<sub>2</sub> films are integrated into metal/HfO<sub>2</sub>/metal crossbar structures of about 2 μm<sup>2</sup> size. The influence of the film quality and film thickness on the switching behavior is studied with respect to electroforming, SET and RESET steps, and the OFF/ON resistance ratio. The results are discussed in comparison to literature reports.

DS 36.22 Thu 9:30 Poster A

**Structural and electrical characterization of Ar<sup>+</sup> irradiated TiO<sub>2</sub> thin films** — ●DANIEL BLASCHKE<sup>1</sup>, AGNIESZKA BOGUSZ<sup>1</sup>, RENÉ HÜBNER<sup>1</sup>, FRANS MUNNIK<sup>1</sup>, RENÉ HELLER<sup>1</sup>, ANDREA SCHOLZ<sup>1</sup>, FRANZISKA NIEROBISCH<sup>1</sup>, VIKAS RANA<sup>3</sup>, SIBYLLE GEMMING<sup>1,2</sup>, and PETER ZAHN<sup>1</sup> — <sup>1</sup>Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf — <sup>2</sup>Chair of Scale-bridging Materials Modeling, Physics Department, TU Chemnitz — <sup>3</sup>Peter Grünberg Institut, Forschungszentrum Jülich

Transition metal oxide thin films, like TiO<sub>2</sub>, are promising candidates for future memory storage devices. They are extensively studied to get a better understanding of the role of oxygen for structural changes and electronic transport inside the films. A defective, nonstoichiometric TiO<sub>2-x</sub> layer can act as a reservoir for oxygen vacancies and improves the switching characteristics. Such a layer was introduced into the virgin TiO<sub>2</sub> film by low energy Ar<sup>+</sup> irradiation with different energies and fluencies to modulate the depths and level of the defective region. The impact of the irradiation to the surface morphology and crystal structure was monitored by AFM and TEM measurements and was found to be surface smoothing and amorphization. The role of the preferential sputtering of oxygen to the stoichiometry of the film was investigated with TRIDYN simulations. Electrical properties of the irradiated films were characterized by I-V and C-V measurements and are related to the structural changes caused by the Ar<sup>+</sup> irradiation.

The project is funded by the Initiative and Networking Fund of the Helmholtz Association (Virtual Institute Memriox, VH-VI-422).

DS 36.23 Thu 9:30 Poster A

**Introducing band gap states in MoS<sub>2</sub> monolayers by triangular defects** — TOMMY LORENZ<sup>1,2</sup>, PETER ZAHN<sup>1</sup>, ●SIBYLLE GEMMING<sup>1,3</sup>, ARTUR ERBE<sup>1</sup>, and GOTTHARD SEIFERT<sup>2</sup> — <sup>1</sup>Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden - Rossendorf e.V., 01314 Dresden, Germany. — <sup>2</sup>Theoretical Chemistry, TU Dresden, 01062 Dresden, Germany. — <sup>3</sup>Theoretical Physics, Faculty of Sciences, TU Chemnitz, 09107 Chemnitz, Germany.

Triangular defects in MoS<sub>2</sub> monolayers and their influence on the electronic structure have been studied using the density-functional based tight-binding (DFTB) method. Systems with different defect sizes and concentrations have been compared to find out how these parameters affect the electronic properties of MoS<sub>2</sub> monolayers. Furthermore, two different ways to saturate the defect edges were used to compare their influence. The density of states (DOS) calculations show the presence of additional states in the HOCO-LUCO-Gap of pristine MoS<sub>2</sub> even for small defects in a low concentration. These localized mid-gap states mainly arise from d-orbitals of the molybdenum atoms at the defect edges and their number increases with an increasing defect size. Due to the fact that the molybdenum d-states dominate the valence and conduction band edges of MoS<sub>2</sub>, additional states arise in the band gap, which may impact the electronic transport through the layer.

DS 36.24 Thu 9:30 Poster A

**Exciton Interactions in Two Dimensions** — ●VALENTIN WALTHER, ROBERT JOHNE, and THOMAS POHL — Max-Planck-Institut für Physik komplexer Systeme, Dresden

Recent experiments have shown that excitons with binding energies of up to 1 eV can be produced in a special class of two-dimensional semiconductors known as TMDCs (transition metal dichalogenides) [1].

We study the excited level structure of such excitons accounting for two-dimensional screening effects. Based on these results we explore the possibility to manipulate the properties by external fields. We determine the resulting interactions at asymptotic distances and discuss the importance of non-adiabatic effects.

[1] A. Chernikov et al., Phys. Rev. Lett. 113, 076802 (2014)

DS 36.25 Thu 9:30 Poster A

**Electrical transport studies of the turbostratically disordered ([SnSe]<sub>1+δ</sub>)<sub>m</sub>(NbSe<sub>2</sub>)<sub>1</sub> misfit layer compounds** — ●GEORG HOFFMANN<sup>1</sup>, CORINNA GROSSE<sup>1</sup>, ANDREAS FIEDLER<sup>1</sup>, MATTI B. ALEMAYEHU<sup>2</sup>, DAVID C. JOHNSON<sup>2</sup>, and SASKIA F. FISCHER<sup>1</sup> — <sup>1</sup>Neue Materialien, Institut für Physik, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — <sup>2</sup>Department of Chemistry and Materials Science Institute, University of Oregon, Eugene, Oregon 97403, United States

The control of material properties by combining layers with different properties is of great interest in the field of quasi-two-dimensional multilayer-systems. The turbostratically disordered misfit layer compounds, so called ferecrystals, have been established as promising novel materials, whose electric and magnetic properties can be systematically controlled by changing the stacking sequence. The effect of systematically increasing the SnSe layer thickness on the magnetoelectric transport is studied for ([SnSe]<sub>1+δ</sub>)<sub>m</sub>(NbSe<sub>2</sub>)<sub>1</sub> between 2 K and 300 K. The Hall coefficient and the resistivity increase with increasing *m* (number of SnSe layers between each NbSe<sub>2</sub> layer). While the temperature dependence of ([SnSe]<sub>1+δ</sub>)<sub>1</sub>(NbSe<sub>2</sub>)<sub>1</sub> is metallic, the measurements reveal an unexpected increase of the resistivity with decreasing temperatures below 20 K for *m* > 1. The increase of the resistivity increases with higher *m*. The Hall coefficient decreases with increasing temperature between 4.2 K and 50 K. Above 50 K the Hall coefficient increases with increasing temperature for *m* > 1. The influence of the stacking sequence is discussed.

DS 36.26 Thu 9:30 Poster A

**Global and local Raman characterization of double perovskite thin films** — ●HENDRIK EHLERS, CHRISTOPH MEYER, FLORIAN FISCHGRABE, VASILY MOSHNYAGA, BERND DAMASCHKE, and KONRAD SAMWER — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

B-site ordered double perovskites La<sub>2</sub>CoMnO<sub>6</sub> (LCMO) and Pr<sub>2</sub>CoMnO<sub>6</sub> (PCMO) with monoclinic P12<sub>1</sub>/n<sub>1</sub> structure can be derived from a single perovskite by alternating layers of Co<sup>2+</sup> and Mn<sup>4+</sup> on the B-site. They are promising for spintronic applications due to ferromagnetic ordering, spin-phonon and magnetodielectric coupling. Since the properties are strongly influenced by the type of the rare earth A-cation and by the degree of the ordering, we used Raman spectroscopy as a global and local tool to correlate the phonon spectra with B-site ordering and A-cation influence. Therefore far-field Raman and tip-enhanced Raman spectroscopy (TERS) of LCMO and PCMO thin films on SrTiO<sub>3</sub>(100) and SrTiO<sub>3</sub>(111) substrates, grown by metalorganic aerosol deposition (MAD), was performed. The spectra exhibit a strong A<sub>g</sub> mode in the 600 – 700 cm<sup>-1</sup> range, indicating B-site cation ordering. Applying TERS, the spectra reveal an enhancement in a parallel as well as in the cross-scattering configuration due to a combination of field enhancement and depolarization effects. Additionally we present first TERS results on single perovskite CaMnO<sub>3</sub> thin films with intensity enhancement and an emergence of a new phonon mode at 650 cm<sup>-1</sup>. Financial support for this work by the DFG via project SFB 1073/B04 is gratefully acknowledged.

DS 36.27 Thu 9:30 Poster A

**Bias Voltage Effect and Interfacial Capacitance of Manganite-Titanite Heterostructures** — ●VITALY BRUCHMANN-BAMBERG, MARKUS MICHELMANN, and VASILY MOSHNYAGA — I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Pl. 1, 37077 Göttingen

Dielectric properties and polarization switching in epitaxial thin films

of ferroelectric oxides are governed by both misfit strain and interfacial capacitance (so-called "dead layers"). While BaTiO<sub>3</sub>-based titanites as a thin film show a remarkable enhancement of the Curie-temperature under homogenous compressive strain, strain gradients are discussed as driving force behind the bias voltage and the loss of remanence in ferroelectric hysteresis loops due to the flexoelectric effect.

We prepared epitaxially grown metal-dielectric-metal heterostructures on SrTiO<sub>3</sub> substrates with metallic La<sub>0.7</sub>Sr<sub>0.3</sub>MnO<sub>3</sub>, ferroelectric Ba<sub>0.5</sub>Sr<sub>0.5</sub>TiO<sub>3</sub> and paraelectric SrTiO<sub>3</sub> by means of metalorganic aerosol deposition. By varying the BSTO-layer thickness, different stages of lattice relaxation with an in-plane compressive strain can be observed. Ferroelectric hysteresis is characterized by dielectric spectroscopy and the Positive-Up Negative-Down technique. Furthermore, an interfacial capacitance at the manganite-titanite-interface leads to a significant reduction of dielectric tunability and ferroelectric remanence. The results are discussed within the framework of flexoelectric coupling between strain and polarisation and interfacial Schottky-barrier formation. As an outlook, first results on engineering dead layers via an LaMnO<sub>3</sub> and SrMnO<sub>3</sub> interlayers and heterostructures with lattice matched Ba<sub>1-x</sub>Ca<sub>x</sub>TiO<sub>3</sub> films will be presented.

DS 36.28 Thu 9:30 Poster A

**Electrochemical analysis of LiPON-tungstenoxide thin-film-systems** — ●CHRISTOPHER JAMES, YURONG SU, ANGELIKA POLITY, and BRUNO K. MEYER — 1. physikalisches Institut der Justus Liebig Universität, Gießen, Deutschland

Amorphous glassy solid state electrolyte LiPON (lithiumphosphorousoxynitride) thin films were sputtered on amorphous electrochromic tungstenoxide (WO<sub>x</sub>) in order to investigate the electrochromic properties of tungstenoxide under the presence of a solid state electrolyte. The LiPON films were deposited by sputtering. Before deposition of LiPON, the WO<sub>x</sub> films were either deintercalated (transparent) or intercalated (darkblue). Since during the sputterprocess colouration could not be prevented at any time, sputter parameters were found for homogeneous colouration of the WO<sub>x</sub>. Cyclic voltammetry (CV) was then applied to LiPON/WO<sub>x</sub>- and to raw WO<sub>x</sub>-samples in order to investigate the colouration efficiency of WO<sub>x</sub> with and without LiPON. CV results revealed a significant degradation of included charge densities being incorporated during cycling, which means colouration changes of the tungstenoxide could hardly be enhanced with CV. With CV, only slight bleaching of the pre-coloured WO<sub>x</sub> layer was achieved. It can be suggested, that Li ion sites in the electrochromic film became occupied by pre-colouration, so during sputter process these sites could no more be irreversibly intercalated. EIS (electrochemical impedance spectroscopy) results revealed an ionic conductivity of the LiPON films of the order of  $\mu\text{S cm}^{-1}$ .

DS 36.29 Thu 9:30 Poster A

**Alternative transparent electrode for inorganic solar cells based on amorphous silicon** — ●DANIEL ROSENKRANZ<sup>1</sup>, ALEX NEUMÜLLER<sup>2</sup>, MATIN VEHESE<sup>2</sup>, JÜRGEN PARISI<sup>1</sup>, and MANUELA SCHIEK<sup>1</sup> — <sup>1</sup>Department of Physics, University of Oldenburg, 26111 Oldenburg, Germany — <sup>2</sup>NEXT ENERGY EWE-Forschungszentrum für Energietechnologie e. V., Carl-von-Ossietzky-Straße 15, 26129 Oldenburg

Today there is a great research interest into developing alternative transparent electrodes with high transparency and low sheet resistance for different applications. One candidate are silver nanowires (AgNW) arranged into high transparent, flexible networks with low sheet resistance. These resulting properties are depending on nanowire geometry and network processing. Here a polyol synthesis will be used to get very long and thin nanowires with high aspect ratios. Furthermore, a spray coating method is used to prepare the nanowire networks for a top or back contact in solar cells based on amorphous silicon. At the backside of the solar cell the nanowire network can be smelted to receive well distributed silver spots/particles which can scatter light into the active layer. For dual performance as electrode and light-managing layer they are sandwiched between sputtered aluminium-doped zinc oxide (AZO) layers. In this work we prepare and characterize (optical, electrical and structural) thin stacks of AZO-AgNW-AZO with a defined roughness for light trapping based on the scattering effect of AgNWs.

DS 36.30 Thu 9:30 Poster A

**Electric characterization of single crystalline and polycrystalline CZTS films and bulk material** — ●MARTIN HANDWERG<sup>1,2</sup>, RÜDIGER MITDANK<sup>1</sup>, JUSTUS JUST<sup>2</sup>, SEGEJ LEVCENCO<sup>2</sup>, THOMAS UNOLD<sup>2</sup>, and AND SASKIA F. FISCHER<sup>1</sup> — <sup>1</sup>AG Neue Materi-

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Copper Zinc Tin Sulfide (CZTS) is investigated as absorption layer for solar cells to increase their efficiency. Because of the large number of stoichiometric combinations, detailed and systematic investigations of the electric and thermal transport properties need to be carried out and correlated to the structure and composition. Here, the temperature dependence of the resistivity of polycrystalline films with different composition from high copper ( $2.29 n_{\text{Cu}}/n_{\text{Zn}+\text{Sn}}$ ) to low copper amount ( $0.47 n_{\text{Cu}}/n_{\text{Zn}+\text{Sn}}$ ) is measured out using the van-der-Pauw method. Resistance and Hall measurements were performed on CZTS single crystals as well. All measurements were performed between 4.2 K and 300 K. The measured electric conductivity values can be compared to reported measurements [1] and discussed in relation to their stoichiometric compound.

[1] Wu Xinkun *et al.*, 2012, J. Semicond., **33**(2)

DS 36.31 Thu 9:30 Poster A

**Transparent conductive ZnO layers on polymer substrates: thin film deposition and application in organic solar cells** — ●M DOSMAILOV<sup>1</sup>, LN LEONAT<sup>2</sup>, J PATEK<sup>1</sup>, D ROTH<sup>3</sup>, P BAUER<sup>3</sup>, MC SCHARBER<sup>2</sup>, NS SARICIFTCI<sup>2</sup>, and JD PEDARNIG<sup>1</sup> — <sup>1</sup>Institute of Applied Physics, Johannes Kepler University Linz, A-4040 Linz, Austria — <sup>2</sup>Linz Institute for Organic Solar Cells (LIOS) / Institute of Physical Chemistry, Johannes Kepler University Linz, A-4040 Linz, Austria — <sup>3</sup>Institute of Experimental Physics, Johannes Kepler University Linz, A-4040 Linz, Austria

Aluminum doped ZnO (AZO) and pure ZnO thin films are grown on polymer substrates by pulsed-laser deposition and the optical, electrical, and structural film properties are investigated. Laser fluence, substrate temperature, and oxygen pressure are varied to obtain transparent, conductive, and stoichiometric AZO layers on polyethylene terephthalate (PET) that are free of cracks. At low fluence ( $1 \text{ J/cm}^2$ ) and low pressure ( $10^{-3}$  mbar), AZO/PET samples of high optical transmission in the visible range, low electrical sheet resistance, and high figure of merit (FOM) are produced. AZO films on fluorinated ethylene propylene have low FOM. The AZO/PET substrates are used in inverted organic solar cell devices employing P3HT:PCBM as photovoltaic polymer-fullerene bulk heterojunction. The power conversion efficiency is  $\eta = 2.1 \%$  with the AZO thin films serving as electron transport layer.

DS 36.32 Thu 9:30 Poster A

**Study of the properties of sputtered TCO layers on flexible glass** — ●JASPER WESTPHALEN<sup>1,2</sup>, MANUELA JUNGHÄHNEL<sup>2</sup>, STEPHANIE WELLER<sup>2</sup>, and EDDA RÄDLEIN<sup>1</sup> — <sup>1</sup>Technische Universität Ilmenau, Department of Inorganic-Nonmetallic Materials, Ilmenau, Germany — <sup>2</sup>Fraunhofer Institute for Organic Electronics, Electron Beam and Plasma Technology FEP, Dresden, Germany

Ultra-thin glass is a new flexible substrate material for electronics and display applications. Transparent conductive oxides (TCOs) are a key material for transparent electrodes for photovoltaics. In this study, aluminum doped zinc oxide (AZO) films were deposited by magnetron sputtering on different flexible glasses.

The influence of the deposition parameters including oxygen partial pressure and substrate temperature on the surface morphology, electrical, optical and mechanical properties of the films were investigated.

In order to improve the optical and the electrical properties, we used flash lamp annealing (FLA) as a post-deposition annealing method for ultra-short thermal treatment in the millisecond range.

The film thickness was determined by mechanical measurements with an XP-200 stylus profiler (AMBIOS technology). We measured the transmittance and reflectance with the optical spectrometer Lambda 19 (Perkin Elmer) in the range of 300 to 2000 nm. The sheet resistance R has been measured with a four point probe FPP 5000 from Veeco Instruments.

DS 36.33 Thu 9:30 Poster A

**Optical and electrical characterization of TiO<sub>2</sub>- and SnO<sub>2</sub>-based transparent conductive oxides** — ●FRANK LUNGWITZ<sup>1</sup>, ERIK SCHUMANN<sup>1</sup>, MARCEL NEUBERT<sup>2</sup>, MATTHIAS KRAUSE<sup>1</sup>, and SIBYLLE GEMMING<sup>1,3</sup> — <sup>1</sup>Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstraße 400, 01328 Dresden — <sup>2</sup>DTF Technology GmbH, Am Promberg 16, 01108 Dresden — <sup>3</sup>Chemnitz University of Technology, 09092 Chemnitz

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Transparent conductive oxides (TCOs) are already widely used in the optoelectronic industry e.g. as electrodes for liquid crystal displays (LCDs), organic light emitting diodes (OLEDs), or thin film solar cells. Less attention has been devoted to their optical properties and thermal stability until now. In this work, Tantalum doped TiO<sub>2</sub> and SnO<sub>2</sub> TCO films are investigated with respect to their structural, optical, and electrical properties at temperatures from RT to 700 °C. The films are prepared at room temperature by direct current reactive magnetron sputtering from metallic as well as ceramic targets and subsequently isothermally annealed at temperatures of 425 °C. For compositional and structural analysis x-ray diffraction (XRD), Raman spectroscopy, and Rutherford backscattering spectroscopy (RBS) are used. The optical properties are determined by spectroscopic ellipsometry, spectral photometry, and subsequent modelling. Hall effect measurements are used to determine the electrical properties of the TCO films. The as-deposited layers are amorphous and isolating. By thermal annealing they are activated and become conductive.

DS 36.34 Thu 9:30 Poster A

**A polymer nanogenerator based on silver nanoparticles doped electrospun P(VDF-HFP) nanofibers** — DIPANKAR MANDAL<sup>1</sup>, •KARSTEN HENKEL<sup>2</sup>, and DIETER SCHMEISSER<sup>2</sup> — <sup>1</sup>Organic Nano-piezoelectric Device Laboratory, Department of Physics, Jadavpur University, Kolkata 700032, India — <sup>2</sup>Angewandte Physik - Sensorik, Brandenburgische TU Cottbus-Senftenberg, K.-Wachsmann-Allee 17, 03046 Cottbus, Germany

The rising energy demand within the increasing mobility of human society has driven the development of new alternative power sources for portable devices with ultra-low electric power consumption.

Based on its piezoelectric properties poly(vinylidene fluoride (PVDF) is a good candidate for mechanical energy harvesting for such devices. Moreover the copolymer poly(vinylidene fluoride-hexafluoropropylene) [P(VDF-HFP)] offers better film flexibility and cost-effectiveness than pure PVDF.

We report on a polymer nanogenerator (PNG) based on electrospun P(VDF-HFP) nanofibers doped with silver nanoparticles (Ag-NPs). The electrospun fibers were characterized by FTIR, XPS, SEM and pressure imparting probe. It has been found that the yield of the piezoelectric phase is increased by the addition of Ag-NPs due to an interaction between surface charges of Ag-NPs and the molecular dipoles. Furthermore, defects in the P(VDF-HFP) electrospun fibers are removed. Accordingly, a significant enhancement in the output power of the PNG was found. Similar trends were also observed with Pd-NPs.

DS 36.35 Thu 9:30 Poster A

**RHEED-based investigations of (La<sub>2</sub>/3Sr<sub>1</sub>/3)<sub>x</sub>Mn<sub>y</sub>O<sub>z</sub> thin film growth** — •ALEXANDRA STEFFEN<sup>1</sup>, SABINE PÜTTER<sup>1</sup>, JÜRGEN SCHUBERT<sup>3</sup>, STEFAN MATTAUCH<sup>1</sup>, WILLI ZANDER<sup>3</sup>, STEFAN GEPRÄGS<sup>4</sup>, and THOMAS BRÜCKEL<sup>1,2</sup> — <sup>1</sup>Jülich Centre for Neutron Science JCNS, Forschungszentrum Jülich GmbH, Outstation at MLZ, Lichtenbergstr. 1, 85748 Garching — <sup>2</sup>Jülich Centre for Neutron Science JCNS und Peter Grünberg Institut PGI, JCNS-2, PGI-4: Scattering Methods, Forschungszentrum Jülich GmbH, 52425 Jülich — <sup>3</sup>Peter Grünberg Institut PGI, PGI-9: Semiconductor Nanoelectronics, Forschungszentrum Jülich GmbH, 52425 Jülich — <sup>4</sup>Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching

In transition metal oxide thin films the Ruddlesden-Popper variants of classical perovskite materials are under intense investigation [1]. Here, we focus on a comparison of the relation between two different growth techniques onto in-situ Reflection of High-Energy Electron Diffraction (RHEED) measurements [2] of ferromagnetic (La<sub>2</sub>/3Sr<sub>1</sub>/3)<sub>x</sub>Mn<sub>y</sub>O<sub>z</sub>. Semi-continuous deposition and atomic-layer-by-layer deposition was realized via oxide Molecular Beam Epitaxy. Control of the stoichiometry was monitored in-situ via quartz crystal balance and RHEED and ex-situ via Rutherford Backscattering Spectrometry (RBS). Via additional XRR, XRD and PNR measurements we combine different scattering methods to gain insight into the depth profile of the atomic positions. [1] V. Goian *et al.*, Phys. Rev. B **90**, 174105 (2014); [2] J. Haeni *et al.*, Journal of Electroceramics **4**, 385 (2000)

DS 36.36 Thu 9:30 Poster A

**Magnetic and structural studies of as grown and hydrogenated Mg<sub>2</sub>Fe based thin films** — •THU TRANG TRINH<sup>1</sup>, OSCAR LIEDKE<sup>1</sup>, WOLFGANG ANWAND<sup>1</sup>, ANDREAS WAGNER<sup>1</sup>, OGUZ YILDIRIM<sup>2</sup>, STEFFEN CORNELIUS<sup>2</sup>, BERNARD DAM<sup>3</sup>, KOHTA ASANO<sup>4</sup>,

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Due to chemochromism, Mg<sub>2</sub>MeHx (Me=Fe, Co, Ni) based alloys are low-cost and rare-earth-free candidates for switchable mirrors upon hydrogen loading [1]. In order to understand the basic physical properties of Mg<sub>2</sub>FeH<sub>6</sub> based thin films, as-sputtered metal as well as hydrogen loaded films have been investigated using magnetometry, X-ray diffraction, 4-point probe sheet resistance technique and positron annihilation spectroscopy (PAS). The interplay of hydrogen loading, the magnetic moment, and structural properties like the sizes and chemical decoration of open volume defects in thin films detected by PAS will be presented.

DS 36.37 Thu 9:30 Poster A

**Characterization of titaniumoxide nanolayers by soft X-ray emission spectrometry with an efficient wavelength dispersive spectrometer** — •RAINER UNTERUMSBERGER, MATTHIAS MÜLLER, and BURKHARD BECKHOFF — Physikalisch-Technische Bundesanstalt

In the present work, the detection and analysis of nanoscaled materials by X-ray Emission Spectrometry (XES) was performed by means of an increased sensitivity of a Wavelength Dispersive Spectrometer (WDS) [1]. The increased sensitivity of the WDS was achieved by an effective focusing of monochromatized soft X-ray undulator radiation down to the micrometer range using a high quality single bounce monochromator [2]. Due to the increased sensitivity of the WDS, the chemical speciation of different nanoscaled titanium compounds was achieved and the transition probabilities of titanium L<sub>L</sub>- and L<sub>α</sub>-fluorescence radiation could be determined as a function of the chemical bonding. The measurements were carried out at the plane-grating monochromator (PGM) beamline in the laboratory of the Physikalisch-Technische Bundesanstalt (PTB) at BESSY II using monochromatized undulator radiation and calibrated instrumentation [3,4].

References

[1] M. Müller *et al.*, Phys. Rev. A **79**, 032503 (2009) [2] R. Unterumsberger *et al.*, Spectrochimica Acta Part B **78** (2012) 37-41 [3] B. Beckhoff *et al.*, Anal. Chem. **79**, 7873 (2007) [4] B. Beckhoff, J. Anal. At. Spectrom. **23**, 845 (2008)

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DS 36.38 Thu 9:30 Poster A

**Characterisation of epitaxial Au(111) layers on H-terminated Si(111) using X-ray diffraction** — JUBIN LIRAWI<sup>1</sup>, •TIM WIEGMANN<sup>1</sup>, MARTIN RUGE<sup>1</sup>, JOCHIM STETTNER<sup>1</sup>, and OLAF MAGNUSSEN<sup>1,2</sup> — <sup>1</sup>Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Germany — <sup>2</sup>Ruprecht Haensel Laboratory, Christian-Albrechts-Universität zu Kiel, Germany

The structure of ultrathin epitaxial Au(111) films electrochemically deposited on H-terminated Si(111) [1] was characterised by X-ray diffraction, aiming at applications of these films as substrates for ferromagnetic nanoscale structures. Specular scans and longitudinally diffuse scans have been used to determine the background-corrected surface reflectivity for three samples with a nominal thickness of 23, 33, and 65 monolayers, respectively. Layer thickness and roughness of the Au surface and Au/Si interface were calculated from these measurements, also taking into account substrate oxidation close to the film. With a roughness of approximately 5 Å, the Au(111) film has been found to be very smooth, which makes the studied systems promising for future GISAXS studies. This finding is supported by rocking scans showing correlated roughness on a scale of 6300 Å. Measurements of six different Au Bragg peaks indicate a 180° rotation of the Au(111) relative to the substrate lattice. Future studies will analyse the Au(111)/electrolyte interface in situ using high X-ray energies and a transmission geometry.

[1] P. Prod'homme, F. Maroun, R. Cortès, P. Allongue: Appl. Phys. Lett. **93**, 171901 (2008)

DS 36.39 Thu 9:30 Poster A

**Growth and characterisation of epitaxial Mn<sub>5</sub>Ge<sub>3</sub>C<sub>x</sub> films** — •MAXIMILIAN KAUTH<sup>1</sup>, CHRISTOPH SÜRGER<sup>1</sup>, and HILBERT V. LÖHNESEN<sup>1,2</sup> — <sup>1</sup>Physikalisches Institut, Karlsruhe Institut für Technologie, D-76049 Karlsruhe — <sup>2</sup>Institut für Festkörperphysik,

Karlsruher Institut für Technologie, D-76021 Karlsruhe

Ferromagnetic  $\text{Mn}_5\text{Ge}_3\text{C}_x$  films with Curie temperatures well above room temperature are potential spin-injection materials to be used in CMOS-compatible spintronic devices. Previously sputtered polycrystalline films exhibit a coarse-grain morphology. Alternatively, we have grown [0001]-oriented  $\text{Mn}_5\text{Ge}_3\text{C}_x$  ( $x = 0, 0.8$ ) films on in-situ cleaned Ge(111) substrates by electron-beam evaporation in ultra-high vacuum. The films have been characterised by in-situ high-energy electron diffraction, atomic-force microscopy, x-ray diffraction, and resistivity measurements.  $\text{Mn}_5\text{Ge}_3\text{C}_x$  films obtained by solid-state reaction of Mn or codeposited Mn-C layers on Ge(111) at 300 - 450°C exhibit a rough surface with holes of sub-micrometer diameter extending down to the substrate. Hole formation can be avoided if Mn, Ge, and C are simultaneously deposited at 300°C on a thin  $\text{Mn}_5\text{Ge}_3$  seed layer on Ge(111). The films show a lower corrugation, lower resistivity, higher residual resistance ratio, and an enhanced Hall coefficient compared to polycrystalline films prepared by magnetron sputtering.

DS 36.40 Thu 9:30 Poster A

**Structural ordering and phonon mode behavior in MBE-grown  $\text{Bi}_2\text{Te}_{3-x}\text{Se}_x$  layers** — ●KARL BRUNNER<sup>1</sup>, STEFFEN SCHREYECK<sup>1</sup>, ADRIAN KIRCHNER<sup>1</sup>, CLAUS SCHUMACHER<sup>1</sup>, JEAN GEURTS<sup>1</sup>, GRZEGORZ KARCEWSKI<sup>2</sup>, and LAURENS W. MOLENKAMP<sup>1</sup> — <sup>1</sup>Universität Würzburg, Exp. Physik III, Würzburg, Germany — <sup>2</sup>Institute of Physics, Polish Academy of Sciences, Warsaw, Poland

Layers of  $\text{Bi}_2\text{Te}_{3-x}\text{Se}_x$ , a system with interesting topological and thermoelectrical properties, were grown by MBE on H-passivated Si(111). We varied the Se-flux at constant Bi and Te flux to obtain 70 nm layers with  $x = 0$  to 3.  $\text{Bi}_2\text{Te}_{3-x}\text{Se}_x$  forms chemically bonded quintuple layers (QLs) VI(2)-V-VI(1)-V-VI(2) with Van-der-Waals bonds between the QLs. EDX, Raman spectroscopy and HRXRD reveal a nonlinear increase of Se content  $x$  with Se flux, as well as changes of phonon-mode and XRD properties at  $x = 1$ . All these results are well described based on a kinetic adsorption/incorporation/desorption growth model with an enhanced incorporation probability of Se vs. Te, which is by far most pronounced at the central site VI(1). This results in partial ordering, e.g. 75% of the Se atoms at site VI(1) in  $\text{Bi}_2\text{Te}_2\text{Se}$ .

The Raman-active phonon modes  $E_{2g}$ ,  $A_{1g}^1$  and  $A_{1g}^2$  are described by coupled spring-mass systems. The nearly constant mode frequencies for Se-content  $x = 0$  to 1 verify the preferential incorporation of Se at the center-of-mass site VI(1). XRD reveals peculiar variations of lattice parameter  $c$  and XRD peak intensities with  $x$ . They are directly related to ordering and the different changes in spacings of inequivalent lattice planes within a QL caused by Se on site VI(1) or VI(2).

DS 36.41 Thu 9:30 Poster A

**Topography evolution of Germanium deposited by Pulsed Laser Deposition** — ●PHILIPP SCHUMACHER, ERIK THELANDER, ISOM HILMI, JÜRGEN GERLACH, and BERND RAUSCHENBACH — Leibniz Institute of Surface Modification, 04318 Leipzig, Germany

Pulsed Laser Deposition is a versatile technique to deposit high quality films of nearly all materials. In order to promote this technique and expand its application it is necessary to increase the understanding of growth mechanisms, the influence of process parameters like the pulse frequency or the pulse energy and the influence of the substrate and its roughness.

In this work, germanium thin films have been deposited on single crystal Ge and Si (100) substrates as well as on mica surfaces by PLD. The topography of the surface is investigated by Atomic Force Microscopy (AFM) to evaluate the scaling behavior of the roughness under different deposition conditions as well as the size and the density of islands.

The roughness evolution is shown to be governed by the Kardar-Parisi-Zhang-equation and at significant temperature by the Mullins diffusion equation. For low film thickness the roughness decreases due to a diffusion term and for higher film thickness a roughening term becomes dominant. The presence of growing structures with growing distance has also been shown by analyzing the Height-Height Correlation of the topography.

DS 36.42 Thu 9:30 Poster A

**Crystalline Silicon on Glass by Steady-State Solution Growth** — ●ROMAN BANSSEN, CHRISTIAN EHLERS, JAN SCHMIDTBAUER, FRANZISKA RINGLEB, THOMAS TEUBNER, and TORSTEN BOECK — Leibniz Institute for Crystal Growth, Berlin, Germany

In order to grow crystalline silicon on glass at low temperatures for photovoltaic applications, a two-step process has been developed. In the first step, nanocrystalline Si films are formed at low temperatures in the range of 300 to 450 °C through either metal-induced crystallization, or direct deposition on heated substrates.

In the second step, the seed layers serve as templates for the growth of crystalline silicon by steady-state solution growth. In contrast to common liquid phase epitaxy, the supersaturation in front of the seed layer is established by a stationary temperature difference between a silicon source and the substrate. Micrometer-sized Si crystallites with low impurity concentrations are grown by this technique.

Essential features of steady-state solution growth are compatible with the float glass process in large-scale industrial glass production, which raises hopes for a successive production of glass and silicon films for thin-film solar cells in a continuous process.

DS 36.43 Thu 9:30 Poster A

**Pulsed laser deposition of W-Cu thin films** — ●ARNE DITTRICH, SUSANNE SCHLENKRICH, FELIX SCHLENKRICH, FLORIAN DÖRING, CHRISTIAN EBERL, and HANS-ULRICH KREBS — Institute for Materials Physics, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Pulsed laser deposition (PLD) is a versatile technique for the deposition of all kinds of different materials. At this, in many cases stoichiometry transfer between target and substrate is one of the unique features, but nevertheless, structural changes and deviations from stoichiometry can occur in systems with strong resputtering of one component due to occurrence of particles with energies up to 100 eV during PLD. In our case, the W-Cu alloy system with especially large difference in masses of the constituents was chosen to test, how strong the film properties can be influenced by the deposition of energetic particles. For this study, elementary as well as alloy targets were used. The thin film properties were studied using profilometry, x-ray diffraction (XRD), x-ray reflectivity (XRR), electron microscopy (SEM, EDX), with respect to structure, amount of alloying, and stoichiometry changes. First deposition experiments were also performed in gas atmosphere to look on the differences in film properties due to a reduction of the particle energy. In this contribution, the changes of film properties compared to the target and the dependence on the particle energy are presented.

DS 36.44 Thu 9:30 Poster A

**Silicon nanocrystals of uncontrollable sizes formed in  $\text{SiN}_x/\text{SiO}_2$  hetero-superlattices** — ●ANASTASIYA ZELENINA<sup>1</sup>, ANDREY SARIKOV<sup>2</sup>, DENIS ZHIGUNOV<sup>3</sup>, and MARGIT ZACHARIAS<sup>1</sup> — <sup>1</sup>Georges-Koehler-Allee 103, Freiburg 79110, Germany — <sup>2</sup>45 Nauki Avenue, Kiev 03028, Ukraine — <sup>3</sup>Leninskie Gory 1, Moscow 119991, Russia

$\text{SiN}_x/\text{SiO}_2$  hetero-superlattices with  $\text{SiN}_x$  sublayer thickness of 3 nm and  $\text{SiO}_2$  barrier thicknesses of 3 and 10 nm were prepared by PECVD. In contrast to the number of the publications based on the preparation of silicon nanocrystals (Si NCs) by size-controlled superlattice approach, high-temperature annealing at 1200°C led to the formation of silicon nanocrystals (Si NCs) with various sizes in the range of 2.5 - 12.5 nm embedded in mainly oxynitride matrix. The multilayer structure was completely destroyed after the high-temperature annealing and no periodicity was observed for the sample with 3 nm  $\text{SiO}_2$  barrier. The increasing of  $\text{SiO}_2$  barrier thickness up to 10 nm did not change the results: the multilayer structure was destroyed and Si NCs of uncontrollable sizes were formed. It is worth noting that according to the TEM images the as-prepared structures were well-organized and had smooth sublayer interfaces. To investigate this unusual behavior, the phase separation and PL were investigated at different temperatures of annealing. Based on the experimental results, we conclude that the loss of size control occurs due to the oxygen migration from  $\text{SiO}_2$  barriers into  $\text{SiN}_x$  sublayers. Thermodynamic reasons are assumed to be responsible for this process.

DS 36.45 Thu 9:30 Poster A

**Transmission electron microscopy study of novel DCV5T/C60 blend films for organic solar cells** — ●MONA SEDIGHI<sup>1</sup>, PETR FORMANEK<sup>2</sup>, MARKUS LÖFFLER<sup>1</sup>, and EHRENFRIED ZSCHECH<sup>1,3</sup> — <sup>1</sup>Dresden Center for Nanoanalysis, Technische Universität Dresden, Dresden, Germany — <sup>2</sup>Leibniz-Institut für Polymerforschung Dresden, Dresden, Germany — <sup>3</sup>Fraunhofer Institute for Ceramic Technologies and Systems, Dresden, Germany

Organic solar cells gained increasing attention as renewable energy conversion elements due to the great potential of low-cost produc-

tion and flexible processing technologies. However, their performance and reliability are still worse compared to the inorganic counterparts. Therefore, one of the major tasks in this research field is the development of new materials to reach higher performance. Recently, novel methyl-substituted dicyanovinylcapped quinquethiophenes (DCV5T) have been introduced as small-molecule organic donors in the blend of bulk heterojunction solar cells, which increase power conversion efficiencies when combined with fullerenes (C60) as the acceptor phase. The heterojunction organic solar cells, made of DCV5T/C60 blend perform better than those of zinc phthalocyanine(ZnPc) and C60 blend. Transmission electron microscopy analysis of pure DCV5T variations and DCV5T/C60 blend films gives insights into the morphology of these novel compounds that can be used to build strong structure-property relationships in order to rationalize their improved photovoltaic performance. Here we report analytical TEM characterization (EFTEM and EELS) of the DCV5T/C60 blend.

DS 36.46 Thu 9:30 Poster A

**Analysis of island shape evolution from diffuse x-ray scattering/GISAXS of organic thin films and implications for growth**

— CHRISTIAN FRANK<sup>1</sup>, ●RUPAK BANERJEE<sup>1</sup>, MARTIN OETTEL<sup>1</sup>, ALEXANDER GERLACH<sup>1</sup>, JIŘÍ NOVÁK<sup>1,2</sup>, GONZALO SANTORO<sup>3</sup>, and FRANK SCHREIBER<sup>1</sup> — <sup>1</sup>Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany — <sup>2</sup>Central European Institute of Technology, Masaryk University, Kamenice 5, CZ-62500 Brno, Czech Republic — <sup>3</sup>Photon Science, DESY, Notkestr. 85, 22607 Hamburg, Germany

Understanding the growth of organic semi-conducting molecules with shape anisotropy is of high relevance to the processing of optoelectronic devices. This work provides insight into the growth of thin films of the prototypical rodlike organic semiconductor diindenoperylene on a microscopic level, by analyzing in detail the film morphology. We model our data, which were obtained by high-resolution grazing incidence small angle x-ray scattering (GISAXS), using a theoretical description from small angle scattering theory derived for simple liquids. Based on form factor calculations for different object types we determine how the island shapes change in the respective layers [1]. Atomic force microscopy measurements approve our findings.

[1] C. Frank *et al.* Phys. Rev. B **90**, 205401 (2014).

DS 36.47 Thu 9:30 Poster A

**Comparison of charge neutrality level of Cu/CuO/HfO2 and Si/SiO2/HfO2.** — ●ZIED ROUISSI, SIMONE BRIZZI, SILMA ALBERTON CORRÊA, MASSIMO TALLARIDA, and DIETER SCHMEISSER — Department of Applied Physics and Sensors, Brandenburg University of Technology, 03046 Cottbus, Germany

Copper Oxide (CuO) is a promising metal oxide semiconductor, which can be used in different applications, such as catalysis, solar energy conversion, and water splitting. In this work, we use resonance photoemission spectroscopy (ResPES) to analyse the electronics properties of HfO2 films deposited on Cu/CuO and Si/SiO2. For that, we deposited 10 cycles of HfO2 by atomic layer deposition (ALD) on Cu/CuO and Si/SiO2 samples and investigated the density states for the valence and conduction bands which were determined by the detailed analysis of the O1s resonance profile obtained by ResPES. We compared the positions of valence band maximum and conduction band minimum, the excitation range for the polaronic states and the range of charge transfer band in Cu/CuO/HfO2 and Si/SiO2/HfO2. Also, we determined the band gap and the charge neutrality level (CNL).

DS 36.48 Thu 9:30 Poster A

**Tunable Coordinative Defects in UHM-3 Surface-Mounted MOFs for Gas Adsorption and Separation: A Combined Experimental and Theoretical Study** — ●ZHENGANG WANG<sup>1</sup>, HIKMET SEZEN<sup>1</sup>, JINXUAN LIU<sup>1</sup>, CHENGWU YANG<sup>1</sup>, STEPHANIE ROGGENBUCK<sup>2</sup>, KATHARINA PEIKERT<sup>2</sup>, MICHAEL FRÖBA<sup>2</sup>, ANDREAS MAVRANTONAKIS<sup>3</sup>, BARBARA SUPRONOWICZ<sup>3</sup>, THOMAS HEINE<sup>3</sup>, HARTMUT GLIEMANN<sup>1</sup>, and CHRISTOF WÖLL<sup>1</sup> — <sup>1</sup>Institute of Functional Interfaces, Karlsruhe Institute of Technology — <sup>2</sup>Institute of Inorganic and Applied Chemistry, Department of Chemistry, University of Hamburg — <sup>3</sup>Engineering and Science, Jacobs University Bremen

Here, we first report on the growth of oriented, homogeneous and virtually defect-free (below 1 %) UHM-3 MOF thin films on a modified solid substrate using a room-temperature liquid phase epitaxy (LPE) method. Thermal postsynthetic treatment allowed to induce Cu(I) defect sites in a controlled fashion. The interaction of CO and CO2 with the Cu(II) and Cu(I) sites was then studied using X-ray photo-

electron spectroscopy (XPS) and IR-spectroscopy. The binding energy of these two species was determined using temperature-induced desorption. The interaction between the guest molecules and the Cu(I) and Cu(II) sites were also analyzed using density-functional theory (DFT). Surprisingly, both experiment and theory show that the binding energy of CO2 to Cu(I) and Cu(II) sites are essentially identical, in pronounced contrast to CO, which binds much stronger to Cu(I).

DS 36.49 Thu 9:30 Poster A

**Controlling the Phase Transition of Sputtered TiO2 Thin Films by Doping** — ●ANTON NEUMANN<sup>1</sup>, SEBASTIAN MÄDER<sup>1</sup>, ROLAND SITTNER<sup>1</sup>, RÜDIGER SCHMIDT<sup>1</sup>, and MATTHIAS WUTTIG<sup>1,2</sup>

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Coated glasses play a significant role in our everyday life, for example in windows, eyeglasses, mobile devices or solar cells. All these applications demand very different requirements like anti-reflex-, self-cleaning-, scratch-resistant- or optical index matched surfaces. Glasses coated with thin TiO2 films can provide any of these properties. By carefully adjusting the deposition conditions, the film characteristics can be significantly altered as the two acquirable crystalline phases, Anatase and Rutile, differ significantly in their physical properties. Due to its very good scalability, magnetron sputtering is the most utilized technique to deposit these TiO2 thin films.

In this study, we show that by adjusting the cationic dopant concentration in the TiO2 films produced by magnetron sputtering, one is able to tailor the onset temperature and speed of the phase transition from Anatase to Rutile. To investigate the crystalline structure of our samples, X-ray diffraction was performed before and after annealing the samples at various temperatures. In addition optical properties were investigated via UV/VIS-spectrometry and ellipsometry.

DS 36.50 Thu 9:30 Poster A

**Ion beam analysis of defects in irradiated lithium niobate** —

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In this presentation ion implanted lithium niobate is investigated applying Rutherford backscattering spectrometry (RBS) in channeling configuration. It is commonly known that the measured defect concentration exhibits a different visibility in x- and z-cut lithium niobate. Generally, this effect has been attributed to the preferred location of displaced niobium atoms at vacant octahedral sites. However, the influence of the implantation for the differently orientated substrates could not be ruled out. Therefore in our investigations lithium niobate samples were used which were cut 45 degrees to the x- and z-direction, respectively. In this case the damage concentration could be measured in both x- and z-direction on one and the same sample. Our results reproduce those obtained from x- and z-cut samples. This proves the assumption that displaced niobium atoms occupy free octahedral sites. Applying RBS only the niobium sublattice can be investigated. Therefore an attempt is made to use nuclear reaction analysis (NRA) for studying the lithium sublattice. For that the Li(p,α0)He reaction is examined. Measurements of the cross-section of this reaction under the given experimental conditions allow for estimates of the depth resolution and the lower detection limit. First results for damage studies with NRA will be presented.

DS 36.51 Thu 9:30 Poster A

**Mechanisms of metal induced crystallization analyzed by in situ Rutherford Backscattering Spectroscopy** — ●ROBERT WENISCH<sup>1</sup>, DANIEL HANF<sup>1</sup>, FRANK LUNGWITZ<sup>1</sup>, RENÉ HELLER<sup>1</sup>, RENÉ HÜBNER<sup>1</sup>, SIBYLLE GEMMING<sup>1,2</sup>, and MATTHIAS KRAUSE<sup>1</sup>

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Metal induced crystallization (MIC) is a promising technique for low temperature thin film transistor fabrication and graphene synthesis. In MIC, a transition metal acts as seed for the crystallization of an amorphous group IV element. Bond screening near the interface and facilitation of nucleation are recently discussed as mechanisms for MIC. So far, *in situ* studies have been performed using X-ray diffraction, which is sensitive to the degree of crystallinity but lacks depth resolution. A better insight into the MIC mechanisms requires depth resolved *in situ* studies in order to determine the concentration profiles of the diffusing components.

Here, the Si/Ag and C/Ni bilayer systems are studied. They are annealed at temperatures of up to 750 °C. Simultaneously, the layer

composition and the compositional profiles are investigated with *in situ* Rutherford backscattering spectroscopy revealing the diffusion kinetics of the components. Both, the quick initial nucleation and the ensuing growth processes are investigated. Further characterization is performed employing *in vacuo* Raman spectroscopy revealing the phase structure of the resulting films and scanning electron microscopy to investigate the surface structure.

DS 36.52 Thu 9:30 Poster A

**Diffuse Scattering from Multilayer Mirrors for EUV Lithography and the Water Window** — ●ANTON HAASE<sup>1</sup>, SAŠA BAJT<sup>2</sup>, VICTOR SOLTWISCH<sup>1</sup>, CHRISTIAN LAUBIS<sup>1</sup>, and FRANK SCHOLZE<sup>1</sup> — <sup>1</sup>Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin, Germany — <sup>2</sup>Center for Free-Electron Laser Science/DESY, Notkestr. 85, 22609 Hamburg, Germany

Optical elements for the EUV and soft X-ray spectral range are of great interest for various scientific and technological applications. Today, the semiconductor industry is driving the development of high reflective multilayer coatings for the use with EUV light at a wavelength of 13.5 nm. On the other hand, soft X-rays in the so called water window spectral range between 2.3 nm and 4.4 nm can penetrate water with high attenuation lengths while being absorbed by the proteins. With the availability of coherent radiation of this wavelength, there is a new demand of high-reflectance mirrors in this spectral range.

We characterize high-reflectance Mo/Si and Cr/Sc multilayer mirrors with respect to interface roughness using scattering of EUV radiation of the respective wavelength near-normal incidence. The resulting intensity distribution of diffusely scattered light provides information on vertical and lateral correlations of roughness through the appearance of resonant diffuse scattering (RDS) sheets. It thus serves as a versatile tool for the investigation of interfacial roughness power spectral densities (PSD). We employ the distorted-wave Born approximation to derive the roughness properties considering the impact of dynamic scattering processes on the diffuse scattering intensity.

DS 36.53 Thu 9:30 Poster A

**Boron carbide coatings for neutron detection probed by x-rays, ions, and neutrons** — ●GREGOR NOWAK<sup>1</sup>, MICHAEL STÖRMER<sup>1</sup>, HANS-WERNER BECKER<sup>2</sup>, CHRISTIAN HORSTMANN<sup>1</sup>, REINHARD KAMPMANN<sup>1</sup>, DANIEL HÖCHE<sup>1</sup>, MARTIN HAESE-SEILLER<sup>1</sup>, JEAN-FRANCOIS MOULIN<sup>1</sup>, CHRISTIAN RANDAU<sup>3</sup>, UWE LORENZ<sup>1</sup>, RICHARD HALL-WILTON<sup>4</sup>, MARTIN MÜLLER<sup>1</sup>, and ANDREAS SCHREYER<sup>1</sup> — <sup>1</sup>Helmholtz-Zentrum Geesthacht, 21502 Geesthacht, Germany — <sup>2</sup>RUBION - Zentrale Einrichtung für Ionenstrahlen und Radionuklide, Ruhr-Universität Bochum, 44780 Bochum, Germany — <sup>3</sup>Georg-August Universität Göttingen, 37077 Göttingen, Germany — <sup>4</sup>European Spallation Source ESS AB, 221 00 Lund, Sweden

Due to the present shortage of <sup>3</sup>He, the supply of large neutron detection systems becomes unaffordable. Alternative neutron detection concepts based on solid <sup>10</sup>B are envisaged and require development in thin film deposition techniques regarding high adhesion, thickness uniformity and chemical purity of the converter coating. We report on the sputter deposition of precise <sup>10</sup>B<sub>4</sub>C coatings of up to several microns thickness on Al substrates using the HZG large area sputtering system. Complementary film analysis using x-rays, ions, and neutrons reveal a high quality <sup>10</sup>B<sub>4</sub>C coating. Especially XPS, SIMS, and RBS show low chemical impurities concentrations in the coatings. The isotope composition determined by SIMS, RBS evidences a very high <sup>10</sup>B isotope content. Neutron detection test measurements demonstrate an average relative quantum efficiency ranging from 65 % to 90 % for cold neutrons as compared to a black <sup>3</sup>He-monitor.

DS 36.54 Thu 9:30 Poster A

**critical current density scaling of FeSe<sub>0.5</sub>Te<sub>0.5</sub> thin films on different substrates** — ●FEIFEI YUAN<sup>1,2</sup>, KAZUMASA IIDA<sup>2,3</sup>, MARCO LANGER<sup>2</sup>, JENS HÄNISCH<sup>2</sup>, ATARU ICHINOSE<sup>4</sup>, ICHIRO TSUKADA<sup>4</sup>, ALBERTO SALA<sup>5</sup>, MARINA PUTTI<sup>5</sup>, RUBEN HÜHNE<sup>2</sup>, LUDWIG SCHULTZ<sup>2</sup>, and ZHIXIANG SHI<sup>1</sup> — <sup>1</sup>Department of Physics and Key Laboratory of MEMS of the Ministry of Education, Southeast University, Nanjing, China — <sup>2</sup>Institute for Metallic Materials, IFW Dresden, Dresden, Germany — <sup>3</sup>Department of Crystalline Materials Science Graduate School of Engineering, Nagoya University, Nagoya, Japan — <sup>4</sup>Central Research Institute of Electric Power Industry, 2-6-1 Nagasaka, Yokosuka, Kanagawa, Japan — <sup>5</sup>Dipartimento di Fisica, Università di Genova, Via Dodecaneso, Genova, Italy

FeSe<sub>0.5</sub>Te<sub>0.5</sub> thin films grown by pulsed laser deposition on CaF<sub>2</sub>, LaAlO<sub>3</sub> (LAO) and MgO substrates were structurally and electro-

magnetically characterized. The in-plane lattice mismatch between FeSe<sub>0.5</sub>Te<sub>0.5</sub> and the substrates shows no influence on the lattice parameters of the films. While the type of the substrates, crystallinity and epitaxy of the films affect the superconducting properties. The film on MgO showed an extra peak in the angular dependence of  $J_c$  at  $\theta=180^\circ$ , which arises from c-axis defects as confirmed by transmission electron microscopy. In contrast, no c-axis  $J_c(\theta)$  peaks were observed in films on CaF<sub>2</sub> and LAO. A successful scaling of the  $J_c(\theta)$  can be realized for both films without c-axis correlated defects by the anisotropy ginzburg-landau (AGL) approach with appropriate anisotropy ratio  $\gamma$ . The AGL scaling parameter  $\gamma$  is decreasing with decreasing temperature.

DS 36.55 Thu 9:30 Poster A

**Structural and magnetic properties of ultrathin epitaxial Fe<sub>3</sub>O<sub>4</sub>/NiO bilayers and Fe<sub>3</sub>O<sub>4</sub> films grown on SrTiO<sub>3</sub>(001)** — ●OLGA SCHUCKMANN<sup>1</sup>, TOBIAS SCHEMME<sup>1</sup>, NICO PATHÉ<sup>1</sup>, FREDERIC TIMMER<sup>1</sup>, RALPH BUS<sup>1</sup>, TIMO KUSCHEL<sup>2</sup>, KARSTEN KUEPPER<sup>1</sup>, and JOACHIM WOLLSCHLÄGER<sup>1</sup> — <sup>1</sup>Physics Department, Osnabrück University, Germany — <sup>2</sup>CSMD, Physics Department, Bielefeld University, Germany

The understanding of magnetic interactions between a ferrimagnet and an antiferromagnet has become of considerable interest for various of applications in information storage technology, e.g., magnetoresistive (MR) devices. In this study, the influence of an NiO interlayer on magnetic and structural properties of ultrathin Fe<sub>3</sub>O<sub>4</sub> films was investigated. Epitaxial Fe<sub>3</sub>O<sub>4</sub>/NiO bilayers and Fe<sub>3</sub>O<sub>4</sub> films were grown on niobium doped SrTiO<sub>3</sub>(001) substrates by reactive molecular beam epitaxy. The stoichiometry and surface structure of the oxide films were controlled in-situ by x-ray photoelectron spectroscopy (XPS) and low energy electron diffraction (LEED), respectively. The film structure was characterized ex-situ by x-ray diffraction (XRD) using a photon energy of 10keV. In addition, the magnetic behavior of the magnetite films was studied by magneto-optic Kerr effect (MOKE) showing that the thickness and epitaxial strain affect the magnetic anisotropy of the films.

DS 36.56 Thu 9:30 Poster A

**Structural characterisation of epitaxial thin magnetite films grown on SrTiO<sub>3</sub>(001)** — ●WANJA SPIESS, OLGA SCHUCKMANN, TOBIAS SCHEMME, KARSTEN KÜPPER, and JOACHIM WOLLSCHLÄGER — Physics Department, Osnabrück University, Germany

Magnetite is a promising material for various physical and chemical applications in different fields as spintronics [1] and catalysis [2]. It has been demonstrated that the electronic and magnetic properties of Fe<sub>3</sub>O<sub>4</sub> films could be influenced by the difference of the strain, stoichiometry or defect states, e.g., using SrTiO<sub>3</sub>(001) as substrate [3,4]. In this study structural properties of ultrathin magnetite films grown on SrTiO<sub>3</sub>(001) were investigated. The films were deposited at different temperatures on single crystalline niobium doped SrTiO<sub>3</sub>(100) substrates by reactive molecular beam epitaxy (RMBE, Fe evaporation in O<sub>2</sub> atmosphere). The surface stoichiometry and structure of the oxide films was controlled by x-ray photoelectron spectroscopy (XPS) and by low energy electron diffraction (LEED). The film structure was characterized by synchrotron radiation x-ray diffraction (XRD) during growth, showing that the strain of the films is strongly affected by the substrate temperature.

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- [2] S. A. Chambers, Surf. Sci. Rep., 39, 105, (2000)
- [3] J. Cheng et al., J. Cryst. Growth, 310, 3730 (2008)
- [4] F. Bertram et al. J. Appl. Phys., 113, 184103 (2013)

DS 36.57 Thu 9:30 Poster A

**The influence of current density on properties of Ni-Co coating** — ●HIDA RASSAIE and SINA SADREDDINI — Department of Materials Science and Engineering, Science and Research Branch, Islamic Azad University, Tehran, Iran.

Electrodeposited Nickel-Cobalt alloys are exposed to investigate the relationship between applied current density, Co content, microstructure and corrosion resistance. Direct current electrodeposition was applied to create compact coatings. The surface morphology was changed from a mixture of needles to a spherical to sphere by increasing the deposition current density. The current density increase was found to have a reverse effect on Co content, with the percentage of Co decreasing gradually from approximately 64.6 to 55.2 wt%. The corrosion behavior of Ni-Co depositions in chloride solution was affected by Co content and surface morphology.

DS 36.58 Thu 9:30 Poster A

**Tribological properties of Ni-P-SiO<sub>2</sub> nano-composite coating on Aluminum** — ●SAHAR SALEHI<sup>1</sup>, SINA SADREDDINI<sup>2</sup>, and MOHSEN AHMADI<sup>3</sup> — <sup>1</sup>Metallurgical & Materials Engineering Department, School of Chemical & Materials Engineering, Islamic Azad University, Shiraz, Iran. — <sup>2</sup>Department of Materials Science and Engineering, Science and Research Branch, Islamic Azad University, Tehran, Iran. — <sup>3</sup>Department of Mining and Metallurgical Engineering, Amir kabir University of Technology, Hafez Ave., P.O. Box 15875, Tehran 4413, Iran.

In this study, the effect of different concentrations of SiO<sub>2</sub> nano sized particles in the bath on deposition rate, surface morphology and wear behavior of Ni-P-SiO<sub>2</sub> Composite coatings were investigated. The deposition rate of coating was influenced by incorporation of SiO<sub>2</sub> Particles. The microstructural observations were performed with field emission scanning electron microscopy (FESEM). The amount of SiO<sub>2</sub> was examined by Energy Dispersive Analysis of X-Ray (EDX). Results showed that for the coating produced at 12.5 g/l of nano SiO<sub>2</sub> in the bath, the amount of SiO<sub>2</sub>nanoparticles co-deposited and microhardness reached a maximum value at 4.5 wt% and 453 VH, respectively. Furthermore, the wear behavior of the coating was studied. Nano-composite coating led to improve the wear resistance of the aluminum substrate.

DS 36.59 Thu 9:30 Poster A

**Effect of current density on properties of Ni-W coating** — ●HIDA RASSAIE and SINA SADREDDINI — Department of Materials Science and Engineering, Science and Research Branch, Islamic Azad University, Tehran, Iran.

In this study, the Ni-W coating was electrodeposited on aluminum at different current densities. Various current densities were applied to investigate the effect of current density on tungsten content, grain size, surface morphology and corrosion behavior. The morphology of Ni-W coating was investigated by FESEM. Also, spherical morphology was observed at 1, 3 and 5 A/dm<sup>2</sup>. The study demonstrated that tungsten concentration decreased by increasing the current density. Fcc peak was observed in all three Ni-W coatings in XRD patterns. Electrochemical polarization proved that the reduced corrosion resistance of Ni-W nanocrystalline electrodeposit was due to the increment of applied current density.

DS 36.60 Thu 9:30 Poster A

**Effect of Co concentration in the bath on composition, microstructure, morphology aspects and electrochemical properties of Ni-Co coatings on aluminum** — ●SINA SADREDDINI and HIDA RASSAIE — Department of Materials Science and Engineering, Science and Research Branch, Islamic Azad University, Tehran, Iran.

In this study, the surface morphology of Ni-Co composite coating was investigated by field emission scanning electron microscopy (FESEM). The crystalline structure was examined by X-Ray diffraction (XRD) and the Corrosion behavior of coating was evaluated by electrochemical impedance spectroscopy (EIS) and polarization techniques. Different amounts of cobalt in the bath affected the morphology of Ni-Co deposited. By increasing the alloying element in bath, structure of Ni-Co coating changed from face centered cubic to hexagonal closed-pack and consequently influenced the corrosion behavior in chloride solution. In addition, increment the alloy element in the bath affected the charge transfer.

DS 36.61 Thu 9:30 Poster A

**Application of magnesium phosphate coating on low carbon steel via electrochemical cathodic method and investigation of its corrosion resistance** — ●MOHAMMADREZA DAYYARI and SINA SADREDDINI — Department of Materials Science and Engineering, Science and Research Branch, Islamic Azad University, Tehran, Iran.

In this study, magnesium phosphate coating was applied on low carbon steel, its morphology was examined by scanning electron microscopy (SEM) and its crystalline structure was investigated by X-ray diffraction (XRD). The corrosion behavior of coated aluminum was evaluated by electrochemical impedance spectroscopy (EIS) and polarization techniques. The results showed that the application of magnesium phosphate coating significantly improved corrosion resistance behavior by forming Newbryite phase.

DS 36.62 Thu 9:30 Poster A

**The effect of current density on electrochemical magnesium**

**phosphate of low carbon steel and its corrosion resistance** — ●MOHAMMADREZA DAYYARI and SINA SADREDDINI — Department of Materials Science and Engineering, Science and Research Branch, Islamic Azad University, Tehran, Iran.

In this study, the magnesium phosphate coating was electrodeposited on aluminum at different current densities. Various current densities were applied to investigate the effect of current density on thickness, surface morphology and corrosion behavior. The related morphology was investigated by scanning electron microscopy (SEM) and crystalline structure was examined by X-Ray diffraction (XRD). The corrosion behavior was evaluated using electrochemical impedance spectroscopy (EIS) and polarization techniques. The results showed that by applying magnesium phosphate coating, the Newbryite structure was formed in the coating structure and at a current density of 5mA/cm<sup>2</sup>, finer morphology, reduced porosity and increased corrosion resistance were observed.

DS 36.63 Thu 9:30 Poster A

**Effect of W concentration in the bath on composition, microstructure, morphology aspects and electrochemical properties of Ni-W coatings on aluminum** — ●HIDA RASSAIE, SINA SADREDDINI, and GOLSA RASSAIE — Department of Materials Science and Engineering, Science and Research Branch, Islamic Azad University, Tehran, Iran.

In this study, the surface morphology of Ni-W composite coating was investigated by field emission scanning electron microscopy (FESEM). The crystalline structure was examined by X-Ray diffraction (XRD) and the Corrosion behavior of coating was evaluated by electrochemical impedance spectroscopy (EIS) and polarization techniques. Increment of W percentage in the bath caused to refine grain size and changed the crystalline structure. FESEM testes demonstrated spherical morphology in all exams. Corrosion resistance in chloride solution was improved by increasing the concentration of tungsten in coating. In addition, increment the alloy element in the bath affected the charge transfer.

DS 36.64 Thu 9:30 Poster A

**The influence of pH on properties of Ni-Co coating** — ●GOLSA RASSAIE<sup>1</sup>, HIDA RASSAIE<sup>2</sup>, and SINA SADREDDINI<sup>2</sup> — <sup>1</sup>Department of engineering management, upm university, Malaysia. — <sup>2</sup>Department of Materials Science and Engineering, Science and Research Branch, Islamic Azad University, Tehran, Iran.

Electrodeposited Nickel-Cobalt alloys are exposed to investigate the relationship between pH, Co content, microstructure and corrosion resistance. Direct current electrodeposition was applied to create compact coatings. The microstructural observations were performed with field emission scanning electron microscopy (FESEM). The amount of SiO<sub>2</sub> was examined by Energy Dispersive Analysis of X-Ray (EDX) and crystalline structure was examined by X-Ray diffraction (XRD). The Corrosion behavior was evaluated through electrochemical impedance spectroscopy (EIS) and polarization techniques.

DS 36.65 Thu 9:30 Poster A

**The influence of heat treatment on properties of Ni-P-SiO<sub>2</sub> nanocomposite coating** — ●SINA SADREDDINI<sup>1</sup>, HIDA RASSAIE<sup>1</sup>, and MOHSEN AHMADI<sup>2</sup> — <sup>1</sup>Department of Materials Science and Engineering, Science and Research Branch, Islamic Azad University, Tehran, Iran. — <sup>2</sup>Department of Mining and Metallurgical Engineering, Amir kabir University of Technology, Hafez Ave., Tehran, Iran.

In this study, the surface morphology of Ni-P-SiO<sub>2</sub> composite coating was investigated with field emission scanning electron microscopy (FESEM). The amount of SiO<sub>2</sub> in the coating was examined by Energy Dispersive Analysis of X-Ray (EDX). Corrosion behavior of coating was evaluated by electrochemical impedance spectroscopy (EIS) and polarization techniques and showed that corrosion resistance of Ni-P-SiO<sub>2</sub> was diminished after heat treatment.

DS 36.66 Thu 9:30 Poster A

**Nano structuring of lithium niobate by ion beams** — ●SVEN BAUER, HENRY HOLLAND-MORITZ, and CARSTEN RONNING — Friedrich-Schiller-Universität, Institut für Festkörperphysik, Helmholtzweg 3, 07743 Jena

Lithium niobate (LiNbO<sub>3</sub>) is a promising material for a wide range of electro-optical applications, because of its excellent properties, e.g. large electro-optical and non-linear optical coefficients. Structuring of LiNbO<sub>3</sub> by standard etching technologies is difficult due to its chem-

ical inertness. Ion beam enhanced etching has proven to be the most promising method for structuring the material for optical applications, whereas the final structure is defined by a mask. This mask is usually produced by electron beam lithography, which is an expensive and time consuming method when it comes to large areas to process. Instead one may just use self-assembled nanostructures as a mask, such as nanowires or nanoparticles. First, simulations were performed by the Monte-Carlo-code iradina [C. Borschel et al., Nucl Instr Meth B 269, 2133-3138 (2011)] for the ion irradiation of CdS, ZnO nanowires and Gold nanoparticles. Thus, LiNbO<sub>3</sub> samples, which were covered by such nanostructures, were irradiated with Argon, Krypton and Neon ions with energies ranging from 40 to 200 keV. Consecutively, all samples were etched in liquid HF-solution. Furthermore, Rutherford backscattering spectrometry and scanning electron microscopy methods were used for investigating the damage formation and morphological effects.

DS 36.67 Thu 9:30 Poster A

**Noble gas ion-induced ripple pattern formation on carbon surfaces** — ●OMAR BOBES, KUN ZHANG, and HANS HOFSSÄSS — Georg-August-Universität Göttingen, II. Physikalisches Institut, Göttingen, Germany

Ion induced ripple pattern formation on HOPG, diamond and amorphous carbon surfaces were studied previously and a qualitative agreement with the predictions of the Bradley-Harper model, but also differences between HOPG and a-C were found [1,2,3]. Here we present new experiments for Ne, Ar and Xe ion irradiation of a-C surfaces as function of ion incidence angle and for ion energies between few hundred eV and 100 keV. We find a disappearance of patterns for Ne and Ar ion irradiation at ion energies higher than several keV. Monte Carlo simulations of the curvature coefficients applied to the Bradley-Harper and Carter-Vishnyakov models, including the recent extensions, are able to explain the absence of pattern formation in these cases. Moreover, simulations indicate that pattern formation on a-C should be possible for low energy Ne ions and even He ions with 250 eV. Indeed we find ripple patterns for 850 eV Ne irradiated a-C.

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- [2] K. Takahiro et al., Nucl. Instr. Meth. B 256, 378 (2007).
- [3] O. Bobes, K. Zhang, H. Hofssäss, Phys. Rev. B 86, 235414 (2012).

DS 36.68 Thu 9:30 Poster A

**Resolution limits of ohmic simulations for proton beam writing in p-GaAs** — ●ALRIK STEGMAIER, TRISTAN KOPPE, CHARLOTTE ROTHFUCHS, ULRICH VETTER, and HANS HOFSSÄSS — 2. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Microelectromechanical systems (MEMS) combine electrical and mechanical features on the micrometer scale. An increasing number of applications for this technology exist, including energy harvesters, accelerometers and pressure sensors [1,2]. Proton beam writing is a maskless lithographic method for the production of microstructures for such applications [3]. It is possible to produce three dimensional structures by varying only the fluence of the proton irradiation on a p-GaAs sample, followed by electrochemical etching [4].

High precision and reproducibility of the final structures requires accurate simulations of the effects of proton irradiation and the subsequent electrochemical etching. The simplest approach for such simulations is an ohmic model [5]. The resolution limits of such a model are explored and extended. The model is also adjusted with non-ohmic elements to reproduce the experimentally measured I-V characteristics.

- [1] V. Cimalla et al., J. Phys. D: Appl. Phys., 40(20), 6386, 2007
- [2] J.A. Paradiso et al., IEEE Pervasive Comput., 4(1), 18-27, 2005
- [3] J.A. van Kan et al., Appl. Phys. Lett., 83(8), 1629, 2003
- [4] P. Mistry et al., Nucl. Instr. Meth. Phys. Res. B, 237, 188-192, 2005
- [5] T. Koppe et al., J. Microelectromech. Syst., 23(4), 955-960, 2014

DS 36.69 Thu 9:30 Poster A

**Drift diffusion model for proton beam writing in p-GaAs** — ●ALRIK STEGMAIER, TRISTAN KOPPE, CHARLOTTE ROTHFUCHS, ULRICH VETTER, and HANS HOFSSÄSS — 2. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Microelectromechanical systems (MEMS) are micrometer scale systems that combine electrical and mechanical functionality for applications like energy harvesters, accelerometers and pressure sensors [1,2].

Proton beam writing (PBW) is a relatively new, maskless litho-

graphic method for the production of microstructures for such applications [3]. It has been shown that it is possible with PBW to produce 3D structures by varying only the fluence of the proton irradiation on a p-GaAs sample, followed by electrochemical etching [4].

Optimization of the resolution of PBW in p-GaAs requires precise models of the irradiation and etching process. Progress has been made in the past with ohmic simulations of the process [5]. Here a drift-diffusion model for the semiconductor material, together with an empirical model for proton irradiation induced defects and a model for the surface electrochemistry is presented.

- [1] V. Cimalla et al., J. Phys. D: Appl. Phys., 40(20), 6386, 2007
- [2] J.A. Paradiso et al., IEEE Pervasive Comput., 4(1), 18-27, 2005
- [3] J.A. van Kan et al., Appl. Phys. Lett., 83(8), 1629, 2003
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- [5] T. Koppe et al., J. Microelectromech. Syst., 23(4), 955-960, 2014

DS 36.70 Thu 9:30 Poster A

**Noble gas ion-induced ripple pattern formation on carbon surfaces** — ●OMAR BOBES, KUN ZHANG, and HANS HOFSSÄSS — Georg-August-Universität Göttingen, II. Physikalisches Institut, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

We present here some experiments for Ne, Ar and Xe ion irradiation of amorphous carbon surfaces as function of ion incidence angle and for a rather broad ion energy regime between few hundred eV and 60 keV. We find a disappearance of patterns for Ne and Ar ion irradiation at intermediate ion energies of several keV. Patterns reappear again at even higher ion energies. Monte Carlo simulations of the curvature coefficients applied to the Bradley-Harper and Carter-Vishnyakov models, including the recent extensions are able to explain the absence of pattern formation in certain cases. Moreover, simulations indicate that pattern formation on a-C should be possible for low energy Ne ions and even He ions with 250 eV. Indeed we find ripple patterns for 950 eV Ne irradiated a-C. Our experimental results are compared with predictions using current linear theoretical models and applying the crater function formalism as well as Monte Carlo simulations to determine curvature coefficients.

DS 36.71 Thu 9:30 Poster A

**Stable phases of Si(111)-(5×2)-Au surface: Dependence on Au and Si adatom coverages** — ●KAORI SEINO and FRIEDHELM BECHSTEDT — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Jena, Germany

Over a few decades, the Si(111)-(5×2)-Au surface has been attracted wide interest in experimental and theoretical studies, because it belongs to the family of Si surfaces on which metal-induced atomic nanowires appear. The experimental determination of the Au coverage has been revised to be 0.6 monolayer (ML) instead of 0.4 ML. Correspondingly, several structural models have been proposed and discussed [1]. However, recently a model with seven Au atoms per (5×2) cell was proposed by using density functional theory calculations [2].

Si adatoms are observed on the Si(111)-(5×2)-Au surface by STM. The effect for their stability was discussed using first-principles calculations with contradictory results [1-3]. The adatom stability of the model with 7 Au atoms decreases with the density of Si adatoms [2], although the surface energy is lowest for the Si-adatom coverage of 1/4 ML per (5×1) cell for the model with 0.6 ML [3]. Here we present *ab-initio* calculations of Si(111)-(5×2)-Au in order to identify stable phases and their variation with Au coverage and Si adatom decoration.

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- [2] S. G. Kwon and M. H. Kang, Phys. Rev. Lett. 113, 086101 (2014).
- [3] S. C. Erwin *et al.*, Phys. Rev. B 80, 155409 (2009).

DS 36.72 Thu 9:30 Poster A

**Infrared optical investigation of plasmonic excitations in finite atom wires on Si(111)-5x2-Au** — ●FABIAN HÖTZEL, CHRISTIAN HUCK, and ANNEMARIE PUCCI — Kirchhoff-Institute for Physics, Heidelberg University, Heidelberg, Germany

Self-assembled gold atom wires on vicinal Si(111), resulting in the 5x2 reconstruction, are investigated by Fourier transform infrared spectroscopy in transmittance geometry. According to reflection high energy electron diffraction patterns the wires are oriented preferably along the step edges. Relative transmittance spectra show a broad, anisotropic absorption feature at 728 cm<sup>-1</sup> at room temperature which shifts to 822 cm<sup>-1</sup> upon cooling down to 20 K. The signal can be at-

tributed to a localized plasmonic excitation, forming a standing wave due to the finite length of the wires, which enables optical detection. For that reason, a metal-to-insulator transition can be excluded for Si(111)-5x2-Au in this temperature range. The chain length is confined by structural defects [1,2] and domain boundaries [3]. For the fundamental plasmon mode the plasmon wavelength is twice the chain length which results in an average gold chain length of 67 nm. The spectral line shape can be described classically within the electrostatic approximation and yields reasonable results for electron scattering rate, plasma frequency and chain length distribution. This contribution is part of the DFG Research Unit FOR 1700.

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DS 36.73 Thu 9:30 Poster A

**Atomically resolved Pb structures on vicinal Si(557)** — ●MONIKA JÄGER, CHRISTIAN BRAND, HERBERT PFNÜR, and CHRISTOPH TEGENKAMP — Institut für Festkörperphysik, Leibniz Universität Hannover, Germany

Vicinal Si(557) surfaces covered by 1.31 ML Pb reveal a 1D transport behavior below 78 K [1]. Furthermore, recent spin resolved ARPES measurements have shown that the insulating behavior across the direction of the wires is associated with the formation of a spin-orbit density wave [2]. In order to correlate these findings with the morphology the atomic structure was investigated by means of STM. Adsorption of Pb at 600 K gives rise to a refaceting of the Si surface into a local (223) orientation with an average spacing of 1.58 nm. High resolution STM images have clearly identified  $\sqrt{3} \times \sqrt{3}$  reconstructions on the  $4\frac{2}{3} \times 0.332$  nm wide (111) terraces. Furthermore, the step edges remain uncovered and reveal the periodicity of the Si-dimers. In addition, the 0.665 nm periodicity along the terraces is superimposed by an additional intensity modulation which is compatible with a 10-fold periodicity deduced from the spot-splitting seen in former high resolution LEED measurements. Phase shifts along the quasi-atomically resolved structures are reminiscent of domain wall structures with  $\sqrt{7} \times \sqrt{3}$ -symmetry. Our findings show strong similarities with a recent high resolution STM and DFT study for Pb/Si(553) [3].

[1] C. Tegenkamp *et al.* PRL **95**, 176804 (2005).

[2] C. Tegenkamp *et al.* PRL **109**, 266401 (2012).

[3] M.Kopciuszyński *et al.* PRB **88**, 155431 (2013).

DS 36.74 Thu 9:30 Poster A

**Electronic Structure and Doping of quasi-1D Ag Nanowires** — ●CHRIS NICHOLSON<sup>1</sup>, CLAUDE MONNEY<sup>1</sup>, ULRICH KRIEG<sup>2</sup>, KARSTEN HORN<sup>1</sup>, and MARTIN WOLF<sup>1</sup> — <sup>1</sup>Abteilung PC, Fritz-Haber-Institut der MPG, Faradayweg 4-6, 10825 Berlin — <sup>2</sup>Institut für Festkörperphysik, Leibniz Universität, Appelstraße 2, 30167 Hannover

Control over the electronic properties in nanoscale structures is an area which has both fundamental and technological importance. Self-assembled systems of metals on semiconducting substrates offer a versatile and tuneable environment within which such control can be achieved. Ag nanowires grown on a vicinal Si substrate, Si(557), at a coverage around 1 monolayer have previously been observed to have a highly anisotropic plasmon dispersion in electron energy loss spectra (EELS) [1], which may be the signal of a 1D electron gas at the surface. Additionally, dosing the surface with additional Ag or residual gas produced a shift of the plasmon frequency as a function of exposure time [2], which is likely to be the filling of the 1D electronic band. We employ angle-resolved photoemission spectroscopy (ARPES) to reveal that the plasmonic behaviour of the AgSi(557) system can be understood in terms of the electron interaction with the vicinal Si substrate. Additionally we show the important role played by residual gas adsorption in filling electronic states at the Fermi level.

[1] Krieg *et al.* J. Phys. Condens. Matt. **25** (2013) 014013

[2] Krieg *et al.* New J. Phys **16** 0430076 (2014)

DS 36.75 Thu 9:30 Poster A

**Ginzburg-Landau theory for collective excitations in In/Si(111)** — ●YASEMIN ERGÜN and ERIC JECKELMANN — Leibniz Universität Hannover, Germany

We investigate the dynamics of collective excitations in Peierls insulators using the Ginzburg-Landau (GL) theory for quasi-one-dimensional charge-density-wave systems. Starting from a microscopic Su-Schrieffer-Heeger-like model for In/Si(111), we generalized the GL theory for systems with several Peierls modes. This formalism allows us to study the vibrations and the non-equilibrium dynamics of col-

lective "amplitude" modes (lattice distortion and density modulation) which are involved in a Peierls transition. We discuss our theoretical results in relation to spectroscopy experiments for In/Si(111). Support from the DFG through the Research Unit FOR 1700 is gratefully acknowledged.

DS 36.76 Thu 9:30 Poster A

**Controlled electromigration of copper and gold thin films on different substrates** — ●DANIEL ARNOLD<sup>1</sup>, MICHAEL MARZ<sup>1</sup>, CHRISTOPH SÜRGER<sup>1</sup>, HILBERT V. LÖHNEYSEN<sup>1,2</sup>, and REGINA HOFFMANN-VOGEL<sup>1</sup> — <sup>1</sup>Karlsruher Institut für Technologie, Physikalisches Institut, D-76131 Karlsruhe — <sup>2</sup>Karlsruher Institut für Technologie, Institut für Festkörperphysik, D-76021 Karlsruhe

The fabrication of planar nanocontacts for single-molecule electronics is a challenging task because the distance between the electrodes should be on the order of 1 nm. A technique to produce such contacts is controlled electromigration (EM) where a current is flowing through a metallic thin film ramped in a cyclic way [1]. This current leads to the motion of metal atoms causing a controlled thinning of the structured film. Recent simulations show that EM in thin films is strongly affected by the thermal conductivity of the substrate [2]. We have performed controlled EM in a four-terminal setup on sputtered gold and copper films with an optimized structure to avoid failure by EM at the macroscopic contacts. We have used mica and sapphire as substrates. Both materials are good electrical insulators, with sapphire showing a higher thermal conductivity. We have observed a significant inclusion of the substrate material on the amount of power needed for EM. Moreover, our study shows substantial differences in the microstructure of the samples, although their current-voltage characteristics show the same EM behavior.

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[2] B. Kiessig *et al.*, New J. Phys. **16**, 013017 (2014).

DS 36.77 Thu 9:30 Poster A

**Density functional theory investigation of rare earth silicide nanowires** — ●KRIS HOLTGREWE, SIMONE SANNA, and WOLF GERO SCHMIDT — Lehrstuhl für Theoretische Physik, Universität Paderborn

Quasi one-dimensional electron systems are of both fundamental interest because of their unusual physical properties as well as potentially interesting for devices on the nanometer scale. In this respect, rare earth silicide nanowires have been studied experimentally [1]. Unfortunately, the exact knowledge of their atomic structure, which is crucial for understanding their physical properties, is still incomplete. As a first step towards the understanding of the nanowires structural and electronic properties, we have investigated different wire models from first-principles within the density functional theory. Thereby erbium is chosen as prototypical trivalent rare earth ion and its 4f-electrons are treated as frozen state in the atomic core. After comparing the formation energy of the different models, electronic band structures and density of states are calculated for the stable wires. Structural and electronic properties are discussed and compared with available STM and ARPES measurements [1].

[1] M. Wanke *et al.*, Phys. Rev. B **83**, 205417 (2011)

DS 36.78 Thu 9:30 Poster A

**Manipulation of atomic chains on Ge(001) surface** — ●DENİZ AŞAN ACAR, UMUT KAMBER, DILEK YILDIZ, and OĞUZHAN GÜRLÜ — Istanbul Technical University, Istanbul, Turkey

Single atom thick self organized nanowires (NW) form on Ge(001) surface due to Au or Pt atoms adsorbed on to clean surfaces. Upon annealing of Pt deposited Ge(001) surface at 1000 K such atomic chains form along with two different types of terraces, namely the alpha and beta terraces [1]. Although the alpha terraces resemble the Ge(001) surface, beta terraces are due to a surface confined phase of platinum-germanide. Pt induced NWs form only on the beta terraces. Interestingly the wires only exist between surface defects resembling ropes fixed between two walls. Yet it is possible to generated artificial defects with the scanning tunneling microscope (STM) tip and the wires can be cut in to smaller sizes. Moreover the individual pieces of the wires can be picked up and put back on to the surfaces at room temperature by STM [2]. When the pieces of the nanowires were removed, the atomic structure of the underlying lattice of the wires was observed to differ from the beta terraces. Here we report the existence of a new domain on the Pt/Ge(001) system and we name these zones as the gamma zones. [1] O. Gurlu *et al.*, APL **83**, 22 (2003). [2] O. Gurlu *et al.*, Nanotechnology **18**, (2007) 365305 (4pp)

DS 36.79 Thu 9:30 Poster A

**DFT simulations for functionalized Si(553)-Au surface** — ●SVETLANA SUCHKOVA<sup>1</sup>, EUGEN SPEISER<sup>1</sup>, SANDHYA CHANDOLA<sup>1</sup>, CONOR HOGAN<sup>2</sup>, JULIAN PLAICKNER<sup>1</sup>, and NORBERT ESSER<sup>1</sup> — <sup>1</sup>Leibnitz-Institut für Analytische Wissenschaften - ISAS - e.V., Department Berlin, Schwarzschildstr. 8-10, 12489 Berlin, Germany — <sup>2</sup>Universita di Roma "Tor Vergata", Via della Ricerca Scientifica 1, 00133 Roma, Italy

The Si(553)-Au surface will be used as a template for functionalization using self-assembled arrays of toluene-3,4-dithiol molecules. The ordering, orientation, structure and interaction of the molecules with the metal nanowire terminated surface and the intermolecular interaction will be investigated depending on various preparation parameters and coverage. The structure and chemistry will be analyzed by means of Density functional theory calculations (DFT) and compared to reflectance anisotropy spectroscopy (RAS) measurements.

DS 36.80 Thu 9:30 Poster A

**Calculation and Measurement of the Transport Parameters of Fe<sub>x</sub>Co<sub>1-x</sub>Sb<sub>3</sub> Skutterudite Thin Films** — ●FELIX TIMMERMANN<sup>1</sup>, MARCUS V. DANIEL<sup>2</sup>, AYHAM DALLA<sup>2</sup>, and MANFRED ALBRECHT<sup>1</sup> — <sup>1</sup>Institute of Physics, University of Augsburg, Universitätsstr. 1, 86159 Augsburg, Germany — <sup>2</sup>Institute of Physics, Technische Universität Chemnitz, 09107 Chemnitz, Germany

Increasing interest in the development of alternative energy sources led to an extended research in the field of thermoelectricity. For a good efficiency of thermoelectric generators, there is a need of materials with special transport properties. The goal is to find compounds with a large Seebeck coefficient, good electrical conductivity and low thermal conductivity. Skutterudites, such as CoSb<sub>3</sub>, are materials that meet those criteria well. Substituting Fe with Co gradually could improve the properties further.

In this work, the transport parameters of Fe<sub>x</sub>Co<sub>1-x</sub>Sb<sub>3</sub> have been calculated with equations derived from the Boltzmann equation. Under the assumption that the substitution of Co-atoms with iron acts as p-doping of CoSb<sub>3</sub>, the electrical conductivity and the Seebeck coefficient were simulated for different values of the Fermi level.

For comparison 30 nm thick thin Fe<sub>x</sub>Co<sub>1-x</sub>Sb<sub>3</sub>-films were deposited at room temperature by molecular beam deposition and post-annealed in vacuum at 450 °C. The substitution level x was varied from 0 to 0.7. The electrical conductivity and the Seebeck coefficient of these films have been measured and show good agreement with the theoretical results.

DS 36.81 Thu 9:30 Poster A

**Influence of interfaces on the thermoelectric efficiency** — ●MICHAEL BACHMANN, JONAS SCHÄFER, MICHAEL CZERNER, and CHRISTIAN HEILIGER — I. Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany

We present our results on phonon- and electron transport across nanostructured interfaces and the resulting impact on the thermoelectric properties. For the electron transport we focus our investigations on the energy filtering at grain boundaries [1]. Our results are based on a model that we developed to describe electron transport in nanograined materials. The grain boundaries are described using the model introduced by Seto [2]. It is believed that such barriers can increase the efficiency of thermoelectric materials by energy filtering effects. We conclude that electrostatic barriers play no role for thermoelectric devices. For the phonon transport we use an atomistic Greens function method to investigate the phonon scattering Si isotope-multilayer. Our calculations [3] show that a periodic arrangement of the layer-system cannot decrease the phonon thermal conductivity substantially, whereas a random arrangement of the layer-system can lead to a strong decrease in the phonon conductivity. We also show that small deviations from the periodic arrangement are enough to end up in the random regime.

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[3] M Bachmann et al 2014 Semicond. Sci. Technol. 29 12400

DS 36.82 Thu 9:30 Poster A

**Calculation of Thermal Conductivity across an Interface using Beam Matching** — DEBANJAN BASU<sup>1</sup>, ●PETER BLÖCHL<sup>1</sup>, CYNTHIA VOLKERT<sup>2</sup>, and CHRISTIAN JOOSS<sup>2</sup> — <sup>1</sup>Institute for Theoretical Physics, Clausthal University of Technology — <sup>2</sup>Institute for Material

Physics, University of Göttingen

Thermal conductivity is an important factor affecting the efficiency of thermoelectric devices. Our goal is to explore the thermal transmission due to phonons in multilayered structures on a mode-by-mode basis using the Beam Matching Technique. For this purpose, we determine the “complex bandstructure”, which describes propagating as well as evanescent phonon modes of the individual materials of this multilayer. We also describe how to extract the matching conditions from the classical equations of motion for the atoms. The connection between our method and the Landauer-Buttiker description of conductivity for phonons shall be discussed.

This work is funded by the DFG Schwerpunktprogramme 1386.

DS 36.83 Thu 9:30 Poster A

**Tuning the thermoelectric properties of cobaltates by epitaxial strain** — ●MARKUS ERNST GRUNER<sup>1,2</sup> and ROSSITZA PENTCHEVA<sup>2,1</sup> — <sup>1</sup>Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), Technische Universität München, Lichtenbergstraße 1, 85748 Garching, Germany — <sup>2</sup>Faculty of Physics and Center for Nanointegration, CENIDE, University of Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany

The hexagonal delafossites PdCoO<sub>2</sub> and PtCoO<sub>2</sub> exhibit highly anisotropic transport properties and have been identified as potential thermoelectric materials. For instance, along the hexagonal a-b-plane the thermopower  $S_{xx}$  exhibits positive values characteristic of a regular metal, while negative values  $S_{zz}$  are encountered in direction of the c-axis, with a much higher absolute value [1]. By means of density functional theory calculations in connection with Boltzmann transport theory we investigate the effect of epitaxial strain on the thermoelectric properties. We find that for PdCoO<sub>2</sub> the anisotropic properties of conductivity and thermopower are essentially maintained under in-plane strain. Moreover, a 30% variation of  $S_{zz}$  is found in the considered strain regime. The transport results are related to the specific properties of electronic structure and Fermi surface. Funding by the DFG (SFB/TR80, project G8) is gratefully acknowledged.

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DS 36.84 Thu 9:30 Poster A

**Synthesis and thermoelectric properties of Bismuth Sulfide and Bismuth Sulfide Selenide alloys** — ●MAIK MATTHIESEN, LEWIS AKINSINDE, HEIKO REITH, and KORNELIUS NIELSCH — Institute of Nanostructure and Solid State Physics, Universität Hamburg, Hamburg, Germany

Thermoelectric Generators (TEG) enable the direct conversion of heat into electrical energy. Materials with high thermoelectric figure of merit ( $ZT = \alpha^2 \sigma T / \kappa$ ) are required for efficient energy conversion. TE materials should be non-toxic, use abundant elements and the synthesis should be simple and scalable. In recent years, a large variety of semi-conducting material systems have been investigated in the search for new high performance TE-materials. It has been demonstrated that doping of Bi<sub>2</sub>S<sub>3</sub> and Bi<sub>2</sub>S<sub>3</sub>-Bi<sub>2</sub>Se<sub>3</sub> alloys can increase their thermoelectric performance significantly. In this study we have synthesized Bi<sub>2</sub>S<sub>3</sub> and Bi<sub>2</sub>S<sub>3</sub>-Bi<sub>2</sub>Se<sub>3</sub> alloys using sealed quartz ampule synthesis. To tune the charge carrier concentration we added slight amounts of dopants. The obtained materials are characterized with regard to their TE properties (electrical/thermal conductivity and Seebeck coefficient:  $\sigma, \kappa$  and  $\alpha$ ) on commercial equipment. The chemical composition and crystal structure are also examined. We observed a larger power factor ( $\alpha^2 \sigma$ ) in rapidly cooled melts of Chlorine doped Bi<sub>2</sub>S<sub>3</sub> compared to slowly cooled melts. This may be connected with stronger defect doping in the rapidly cooled Ingots. The synthesis method and parameters such as temperature and time need to be taken into account when optimizing such materials.

DS 36.85 Thu 9:30 Poster A

**Nonlinear Dielectric Response of Anisotropically Strained Epitaxial Ferroelectric Films** — ●YANG DAI, JÜRGEN SCHUBERT, EUGEN HOLLMANN, and ROGER WÖRDENWEBER — Peter Grünberg Institute (PGI), Forschungszentrum Jülich, D-52425 Jülich, Germany

Strain can not only strongly modify the electronic characteristics of ferroelectric material, it can also induce interesting partially novel properties in these systems. In this work, the impact of ac and dc electric field and the field orientation on the dielectric properties of anisotropically strained epitaxial SrTiO<sub>3</sub> films grown on DyScO<sub>3</sub> are examined. The anisotropic lattice mismatch between the SrTiO<sub>3</sub> film and DyScO<sub>3</sub> leads to different in-plane tensile strain in the different

crystalline direction of 0.95% and 1.05%, respectively. As a result, (i) the tensile strain causes an increase of the ferroelectric-dielectric phase transition temperature to  $T_{\text{max}}=258$  K and  $T_{\text{max}}=288$  K for small and large tensile strain, respectively. (ii) With increasing amplitude of the ac electric field, the extrinsic contribution to the dielectric permittivity increases nonlinearly, which provides indication on the dynamic and pinning of domain wall. (iii) The dielectric permittivity is strongly suppressed by an additional dc bias electric field for a restricted temperature regime ranging from 180 K to 320 K. The different dielectric responses are discussed in the term of domain wall dynamic and pinning inducing relaxor type models.

DS 36.86 Thu 9:30 Poster A

**Ferroelectric properties of anisotropically strained epitaxial  $\text{NaNbO}_3$  films grown on  $\text{NdGaO}_3$**  — ●BIYA CAI<sup>1</sup>, JUTTA SCHWARZKOPF<sup>2</sup>, EUGEN HOLLMANN<sup>1</sup>, DOROTHEE BRAUN<sup>2</sup>, MARTIN SCHMIDBAUER<sup>2</sup>, and ROGER WÖRDENWEBER<sup>1</sup> — <sup>1</sup>Peter Grünberg Institute (PGI) Jülich, D-52425 Jülich, Germany — <sup>2</sup>Leibniz Institute for Crystal Growth, Max-Born-Str. 2, D-12489 Berlin, Germany

Due to the lattice mismatch between the film and substrate, an anisotropically in-plane strain can be imposed to an epitaxially grown film.  $\text{NaNbO}_3$  films are epitaxially deposited on (110)  $\text{NdGaO}_3$  via Metal Organic Chemical Vapor Deposition. X-ray analysis shows that above 15nm, relaxation of the compressive strain starts. The analysis of the complex permittivity of different thickness films (27 \* 80nm) as a function of temperature, electric field direction, AC and DC electric field reveals that (i) the compressive strain shifts the temperature of maximum permittivity from about 628K of a bulk  $\text{NaNbO}_3$  to close to room temperature of thin films, (ii) the room temperature permittivity of these strained films is enhanced by up to a factor of almost 3 compared to that of bulk material, (iii) there is a strong anisotropy in all ferroelectric characteristics for electric field orientations and (iv) a strong dependence of the permittivity on the ac amplitude of the electric field as well as the dc component of the electric field. The experimental results are discussed in terms of theories on domain wall motions and effect of relaxor ferroelectrics. These strained films represent interesting candidates for the applications of surface acoustic wave sensors.

DS 36.87 Thu 9:30 Poster A

**A Novel Concept of an Oxide Thin Film Sensor for Integrated Filtering and Local Signal Detection** — ●ALEKSANDR MARKOV, EUGEN HOLLMANN, and ROGER WÖRDENWEBER — Forschungszentrum Jülich GmbH, Wilhelm-Johnen-Straße, 52428, Jülich

Engineering of a frequency dependence of permittivity can be of interest for various sensor application. In this work a strong modification of the frequency dependence of ferroelectric properties is achieved via a controlled deposition process of the metal electrode (Pt) into the ferroelectric layer ((Ba,Sr)TiO<sub>3</sub>). For this purpose a series of Ba<sub>0.5</sub>Sr<sub>0.5</sub>TiO<sub>3</sub> layers has been deposited onto Pt coated sapphire at various temperatures range from 660 °C to 760 °C. Additionally a top electrode is deposited at room temperature. The electronic properties of the capacitors are investigated via frequency dependent cryoelectronic measurements, structure and stoichiometry are analyzed via X-ray and RBS measurements, respectively. The analysis of the permittivity and tangent loss show a strong frequency dependence of the permittivity in a small region of the deposition temperatures (680 °C - 710 °C), i.e. the permittivity changes from  $\epsilon_{\text{eff}}$  of 600 at low frequency to  $\epsilon_{\text{eff}}$  of 20 at high frequency. This behavior is caused by a partial diffusion of Pt into the ferroelectric layer and can be explained by the Maxwell-Wagner model. The diffusion is supported by RBS data obtained for the samples deposited at different temperatures. Potential application of these layers for sensors with integrated filtering are sketched.

DS 36.88 Thu 9:30 Poster A

**Experimental and Theoretical Investigations on an in situ k-restore Process with Plasma Enhanced Fragmentation for Damaged ULK Materials** — ●ANJA FÖRSTER<sup>1,5</sup>, NICOLE KÖHLER<sup>2</sup>, SVEN ZIMMERMANN<sup>1,2</sup>, TOBIAS FISCHER<sup>2</sup>, CHRISTIAN WAGNER<sup>2</sup>, JÖRG SCHUSTER<sup>1</sup>, SIBYLLE GEMMING<sup>3,4</sup>, STEFAN SCHULZ<sup>1,2</sup>, and THOMAS GESSNER<sup>1,2</sup> — <sup>1</sup>Fraunhofer ENAS, Chemnitz — <sup>2</sup>Center for Microtechnologies, TU Chemnitz, Chemnitz — <sup>3</sup>Institute of Physics, TU Chemnitz, Chemnitz — <sup>4</sup>Helmholtz-Zentrum Dresden-Rossendorf, Dresden — <sup>5</sup>cfaed, TU Dresden, Dresden

We present an in situ repair process for damaged ultra-low-k (ULK) materials. We use repair fragments to replace damaged bonds (Si-

H and Si-OH) and to reinsert lost methyl groups to restore the k-value. The repair fragments are gained from plasma enhanced fragmentation of the silylation precursor Octamethylcyclotetrasiloxane (OMCTS) and Bis(dimethylamino)-dimethylsilane (DMADMS).

We show that the plasma fragments of both silylation precursors can repair the damage. Further, the oxygen containing OMCTS precursor displays a better repair performance than DMADMS. The influence of the reaction temperature and of an oxygen pretreatment was investigated.

The fragmentation of DMADMS and OMCTS is studied using density functional theory (DFT), confirming the ratio of the repair fragments in the experimental repair plasma. The repair process was also analyzed with DFT and molecular dynamics methods. An explanation for the OMCTS's fragments better repair performance was found.

DS 36.89 Thu 9:30 Poster A

**Modification of resistive switching of  $\text{TiO}_2$  by noble gas ion implantation** — ●SOLVEIG RENTROP<sup>1</sup>, BARBARA ABENDROTH<sup>1</sup>, WOLFRAM MÜNCHGESANG<sup>1</sup>, JULIANE WALTER<sup>1</sup>, JURA RENSBERG<sup>2</sup>, HARTMUT STÖCKER<sup>1</sup>, and DIRK C. MEYER<sup>1</sup> — <sup>1</sup>TU Bergakademie Freiberg, Deutschland — <sup>2</sup>Friedrich-Schiller-Universität Jena, Deutschland

Ion beam modification is one of the possible routes to specifically modify resistive switching characteristics of metal-insulator-metal (MIM) capacitor structures for future non-volatile random access memories. The effects of noble gas ion implantation on structural, optical and electrical properties were investigated for  $\text{TiO}_2$ -based MIM devices, as  $\text{TiO}_2$  is one of the most studied and well known binary dielectric for resistive switching.

Here, we used TiN-TiO<sub>2</sub>-Au devices with oxide layer thickness ranging from 16-44 nm.  $\text{TiO}_2$  layers are deposited by atomic layer deposition and are either amorphous or crystalline in the anatase phase. Ion implantation of Kr<sup>+</sup> at 28-40 keV was applied to induce structural modifications within the oxide layer leading to full amorphisation of anatase layers for fluences of  $F = 1 \times 10^{15}$  ions/cm<sup>2</sup>. We demonstrate stable and reproducible non-volatile switching behaviour for as deposited amorphous  $\text{TiO}_2$  and the change in resistive switching parameters such as  $R_{\text{ON/OFF}}$  ratio and current compliance induced by ion implantation and in dependence on the ion fluence. Volatile switching with a very high  $R_{\text{ON/OFF}}$  ratio of 946 was found for anatase layers after ion implantation using small fluences of  $F = 1 \times 10^{13}$  ions/cm<sup>2</sup>.

DS 36.90 Thu 9:30 Poster A

**CEMS study of iron silicide formation on silicon surfaces induced by surfactant sputtering** — CLEMENS BECKMANN, ●CHRISTOPH BRÜSEWITZ, OMAR BOBES, ULRICH VETTER, and HANS HOFSSÄSS — Georg-August-Universität Göttingen, II. Physikalisches Institut, Göttingen, Germany

We investigate ripple pattern formation on Si during normal incidence ion beam erosion under simultaneous co-deposition of Fe surfactant atoms. In previous work we proposed that chemical interaction between Fe and Si and phase separation towards a disilicide phase of the mixed  $\text{Fe}_x\text{Si}_{1-x}$  surface layer is a dominant contribution to self-organized pattern formation [1,2,3]. Isotopically enriched <sup>57</sup>Fe is used as surfactant and the generated patterns were analyzed with conversion electron Mössbauer spectroscopy (CEMS) in addition to RBS and AFM. Samples were irradiated with keV Ar and Xe ions at normal incidence and simultaneous <sup>57</sup>Fe co-deposition. CEMS measurements show a quadrupole splitting of 0.65(1) mm/s and isomer shift of 0.18(1) mm/s, typical for amorphous  $\text{Fe}_x\text{Si}_{1-x}$ . From a comparison with literature data, quadrupole splitting and isomer shift are consistent with a composition  $x = 0.3-0.35$  and support phase separation as relevant mechanism.

[1] K. Zhang et al., New.J.Phys. 13,013033(2011).

[2] H. Hofsäss et al., AIP Advances 2,032123(2012).

[3] H. Hofsäss et al., Appl.Phys.A: Mat.Sci.Proc. 111,653 (2013).

DS 36.91 Thu 9:30 Poster A

**Formation of hybrid Ge:Mn structures during flashlamp annealing** — ●DANILO BÜRGER<sup>1</sup>, STEFAN BAUNACK<sup>2</sup>, JÜRGEN THOMAS<sup>2</sup>, DANIEL BLASCHKE<sup>3</sup>, THOMAS SCHUMANN<sup>3</sup>, SHENGQIANG ZHOU<sup>3</sup>, OLIVER G. SCHMIDT<sup>1,2</sup>, and HEIDEMARIE SCHMIDT<sup>1</sup> — <sup>1</sup>Material Systems for Nanoelectronics, Chemnitz University of Technology — <sup>2</sup>Institute for Integrative Nanosciences, IFW Dresden — <sup>3</sup>Institute of Ion Beam Physics and Materials Research, Helmholtz-

The formation of ordered hybrid structures opens the way to several applications, e.g. in the field of nanoimprint lithography and solar cell

processing [1]. The formation of hybrid Ge:Mn structures by pulsed laser annealing of Mn-implanted Ge wafers has already been experimentally verified [2]. In this work, we co-sputtered Germanium and Manganese to produce amorphous GeMn-films with an initial homogeneous Mn distribution on a (001)-Ge substrate. Afterwards, flashlamp annealing on the ms-timescale has been performed to crystallize the Ge:Mn films. Transmission electron microscopy reveal a polycrystalline structure and an inhomogeneous Mn-distribution. Magnetotransport measurements indicate that the secondary Mn-rich phases do not form a percolating Mn-rich nanonet as known from pulsed laser annealed Mn-implanted Ge [2]. Furthermore, systematic investigations on annealed, co-sputtered Ge:Mn films with different Mn concentration will be presented. The project was supported by the DFG, project BU 2956/1-1. [1] Optics Express **21**, A60-A76 (2013), [2] APL **100**, 012406 (2012)

DS 36.92 Thu 9:30 Poster A

**Spatial Patterning of molecule modified surfaces** — ●JOHANNES VÖLKNER and GREGOR WITTE — Molekulare Festkörperphysik, Philipps-Universität Marburg, 35032 Marburg

Self-assembling monolayers (SAMs) are commonly used for modification of metal surfaces with molecules. It results in a variation of surface properties such as wetting behavior, friction and biofunctionality. Microcontact printing (muCP) enables lateral patterning of such layers by spatially controlled adsorption of molecules through a polysiloxane matrix. It opens the possibility to structure further layers on top, for instance, containing nanoparticles and proteins with different properties.

Here, an array of alternating methyl- and hydroxyl-terminated molecule regions is fabricated. Hence exhibiting hydrophobic and -philic character, the layer serves as template for selective assembly of respectively coated nanoparticles. Optical and fluorescence micrographs reveal the microstructure of juxtaposed regions of nanoparticles exhibiting different photoelectric character. Furthermore, AFM and DLFM serve as means to image patterns on small scale. This successful and reproducible spatial arrangement of nanoparticles is a mandatory step towards the realization of multi-analyte photoelectrochemical detection systems which are based on a spatially resolved optical excitation of functionalized quantum dot arrays.

DS 36.93 Thu 9:30 Poster A

**CIGS Islands for Micro-Concentrator Solar Cells** — ●FRANZISKA RINGLEB<sup>1</sup>, TORSTEN BOECK<sup>1</sup>, BERIT HEIDMANN<sup>2</sup>, MARTINA SCHMID<sup>2</sup>, CHRISTIAN SYMIETZ<sup>3</sup>, JÖRN BONSE<sup>3</sup>, and JÖRG KRÜGER<sup>3</sup> — <sup>1</sup>IKZ, Max-Born-Straße 2, 12489 Berlin — <sup>2</sup>HZB, Hahn-Meitner-Platz 1, 14109 Berlin — <sup>3</sup>BAM, Unter den Eichen 44-46, 12203 Berlin

Cu(In,Ga)Se<sub>2</sub> (CIGS) is a commonly used absorber material in thin film photovoltaics. However, the high costs of raw materials constitute a challenge for industrial production, such that there is a demand for alternative, more efficient cell designs. In demonstration experiments, CIGS micro-concentrator cells have in principle been shown to increase the efficiency while saving source material. A bottom-up process for the preparation of ordered arrays of isolated micro-absorbers is being developed based on arranging precursor islands on a laser patterned substrate.

DS 36.94 Thu 9:30 Poster A

**Pulsed Laser Deposition of Multilayers designed for Phonon Blocking and Minimizing Thermal Conductivity** — ●FLORIAN DÖRING<sup>1</sup>, CHRISTIAN EBERL<sup>1</sup>, SINJA PAGEL<sup>1</sup>, CHRISTINA KLAMT<sup>1</sup>, ANNA MAJOR<sup>1</sup>, HENNING ULRICHS<sup>2</sup>, MARIA MANSUROVA<sup>2</sup>, MARKUS MÜNZENBERG<sup>3</sup>, and HANS-ULRICH KREBS<sup>1</sup> — <sup>1</sup>Institute for Materials Physics, University of Göttingen — <sup>2</sup>1st Institute of Physics, University of Göttingen — <sup>3</sup>Institute for Physics, University of Greifswald

Pulsed Laser Deposition (PLD) is a versatile thin film method for producing thin layers consisting of various materials, as metals (e.g. W, Ti, or Cu), oxides (e.g. ZrO<sub>2</sub>, MgO, or Ta<sub>2</sub>O<sub>5</sub>) and polymers (e.g. PC). This allows combining different kinds of materials to design multilayers with high acoustic mismatch at the interfaces resulting in different phonon dispersion relations in adjacent materials. By increasing the number of interfaces between such materials, the phonon mean free path is shortened and interface effects like reflection and scattering become more important leading to phonon blocking and henceforth to a decrease in phonon thermal conductivity. In this work, first the results of the structural properties (roughness, film thickness, composition and thermal stability) of laser deposited multilayers of different

material combinations, which were carefully analyzed using x-ray reflectometry, x-ray diffraction and electron microscopy, are presented. Then, the phonon propagation and heat dissipation measured by ultrafast pump-probe reflectivity and transient thermal reflectometry experiments are shown.

DS 36.95 Thu 9:30 Poster A

**Zinc ferrite based magnetic tunnel junctions** — ●MICHAEL BONHOLZER, KERSTIN BRACHWITZ, MICHAEL LORENZ, and MARIUS GRUNDMANN — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, 04103 Leipzig, Germany

Zinc ferrite (ZFO) thin films show promising properties for spintronic device implementation such as semiconducting behaviour [1, 3] and ferromagnetism at room temperature with a high saturation magnetization and coercive field [2, 3]. Also a high spin polarisation of charge carriers is predicted [4].

On the basis of zinc ferrite we have built magnetic tunnel junctions on MgO(100) single crystals by pulsed laser deposition (PLD). The junction structure is MgO(substrate)/TiN(20 nm)/ZFO(30 nm)/MgO(1 to 5 nm)/Co(20 nm). Junctions are fabricated by Ar ion sputtering. Here a protecting Ti mask defines the contact areas.

In order to reduce the series resistance of the devices we have added a highly conducting TiN layer underneath the ZFO [5]. RHEED intensity oscillations are visible during PLD-growth of the MgO barrier. The resistance-area product (RA) of the contacts shows a clear exponential dependence on barrier thickness, proving tunneling transport.

[1] A. Marcu *et al.*, J. Appl. Phys. **102** 023713 (2007)

[2] C.E. Rodríguez Torres *et al.*, Phys. Rev. B **84**, 064404 (2011)

[3] M. Lorenz *et al.*, Phys. Status Solidi RRL **5**, 438 (2011)

[4] S. Soliman *et al.*, Phys. Rev. B **83**, 085205 (2011)

[5] M. Bonholzer *et al.*, Phys. Status Solidi A **211**, 2621 (2014)

DS 36.96 Thu 9:30 Poster A

**Towards high spatial and temporal resolution of attosecond XUV pulse by fractal multilevel zone plate** — ●HUAHAI PAN<sup>1,2,3</sup>, CHRISTIAN SPÄTH<sup>1,3</sup>, ALEXANDER GUGGENMOS<sup>1,3</sup>, SOOHOON CHEW<sup>1,3</sup>, JÜRGEN SCHMIDT<sup>1,3</sup>, QUANZHONG ZHAO<sup>2</sup>, and ULF KLEINEBERG<sup>1,3</sup> — <sup>1</sup>Ludwig-Maximilians-Universität München, Fakultät für Physik, Am Coulombwall 1, 85748 Garching, Germany — <sup>2</sup>State Key Laboratory of High Field Laser Physics, Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, Shanghai 201800, China — <sup>3</sup>Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching, Germany

Multilevel zone plate has been proposed to improve the diffraction efficiency at first diffraction order. Here, we report the theoretical simulation of chirped-pulses diffracted by multilevel zone plate that only consists of outermost successive 10 one-wave zones with other inner zones blocked. This kind of multilevel zone plate is divided into 4 levels for each one-wave zone, every level of which has a certain amount of phase shift for the given wavelength. Molybdenum is chosen to electroplate zone plate and Gaussian pulse centered at 92.02 eV with full bandwidth of approximately 76 ~ 140 eV is employed. This design does not only improve the diffraction efficiency that reach to 56.5% for the effective incident light illuminated on multilevel zone plate but also increase the spatial resolution as well as preserve the temporal structure of focused attosecond pulse at first diffraction order for the first time.

DS 36.97 Thu 9:30 Poster A

**Sol-gel derived composite metal oxide layers for photocatalytic applications** — ●MARINA KULMAS<sup>1</sup>, OLGA LOHSE<sup>1</sup>, MUHAMMAD BASHOUTI<sup>1</sup>, LUBOMIR SPAHEL<sup>3</sup>, and SILKE CHRISTIANSEN<sup>1,2</sup> — <sup>1</sup>Max Planck Institute for the Science of Light — <sup>2</sup>Helmholtz-Center Berlin — <sup>3</sup>Institute of Chemical Sciences Rennes

Development of photocatalytically active and environment friendly materials for water splitting applications rises to new challenges for scientists. In our work, novel composite materials based on TiO<sub>2</sub>/ZnO were studied for photonodic application for water splitting. The fabrication of the designed layers were simplified by usage of nanocolloids. In the present work, we will show how the properties of the composite materials can be changed through the parameters of fabrication. The morphological and microstructural properties were investigated by scanning electron microscopy (SEM), Energy-Dispersive X-ray (EDX) and X-ray photoelectron spectroscopy (XPS). DOS of the new materials were also estimated. From Impedance spectroscopy the modifications of band gap of synthesized layers were analyzed.

DS 36.98 Thu 9:30 Poster A

**Dielectric Laser Acceleration of electrons using anodic alumina nanostructures** — ●ALEXANDER TAFEL<sup>1</sup>, JOSHUA MCNEUR<sup>1</sup>, ANG LI<sup>1</sup>, KENNETH LEEDLE<sup>2</sup>, JONAS HAMMER<sup>1</sup>, NORBERT SCHÖNENBERGER<sup>1</sup>, PEYMAN YOUSEFI<sup>1</sup>, JAMES HARRIS<sup>2</sup>, and PETER HOMMELHOFF<sup>1</sup> — <sup>1</sup>Department of Laserphysics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — <sup>2</sup>Stanford University, USA

Dielectric Laser acceleration (DLA) has evolved quickly during the last few years. Successful experiments have been conducted with electron energies as low as 28 keV, accelerating gradients as high as 375 MeV/m and deflection angles of 8 mrad. Here, we discuss thin anodic alumina honeycomb nanostructures that are being investigated for future experiments. These nanostructures are periodic in two dimensions, resulting in field patterns and particle trajectories potentially leading to transverse microbunching. Moreover, the damage threshold of alumina in the NIR is high, enabling high accelerating gradients and strong deflecting fields. Lastly, thin films for high reflectivity and thus stronger fields are discussed.

- [1] J. Breuer, P. Hommelhoff, Phys. Rev. Lett., 111, 134803 (2013).  
[2] K. Leedle et al., to be published.

DS 36.99 Thu 9:30 Poster A

**A memristor-based hardware cryptography** — ●N. DU<sup>1</sup>, N. MANJUNATH<sup>1</sup>, Y. SHUAI<sup>2</sup>, D. BUERGER<sup>1</sup>, I. SKORUPA<sup>1</sup>, R. SCHUEFFNY<sup>3</sup>, C. MAYR<sup>4</sup>, D. N. BASOV<sup>5</sup>, M. DI VENTRA<sup>5</sup>, O. G. SCHMIDT<sup>1,6</sup>, and H. SCHMIDT<sup>1</sup> — <sup>1</sup>TU Chemnitz — <sup>2</sup>UESTC — <sup>3</sup>TU Dresden — <sup>4</sup>University of Zurich and ETH Zurich — <sup>5</sup>University of California — <sup>6</sup>IFW Dresden

With the rise of big data handling, new solutions are required to drive cryptographic algorithms for maintaining data security. Here we exploit the nonvolatile, nonlinear resistance change in BiFeO<sub>3</sub> memristors [1] by applying a voltage for the generation of second and higher harmonics and develop a new memristor-based encoding system [2] from it to encrypt and obfuscate data. It is found that a BiFeO<sub>3</sub> memristor in high and low resistance state can be used to generate two clearly distinguishable sets of second and higher harmonics as recently predicted theoretically [3]. The computed autocorrelation of encrypted data (0, 1) using higher harmonics generated by a BiFeO<sub>3</sub> memristor (LRS, HRS) shows that the encoded data distribute randomly.

[1] Y. Shuai, X. Ou, W. B. Luo, N. Du, C. Wu, W. Zhang, D. Bürger, C. Mayr, R. Schüffny, S. Q. Zhou, M. Helm, H. Schmidt, IEEE Elec.Dev. Lett. 34, 54-56 (2013). [2] N. Du, N. Manjunath, Y. Shuai, D. Bürger, I. Skorupa, R. Schüffny, C. Mayr, D. N. Basov, M. Di Ventra, O. G. Schmidt, H. Schmidt, J. Appl. Phys. 115, 124501 (2014) [3] G.Z. Cohen, Y. V. Pershin, M. D. Ventra, Appl. Phys. Lett. 100, 133109 (2012).

DS 36.100 Thu 9:30 Poster A

**Yttrium Oxide Coatings as Tritium Permeation Barriers for Fusion Energy Research** — ●JAN ENGELS, ANNE HOUBEN, and CHRISTIAN LINSMEIER — Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung - Plasmaphysik, 42425 Jülich, Germany

In fusion power plants the hydrogen isotopes deuterium and tritium are used as fuel. To prevent the loss of fuel and the accumulation of radioactive tritium in the first wall, the cooling system, and other parts of the fuel vessel, a tritium permeation barrier is necessary. Oxide thin films, e.g. Er<sub>2</sub>O<sub>3</sub> and Y<sub>2</sub>O<sub>3</sub>, are promising candidates as tritium permeation barrier layers. In this contribution magnetron sputtered Y<sub>2</sub>O<sub>3</sub> thin films on Si-wafers are presented. They are annealed at 600 °C to achieve a plenary cubic phase of the Y<sub>2</sub>O<sub>3</sub> system. The phase of the thin films is investigated by X-ray diffraction. To be able to quantify the permeation reduction factor of the Y<sub>2</sub>O<sub>3</sub> thin films, the construction of a new permeation measurement setup is in progress. Therefore, the oxide layers are deposited on Eurofer97, a reduced activation steel developed for fusion applications. Comparing the permeation flux through a bare substrate and a coated substrate, the permeation reduction factor can be determined.

DS 36.101 Thu 9:30 Poster A

**Anode Materials for All Solid-State Thin-Film Batteries** — ●SUSANN NOWAK, GIULIO CALCAGNO, and GUIDO SCHMITZ — Lehrstuhl für Materialphysik, Universität Stuttgart

Promising anode materials for all solid-state lithium ion batteries are alloying materials like tin or silicon due to their safety compared to

lithium metal and their high specific capacity. However they are also known for their low cycle stability due to a huge volume expansion when lithiated. Recent approaches are trying to use a thin coating of high area materials, nano-wires or patterned materials to overcome these constraints. To give a guideline for the desired thicknesses in these processes we prepared thin films of Si and Sn on different substrates which were charged and discharged by chrono-amperometry in liquid (EC:DEC 1M LiClO<sub>4</sub>) and solid electrolyte (LiPON). The results show clearly that coatings of silicon should not exceed a thickness of 50 nm if long cycle lives are desired. Very thin layers of silicon can be charged at very high rates (over 100 C) without showing significant volume decrease or layer destruction.

DS 36.102 Thu 9:30 Poster A

**Photocatalytic titania layers with designed morphologies** — ●ALEXANDER VAHL, BODO HENKEL, OLEKSANDR POLONSKYI, THOMAS STRUNSKUS, and FRANZ FAUPEL — Lehrstuhl für Materialverbunde, Institut für Materialwissenschaften, Technische Fakultät der Christian-Albrechts-Universität zu Kiel

Titania thin films are widely studied due to their high potential for applications as photocatalytic material. For the improvement of photocatalytic performance of titania thin film layers composites of titania layers comprising different morphologies were prepared. The investigated composites rely on a closed titania bottom layer, which has been prepared by pulsed DC reactive sputtering. Increase in photocatalytic relevant surface area of sputtered titania thin films has been effectively realized by addition of an open porous titania cluster top layer. Samples were characterized by SEM, Raman spectroscopy and methylene blue degradation measurements. Raman spectra show pure phase anatase for both layers, cross sectional SEM micrographs indicate a strong increase in surface area by cluster coating. Congruently, methylene blue degradation experiments reveal a noticeable improvement in photocatalytic performance by application of an additional titania cluster layer.

DS 36.103 Thu 9:30 Poster A

**Field effect transistors with a BiFeO<sub>3</sub>/Si<sub>3</sub>N<sub>4</sub> gate** — ●KEFENG LI<sup>1</sup>, TIANGUI YOU<sup>1</sup>, TIM KASPAR<sup>1</sup>, NAN DU<sup>1</sup>, DANILO BÜRGER<sup>1</sup>, ILONA SKORUPA<sup>1</sup>, THOMAS MIKOLAJICK<sup>2</sup>, OLIVER G. SCHMIDT<sup>1,3</sup>, and HEIDEMARIE SCHMIDT<sup>1</sup> — <sup>1</sup>Material Systems for Nanoelectronics, Chemnitz University of Technology, Reichenhainer Strasse 70, D-09107 Chemnitz, Germany — <sup>2</sup>Namlab gGmbH, Noethnitzer Strasse 64, 01187 Dresden, Germany — <sup>3</sup>Institute for Integrative Nanosciences, IFW-Dresden, Helmholtz Strasse 20, D-01069 Dresden, Germany

The nonvolatile ferroelectric memory field effect transistor has many advantages such as random access, high speed, low power, high density, and non-destructive reading operation [1]. Its memory properties can be tailored using a gate stack of dielectrics and ferroelectric films [2]. Nonvolatile resistive switching in BiFeO<sub>3</sub> (BFO) has attracted much attention [3] and has been attributed to flexible barriers [4]. In this work, field effect transistors with a BFO/Si<sub>3</sub>N<sub>4</sub> gate stack have been fabricated and the output characteristics are discussed in dependence on the nonvolatile capacitive switching in the BFO/Si<sub>3</sub>N<sub>4</sub> gate. [1] O. Auciello, J.F.Scott, R. Ramesh, Physics Today, 51,22 (1998) [2] J. T. Evans and R. Womack, IEEE J. Solid-State Circuits. 23, 1171(1988) [3] Y. Shuai, S. Zhou, D. Bürger, M. Helm, and H. Schmidt, J. Appl. Phys., 109, 124117 (2011) [4] T. You, N. Du, S. Slesazek, T. Mikolajick, G. Li, D. Bürger, I. Skorupa, H. Stöcker, B. Abendroth, A. Beyer, K. Volz, O. G. Schmidt, H. Schmidt, ACS Appl. Mater. Interfaces, 6, 19758 (2014)

DS 36.104 Thu 9:30 Poster A

**ZnO Nanostructured Thin Films: Synthesize for Electrochemical Sensor Application** — ●ALI JASIM MOHAMMED<sup>1</sup> and GERHARD WILDE<sup>2</sup> — <sup>1</sup>Department of Physics, College of Science, Al-Mustansiriyah University, Baghdad, IRAQ — <sup>2</sup>Institute of Material Physics, Westfälisch Wilhelm-University, Wilhelm-Klemm-Str.10, Muenster, GERMANY.

Nanostructured zinc oxide thin films has great interest, our presentation focuses on a simple technique of ZnO thin film synthesization by physical vapor deposition (PVD) and chemical vapor deposition (CVD) to form different types of nanostructures as wires, rods, needles, and discs. The morphologies of these films were investigated by scanning electron microscopy (SEM). The sensing response of the films towards gas and salt solutions detection was studied. Zinc oxide nanowires/nanobelts thin films were prepared by thermal evaporation deposition of Zn on both glass and silicon substrates, namely Cr-glass

and Cr-<100> n-type Si. ZnO nanostructured based CO- gas sensing, furthermore the piezoelectrical characteristics employed for detection of sodium and magnesium solutions. As the gas sensing, the sensitivity increased with increasing operating temperature, particularly above 175 °C where it increased by three folds. Typically ZnO nanowires/nanobelts thin film sensor had fast rise times and good recovery times substrates. While, the salt solution sensor had a fast rise time especially for low pulse repetition rate (1 p/s).

DS 36.105 Thu 9:30 Poster A

**Towards a zone plate based ultra compact HHG driven XUV / soft X-ray scanning transmission microscope** — ●CHRISTIAN SPÄTH, ANNIKA SPREEN, JÜRGEN SCHMIDT, HUIHAI PAN, ALEX GUGGENMOS, and ULF KLEINEBERG — Fakultät Physik, LS Laserphysik, Ludwig-Maximilians-Universität München, 85748 Garching/München

X-ray microscopy is an invaluable imaging method in many research areas with applications at physical, medical and biological problems as well as material science. Especially XUV / soft X-ray microscopy offers the great potential for investigating sensitive biological samples in their natural environment with low dose to reduce radiation damage and high spatial and energy resolution to address questions concerning sub cellular features or elemental composition. Here we report on our concept of an ultra compact microscope utilizing laser driven high harmonic radiation with  $\sim 73$  eV energy as a light source and a dedicated zone plate operated in transmission as the main focussing element combined with different detectors which enables us to run this system in scanning mode as a STXM but also in a modified version as a high resolution instrument in diffraction mode employing the CDI technique. Furthermore due to our pulsed light source the possibility of time-resolved microscopic analysis is given with a possible few-femtosecond temporal resolution.

DS 36.106 Thu 9:30 Poster A

**Spectroscopic investigation of the electronic structure of HfO<sub>2</sub> thin films** — ●SILMA ALBERTON CORRÊA, SIMONE BRIZZI, MASSIMO TALLARIDA, and DIETER SCHEISSER — Department of Applied Physics and Sensors, Brandenburg University of Technology, 03046 Cottbus, Germany

HfO<sub>2</sub> is of current interest as a material for memristive and ferroelectric devices. In this work, we used spectroscopic techniques to evaluate the electronic structure and defects mechanisms in thin HfO<sub>2</sub> films deposited by atomic layer deposition and by metal-organic chemical vapour deposition. The partial density of states for the valence and the conduction bands was determined by the detailed analysis of the O1s resonance profile by resonant photoelectron spectroscopy. From the relative contributions we find a CNL 6.5 eV referred to Evac. We also find that the positions of valence band maximum and conduction band minimum, the excitation range for the polaronic states and the range of charge transfer band were not influenced by the preparation conditions. All films exhibit a band gap of 6.2 eV. However, the Fermi level position was found to vary within about 1.2 eV depending on the preparation conditions, which we argue that is due to the presence of charges within the films. This explains why the position of the Fermi level depends on the individual preparation parameters.

DS 36.107 Thu 9:30 Poster A

**Microstructure of Ruddlesden-Popper SrO(SrTiO<sub>3</sub>)<sub>n</sub> films, prepared by means of Atomic Layer Epitaxy with Metalorganic Aerosol Deposition** — ●FRYDERYK LYZWA<sup>1</sup>, MARKUS JUNGBAUER<sup>1</sup>, SEBASTIAN HÜHN<sup>1</sup>, RICARDO EGOAVIL<sup>2</sup>, HAIYAN TAN<sup>2</sup>, JO VERBEECK<sup>2</sup>, GUSTAAF VAN TENDELOO<sup>2</sup>, and VASILE MOSHNYAGA<sup>1</sup> — <sup>1</sup>Physikalisches Institut, Universität Göttingen — <sup>2</sup>EMAT, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerp, Belgium

The Ruddlesden-Popper (RP) films represent a material system, in which perovskite layers of (SrTiO<sub>3</sub>)<sub>n</sub> are separated by SrO layers. Those dielectrics are promising due to low-loss for microwave frequencies. We report RP thin films of SrO(SrTiO<sub>3</sub>)<sub>n</sub> with  $n = 2, 3, 4$  using metalorganic aerosol deposition (MAD) in the atomic layer epitaxial mode (ALE). The films were grown on SrTiO<sub>3</sub>(100) by sequential deposition of Sr-O/Ti-O<sub>2</sub> atomic layers monitored by optical in-situ ellipsometry. The RP structure was confirmed by X-ray diffraction and transmission electron microscopy. A large number of RP defects observed close to the substrate identifies the STO-surface as a source of RP defects under the oxidizing conditions employed during MAD. To

control this behavior we used a buffer between substrate and film and also other types of substrates such as LSAT(100) and DyScO<sub>3</sub>(110). Financial support from EU FP 7 Project IFOX (interfacing oxides) is acknowledged.

DS 36.108 Thu 9:30 Poster A

**Synthesis of TiS<sub>2</sub> Thin Films Based on Atomic Layer Deposition** — ●JANA VON POBLOTZKI, JOHANNES GOOTH, LEWIS AKINSINDE, ROBERT ZIEROLD, and KORNELIUS NIELSCH — Institute of Nanostructure and Solid State Physics, Universität Hamburg, Hamburg, Deutschland

Transition metal dichalcogenides (TMDCs) are layered materials, which have a strong horizontal and a weak layer-to-layer (van der Waals) interaction. Monolayers of TMDCs can be semiconducting and show high electrical mobility and low effective masses of the charge carriers. Recently, the synthesis of TiS<sub>2</sub> thin films is gaining attention because of their promising thermoelectric properties. In the future TiS<sub>2</sub> could become a very important material choice to replace already existing and popular materials such as Bi<sub>2</sub>Te<sub>3</sub>, Sb<sub>2</sub>Te<sub>3</sub>, and Bi<sub>2</sub>Se<sub>3</sub>.

Two different synthesis approaches of TiS<sub>2</sub> are explored: First, TiO<sub>2</sub> anatase thin films of less than 20 nm thickness were prepared by atomic layer deposition (ALD), thermally annealed to modify the crystalline structure of the samples, and subsequently sulfurized through vapor of CS<sub>2</sub> in a tube furnace. Second, the new precursor combination titanium(IV) isopropoxide and bis(trimethylsilyl)sulfide was tested for direct atomic layer deposition of TiS<sub>2</sub>. The temperature range in which these ALD processes proceed allows the use of standard photolithography to obtain micron-sized measurement structures. Such devices are utilized to determine the (thermo)electric transport properties of these films.

DS 36.109 Thu 9:30 Poster A

**Atomic Layer Deposition of metallic copper using novel precursors in a very small ALD setup** — ●MATTHIAS BÜCHELE<sup>1</sup>, MICHAEL LATZEL<sup>1,2</sup>, and SILKE CHRISTIANSEN<sup>1,3</sup> — <sup>1</sup>Max Planck Institute for the Science of Light, Günther-Scharowsky-Straße 1, Erlangen, Germany — <sup>2</sup>Friedrich-Alexander-Universität Erlangen-Nürnberg, Institut of Optic, Information and Photonics, Staudstr. 7, Erlangen, Germany — <sup>3</sup>Helmholtz Centre Berlin of Energy and Materials, Hahn-Meitner-Platz 1, Berlin, Germany

We pursued the goal, to test new precursors for Atomic Layer Deposition of metallic copper thin-films. This was done with an ultra handy evaporator/chamber setup which easily can be combined with an optical microscope or Raman, due to the thin and small chamber with transparent lid.

We have shown, that the growth mechanism is ALD and that the thin layers contain only metallic copper. Furthermore the surface was determined to be very smooth by AFM measurements.

We will show EDX, AFM and PL measurements of our samples. Latter were done in situ, meaning in real time during the process, so one can see the Signal change from cycle to cycle over the whole deposition time.

DS 36.110 Thu 9:30 Poster A

**Phenomenological Monte-Carlo Simulation of Gold Cluster Growth Kinetics during sputter deposition** — ●SVEN-JANNIK WÖHNERT, MATTHIAS SCHWARTZKOPF, STEPHAN V. ROTH, and WILFRIED WURTH — DESY, Notkestr. 85, D-22607 Hamburg, Germany

Sputter deposition routinely applied to install tailored nanostructures on surfaces. One very suitable method retrieve nanoscale information on such surface is grazing incidence small-angle X-ray (GISAXS) scattering. This method can ideally be combined with in-situ investigations and real-time observations of layer deposition [1,2]. Based on experimental results for noble metal sputter deposition, we introduced successful a mean field model of spherical noble metal cluster growth with a near-field hexagonal lattice on oxide surfaces [1,2]. In order to distinguish the influence of different particle properties and deposition parameters, we introduced a phenomenological Monte-Carlo Simulation We present quantitative visualization of the different growth modes of the real-time experiments [1,2]. Especially we are able to compare the influence of kinetic diffusion and aggregation rate on mean cluster size, mean cluster distance and the percolation threshold. We compare our results to different experimental conditions [1,2].

[1] M. Schwartzkopf, *Nanoscale*, 2013,5, 5053-5062 [2] G. Santoro, *Applied Physics Letters* 104 (24), 243107

## DS 37: Focussed Session: Oxide semiconductors II (joint session with HL)

Time: Thursday 15:00–19:00

Location: H 2032

**Invited Talk**

DS 37.1 Thu 15:00 H 2032

**Optical properties and band structure of transparent semi-conducting oxides** — ●RÜDIGER GOLDHAHN — Otto-von-Guericke-Universität Magdeburg, Institut für Experimentelle Physik

Semiconducting metal oxides such as cubic  $\text{In}_2\text{O}_3$  and rutile  $\text{SnO}_2$  have attracted much interest in recent years. High-quality bulk crystals and single-crystalline heteroepitaxial films, covering a wide range of electron concentrations, became available allowing the determination of intrinsic optical properties as well as related fundamental band-structure parameters. This talk summarizes recent achievements.

Spectroscopic ellipsometry from the infrared (IR) into the vacuum-ultraviolet (VUV) spectral region is applied for determining the components of the dielectric tensor. The analysis of the IR dielectric function yields the phonon frequencies and the coupled phonon-plasmon modes from which electron effective mass as a function of carrier density (non-parabolicity of the conduction band) is obtained. Many-body effects such as exciton screening, band-gap renormalization, and band filling have a strong impact on the behavior around the fundamental band gaps, a quantitative description of these properties will be presented. Finally, synchrotron-based studies in VUV provide the transition energies related to critical points of the band structure.

DS 37.2 Thu 15:30 H 2032

**Optical and Magneto-Optical Investigation of Spinel Oxide Thin Films** — ●VITALY ZVIAGIN<sup>1</sup>, PETER RICHTER<sup>2</sup>, CHRISTIAN KRANERT<sup>1</sup>, TAMMO BÖNTGEN<sup>1</sup>, MICHAEL LORENZ<sup>1</sup>, DIETRICH R.T. ZAHN<sup>2</sup>, GEORGETA SALVAN<sup>2</sup>, RÜDIGER SCHMIDT-GRUND<sup>1</sup>, and MARIUS GRUNDMANN<sup>1</sup> — <sup>1</sup>Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, Germany — <sup>2</sup>Technische Universität Chemnitz, Semiconductor Physics, Reichenheiner Str. 70, Germany

We present a (magneto-) optical and structural investigation of  $\text{Co}_3\text{O}_4$ ,  $\text{ZnFe}_2\text{O}_4$ ,  $\text{CoFe}_2\text{O}_4$ ,  $\text{ZnCo}_2\text{O}_4$  and  $\text{Fe}_3\text{O}_4$  spinel oxides grown at different temperatures on  $\text{MgO}$  (100) and  $\text{MgAl}_2\text{O}_4$  (100) substrates by pulsed laser deposition. The optical properties were determined by spectroscopic ellipsometry in the spectral range from 0.5 eV to 8.5 eV and at temperatures from 10 K to 300 K. The magneto-optical response was measured in the range from 1.5 eV to 5.5 eV at room temperature and with an applied magnetic field of 1.7 T. A parametric model for the dielectric function, consisting of Gaussian and Lorentzian functions located at the optical transition energies, as well as the off-diagonal elements of the dielectric tensor were obtained. The magneto-optical response depends markedly on the crystal quality thus indicating the occurrence of mixtures of normal and inverse spinel structures. The study of (magneto-) optical properties is accompanied by structural analysis of the thin films using Raman spectroscopy, atomic force microscopy, and X-ray diffraction.

DS 37.3 Thu 15:45 H 2032

**Spectroscopic signatures of dinitrogen in  $\text{Cu}_2\text{O}:\text{N}$  thin films** — ●JULIAN BENZ, PHILIPP HERING, BENEDIKT KRAMM, BRUNO K. MEYER, and PETER J. KLAR — I. Physikalisches Institut, Justus-Liebig-Universität, Heinrich-Buff-Ring 16, 35392 Gießen

Cuprous oxide ( $\text{Cu}_2\text{O}$ ) is an intrinsically p-type semiconductor with a band gap of 2.1 eV. By doping with nitrogen it is possible to increase the hole density significantly. Thin films of  $\text{Cu}_2\text{O}:\text{N}$  were prepared by reactive RF sputtering, providing  $\text{N}_2$  gas as dopant in the plasma. Raman spectra of the N-doped samples exhibit additional signals in the region of  $2200\text{ cm}^{-1}$  to  $2300\text{ cm}^{-1}$  Raman shift, which scale with the nitrogen content. We assume that these signals can be assigned to the vibration of dinitrogen molecules bound at different sites inside the bulk and at the surface. To support our assumption, the influence of oxygen flow during growth, as well as growth and annealing temperature are investigated.

DS 37.4 Thu 16:00 H 2032

**Structural properties and phonon modes of  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$**  — ●CHRISTIAN KRANERT, MARCUS JENDERKA, JÖRG LENZNER, MICHAEL LORENZ, HOLGER VON WENCKSTERN, RÜDIGER SCHMIDT-GRUND, and MARIUS GRUNDMANN — Universität Leipzig, Institut für Experimentelle Physik II, Semiconductor Physics Group, Leipzig, Germany

We present a combined X-ray diffraction and Raman scattering study

on a 2-inch diameter thin film with a continuous composition spread (CCS) [1] in comparison to bulk-like ceramic samples. For the composition range for which the ceramic materials exclusively exhibit the  $\beta$ -modification, we obtained their individual lattice parameters as a function of the composition. These comply with Vegard's rule. We further investigated these samples by Raman spectroscopy. The obtained phonon energy dependencies on the composition in the  $\beta$ -phase are found to be linear as well.

The CCS approach for the thin films allows us to determine its properties for virtually any composition within the composition range of the sample. The comparison to the ceramic samples shows a reduced out-of-plane lattice parameter for the thin films. Despite that, the phonon energies show a good agreement to the bulk values.

The material  $\beta$ - $\text{Ga}_2\text{O}_3$  is of interest for deep UV optoelectronics. Alloying with  $\text{Al}_2\text{O}_3$  increases its band gap, which makes the alloy  $(\text{Al,Ga})_2\text{O}_3$  suitable for an application in  $\text{Ga}_2\text{O}_3$ -based heterostructures or as barrier material for  $\text{Ga}_2\text{O}_3$  quantum wells.

[1] H. von Wenckstern et al., *CrystEngComm* **15**, 10020 (2013)

DS 37.5 Thu 16:15 H 2032

**Angle dependent Raman investigations of the different phases of  $\text{Sn}_x\text{O}_y$**  — ●CHRISTIAN T. REINDL, MARTIN BECKER, BRUNO K. MEYER, and PETER J. KLAR — I. Physikalisches Institut, Justus-Liebig-Universität Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

The two widely known tin oxide phases  $\text{SnO}_2$  and  $\text{SnO}$  are easily distinguished by examining their Raman spectra. Such Raman spectra contain information about the crystal structure and orientation as well as its quality, impurities, etc. Ion beam sputtered samples of  $\text{SnO}_2$  and  $\text{SnO}$  with well-defined orientations are investigated using rotational Raman spectroscopy, a technique where the sample is rotated in plane with respect to the incident laser polarization. The intensity of the scattered light is analyzed for different polarizations with respect to the incident light. The data obtained is used to confirm the assignments of Raman modes appearing in the spectra of  $\text{SnO}_2$  and  $\text{SnO}$  and to determine the values of the corresponding Raman tensor elements. Samples grown in the regime between the formation of these two phases yield completely different Raman spectra implies the formation of a third tin oxide phase in this intermediate regime. We present first identification of the Raman modes of this additional  $\text{Sn}_x\text{O}_y$  phase. Furthermore, naturally grown crystals are investigated and compared to the samples grown by ion beam sputtering and chemical vapor deposition.

**15 min. break.****Invited Talk**

DS 37.6 Thu 16:45 H 2032

**Thermodynamic stability and electronic structure of TCO surfaces: A computational approach** — ●KARSTEN ALBE, PETER AGOSTON, MANUEL DIEHM, and ARNO FEY — TU Darmstadt, FB 11, Fachgebiet Materialmodellierung, Jovanka-Bontschits-Str. 2, 64287 Darmstadt

A detailed understanding of the surface properties of transparent electrodes is a prerequisite for optimizing optoelectronic devices. In this contribution the thermodynamic stability and electronic properties of several experimentally observed low-index surfaces of bcc indium oxide ( $\text{In}_2\text{O}_3$ ) and tin oxide ( $\text{SnO}_2$ ) are discussed based on results obtained by electronic structure calculations within density-functional theory. The influence of hydrogen, organic surfacants, n-type dopants (Sn), as well as the in-plane lattice strain are studied and compared to results of STM-studies on single crystalline samples. The computed data are also contrasted with results from photoelectron spectroscopy on magnetron-sputtered layers.

DS 37.7 Thu 17:15 H 2032

**Defect studies on  $\text{In}_2\text{O}_3$  thin films grown by pulsed laser deposition** — ●FLORIAN SCHMIDT, MANUEL R. LINDEL, DANIEL SPLITH, STEFAN MÜLLER, HOLGER VON WENCKSTERN, and MARIUS GRUNDMANN — Universität Leipzig, Institut für Experimentelle Physik II, Abteilung Halbleiterphysik, Linnéstraße 5, 04103 Leipzig

$\text{In}_2\text{O}_3$  is a promising oxide semiconducting material for applications in transparent electronics. Highly tin-doped  $\text{In}_2\text{O}_3$  for instance is already

commercially exploited as transparent conducting electrode. However, less is known on the defect structure of the host material. The fabrication of rectifying Schottky contacts on  $\text{In}_2\text{O}_3$  was reported recently [1] and opens up the possibility to apply space-charge spectroscopic methods, such as thermal admittance spectroscopy (TAS) or deep-level transient spectroscopy (DLTS).

We investigated point defects in both undoped  $\text{In}_2\text{O}_3$  and compensated  $\text{In}_2\text{O}_3:\text{Mg}$  thin films by means of TAS and DLTS. While a defect level with a thermal activation energy  $E_t$  of approximately 200 meV and an apparent capture cross-section  $\sigma_n$  of about  $10^{-16} \text{ cm}^2$  was found both materials another deep defect with  $E_t \approx 90 \text{ meV}$  and  $\sigma_n \approx 5 \times 10^{-18} \text{ cm}^2$  was exclusively found in the Mg-doped sample.

[1] H. von Wenckstern *et al.*, APL Materials **2**, 046104 (2014).

DS 37.8 Thu 17:30 H 2032

**Lattice dynamics of Copper-Oxide phases from ab initio calculations** — ●MARCEL GIAR, THOMAS SANDER, MARKUS HEINEMANN, CHRISTIAN T. REINDL, BIANCA EIFERT, PETER J. KLAR, and CHRISTIAN HEILIGER — I. Physikalisches Institut, Justus-Liebig-University, D-35392 Giessen, Germany

Lattice dynamic properties the three copper oxide phases  $\text{Cu}_2\text{O}$ ,  $\text{Cu}_4\text{O}_3$ , and  $\text{CuO}$  are investigated employing DFT calculations using the VASP code. Phonon bandstructure and density of states for all three phases are derived from a supercell small displacement method. The splitting of the LO and TO modes at the  $\Gamma$  point is obtained by properly taking into account the non-analytical contributions to the dynamical matrix in the limit  $\mathbf{q} \rightarrow 0$ . We also examine Raman properties by calculating Raman susceptibilities and derived Raman spectra. Special attention is paid to the role of defects such as simple Cu vacancies ( $V_{\text{Cu}}$ ) and Cu split vacancies ( $V_{\text{Cu}}^{\text{split}}$ ) in the Raman spectrum of  $\text{Cu}_2\text{O}$ . [1] Further, we present calculations on the low-frequency dielectric tensor from which also IR data can be derived.

[1] T. Sander, C. T. Reindl, M. Giar, B. Eifert, M. Heinemann, C. Heiliger, and P. J. Klar, Phys. Rev. B **90**, 045203 (2014)

DS 37.9 Thu 17:45 H 2032

**Determination of subgap states in oxides: a challenge for DFT functionals** — WOLFGANG KÖRNER<sup>1</sup>, ●DANIEL F. URBAN<sup>1</sup>, DAVID MUNOZ RAMO<sup>2</sup>, PAUL D. BRISTOWE<sup>2</sup>, and CHRISTIAN ELSÄSSER<sup>1,3</sup> — <sup>1</sup>Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany — <sup>2</sup>Department of Materials Science and Metallurgy, University of Cambridge, United Kingdom — <sup>3</sup>Institute for Applied Materials, Karlsruhe Institute of Technology

We present a density-functional-theory analysis of crystalline and amorphous Zn- and Sn-based oxide systems which focuses on the electronic defect-states within the band gap [1]. A comparison of these electronic levels reveals that the hybrid DFT exchange-correlation functionals PBE0, HSE06 or B3LYP agree with a self-interaction corrected local-density approximation (SIC-LDA) functional on occupied defect levels when similar treatments of the self-interaction are considered. However, for unoccupied levels the hybrid functionals and the SIC approach lead to very different predictions. We show that a prerequisite for the determination of the energetic position of subgap states in these oxides is that a functional needs to predict correctly the electronic band structure over a wide energy range and not just close to the band gap. We conclude that for accurate defect levels an adequate treatment of the self interaction problem is required especially in the presence of nearby metal-metal interactions.

[1] W. Körner, D. F. Urban, D. Munoz Ramo, P. D. Bristowe, C. Elsässer, Phys. Rev. B **90**, 195142 (2014)

#### Invited Talk

DS 37.10 Thu 18:00 H 2032

**Synthesis and Stability of Indium (III) Oxide Polymorphs** — ●ALEKSANDER GURLO and MAGED BEKHEET — Fachgebiet Keramische Werkstoffe, Technische Universität Berlin, Fakultät III Prozesswissenschaften, Institut für Werkstoffwissenschaften und -technologien, Sekr. BA3, Hardenbergstraße 40, 10623 Berlin, Germany

In our presentation the synthesis, stability and properties of binary indium oxides will be addressed. Our recent works deal with the synthesis and characterization of the known and new polymorphs in indium-oxygen system. In this way (i) a new orthorhombic  $\text{In}_2\text{O}_3$  polymorph has been synthesized under high-pressure high-temperature conditions and recovered to ambient pressure and temperature, (ii) the metastability of corundum-type  $\text{In}_2\text{O}_3$  have been proved both theoretically and experimentally, (iii) new sol-gel methodologies to synthesize high pressure  $\text{In}_2\text{O}_3$  polymorphs under ambient pressure conditions have been developed, (iv) the stabilisation of pseudo-cubic {012} morphology in corundum-type  $\text{In}_2\text{O}_3$  over several length scales have been verified, (v) the mobility and carrier concentration of well-defined corundum- and bixbyite-type  $\text{In}_2\text{O}_3$  nanocrystals have been measured at different temperatures and in different gas atmospheres, (vi) a synthetic methodology for hierarchically organized hollow spheres has been developed, (vii) the crystallization of bixbyite-type  $\text{In}_2\text{O}_3$  has been proven using in-situ time-resolved synchrotron radiation, and (viii) the stabilization of high-pressure corundum-type  $\text{In}_2\text{O}_3$  polymorph in nanocrystals have been explained.

DS 37.11 Thu 18:30 H 2032

**Photocatalysis of Titania Thin Films Prepared by Sputtering versus Evaporation** — BODO HENKEL<sup>1</sup>, THOMAS NEUBERT<sup>2</sup>, SEBASTIAN ZABEL<sup>1</sup>, ●THOMAS STRUNSKUS<sup>1</sup>, MICHAEL VERGÖHL<sup>2</sup>, and FRANZ FAUPEL<sup>1</sup> — <sup>1</sup>Lehrstuhl für Materialverbunde, Institut für Materialwissenschaft, Christian Albrechts Universität zu Kiel — <sup>2</sup>Fraunhofer Institut für Oberflächen- und Schichttechnologie, Braunschweig

To achieve a deeper understanding about reasons for differing photocatalytic efficiencies of titania thin films made by different physical vapor deposition techniques, different grain and phase growth pathways of these titania thin films have been studied. Results are shown for two well established and widely used PVD methods, namely electron beam evaporation and reactive pulsed DC magnetron sputtering. In addition the effect of inducing oxygen vacancy defects by tempering in reducing atmospheres on their photocatalytic efficiency have been tested, as well as aging of these thin films. These titania thin films where characterized with respect to crystallinity, texture and phases (XRD and Raman), roughness and surface area (AFM), light transmission and band gap energy (UV-Vis), refractive index (Ellipsometry), film thickness (Profilometer, Ellipsometry, SEM cross section), grain growth and structure (AFM, SEM of surface and cross section) and photocatalytic efficiency (methylene blue degradation). Results show different nucleation and growth mechanisms for evaporated compared to sputtered titania thin films, which have severe influence on photocatalytic efficiency.

DS 37.12 Thu 18:45 H 2032

**Interdependence of electroformation and hydrogen incorporation in titanium dioxide** — MARA STRUNGARU<sup>1</sup>, MIHAI CERCHEZ<sup>2</sup>, ●SVENJA HERBERTZ<sup>2</sup>, THOMAS HEINZEL<sup>2</sup>, MHAMED EL ACHHAB<sup>3</sup>, and KLAUS SCHIERBAUM<sup>3</sup> — <sup>1</sup>Faculty of Physics, Alexandru Ioan Cuza University, 700506, Iasi, Romania — <sup>2</sup>Solid State Physics Laboratory, Heinrich-Heine-Universität Düsseldorf — <sup>3</sup>Materials Science Laboratory, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf

Nanoporous titanium dioxide films are exposed to molecular hydrogen gas during electroformation. In addition to the usual reversible increase of the conductance of the films as hydrogen is offered, an irreversible decrease of the conductance is observed. The behavior is interpreted in terms of a phenomenological model where current carrying, oxygen-deficient filaments form inside the  $\text{TiO}_2$  matrix in which hydrogen incorporation decreases the carrier density.

[1] M. Cerchez, H. Langer, M. E. Achhab, T. Heinzl, D. Ostermann, H. Lüder, and D. Ostermann, Appl. Phys. Lett. **103**, 033522 (2013). [2] D. B. Strukov, G. S. Snider, D. R. Stewart, and R. S. Williams, Nature **453**, 80 (2008). [3] T. Bjørheim, S. Stølen, and T. Norby, Phys. Chem. Chem. Phys. **12**, 6817 (2010).

## DS 38: Phase change/ resistive switching

Time: Thursday 15:00–18:45

Location: H 0111

DS 38.1 Thu 15:00 H 0111

**Nanosecond laser-induced phase transitions in pulsed laser deposition-deposited GeTe films** — ●XINXING SUN, ERIK THELANDER, JÜRGEN W. GERLACH, and BERND RAUSCHENBACH — Leibniz Institute of Surface Modification, Permoserstr. 15, D-04318, Leipzig, Germany

Phase changes in chalcogenide-based alloys have been widely studied in terms of the application in optical data storage and the same class of phase change materials is a promising candidate for further applications in non-volatile memories. In this study, phase transformations between the amorphous and crystalline state in GeTe thin films grown by pulsed laser deposition (PLD) are investigated. The phase transformations are induced by irradiation with nanosecond laser pulses at 248 nm and pulse duration of 20 ns. The structural and optical properties of the GeTe films were studied by x-ray diffraction and optical reflectivity measurements as a function of the number of irradiation pulses between 0 and 30 pulses and of the laser fluence up to 195 mJ/cm<sup>2</sup>. A reversible phase transition is found by using pulse numbers more than 5 pulses at a fluence above the threshold fluence for crystallization (between 11 and 14 mJ/cm<sup>2</sup>) and single pulse at a fluence of between 162 and 182 mJ/cm<sup>2</sup> for amorphization. The influence of film thickness (6-300 nm) and irradiation with pulse repetition frequency (1-400 Hz) on the crystallization behavior of GeTe films is also discussed. A high optical contrast between the amorphous and crystalline state is achieved, proving that PLD-deposited GeTe films have excellent potential for application in phase change storage.

DS 38.2 Thu 15:15 H 0111

**Growth of Germanium Telluride Thin Films on Passivated Silicon Surfaces by Molecular Beam Epitaxy** — ●RUI NING WANG<sup>1</sup>, JOS BOSCHKER<sup>1</sup>, RAFFAELLA CALARCO<sup>1</sup>, JAMO MOMAND<sup>2</sup>, and BART KOOI<sup>2</sup> — <sup>1</sup>Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — <sup>2</sup>University of Groningen, Zernike Institute for Advanced Materials, Groningen, The Netherlands

As a phase change material, and as a ferroelectric semiconductor, germanium telluride is worth investigating both from the fundamental and technological point of view. And especially for fundamental research, the ability to produce GeTe thin films of great crystalline quality is of prime importance.

Epitaxial growth of GeTe on Si(111)-(7x7) by molecular beam epitaxy was first demonstrated by Giussani et al. [1] and it has been recently shown that the crystalline quality of such GeTe thin films can be significantly improved by growing on a passivated Si(111)-( $\sqrt{3} \times \sqrt{3}$ )R30°-Sb surface [manuscript accepted in J. Phys. Chem. C 19/11/2014].

To better understand the role of the surface passivation in the epitaxy of GeTe, growth on the hydrogen passivated Si(111)-(1x1)-H surface was investigated as well. In this presentation, the growth of GeTe on these different silicon surfaces is reported and compared between each other.

[1] A. Giussani et al., Phys. Status Solidi B, vol. 249, no. 10, pp. 1939-1944, Oct. 2012.

DS 38.3 Thu 15:30 H 0111

**Epitaxial and textured Ge-Sb-Te phase-change thin films investigated by Cs-corrected STEM** — ●ULRICH ROSS, ANDRIY LOTNYK, ERIK THELANDER, and BERND RAUSCHENBACH — Leibniz-Institut für Oberflächenmodifizierung e.V. Permoserstr. 15 D-04318 Leipzig

Chalcogenide phase change compounds are under intense scrutiny for emerging data storage and fast switching electronic memory applications. The unique properties of this class of materials are based on the distinct change in electrical conduction and optical reflectivity upon transition between crystalline and amorphous states. Much interest has been focused on compounds from the stoichiometric tie-line (GeTe)<sub>x</sub>-(Sb<sub>2</sub>Te<sub>3</sub>)<sub>1-x</sub> in the Ge-Sb-Te intermetallic system. For the development of phase change memory in particular, oriented, epitaxial and layered thin films have been reported to display significantly enhanced switching properties.

We have performed a detailed high-resolution scanning transmission electron microscopy (STEM) investigation of fast grown Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub> thin films on native amorphous silicon oxide as well as oriented

BaF<sub>2</sub>(111) and Si(111) substrates, produced by pulsed laser deposition. Formation of the crystalline phases was induced by deposition at elevated temperatures as well as post-deposition heat treatment. An analytical probe aberration-corrected FEI Titan<sup>3</sup> G2 60-300 S/TEM was used in order to correlate treatment conditions and local structure at the atomic scale. The interplay between grain texture, lattice disorder and local composition variations will be discussed.

DS 38.4 Thu 15:45 H 0111

**Optical and structural dynamics of the photoinduced phase transition of GST** — ●LUTZ WALDECKER<sup>1</sup>, TIMOTHY MILLER<sup>2</sup>, ROMAN BERTONI<sup>1</sup>, SIMON WALL<sup>2</sup>, and RALPH ERNSTORFER<sup>1</sup> — <sup>1</sup>Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — <sup>2</sup>ICFO - Institut de Ciències Fotòniques, Castelldefels (Barcelona), Spain

The phase change material Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub> (GST) exhibits large changes in its optical and electronic properties across the structural phase transition between its amorphous and crystalline states. We use single-shot optical and diffraction measurements to follow the system's dynamics after initiating the phase transition with a femtosecond laser pulse. We observe large changes in the dielectric function instantaneously after photoexcitation, when the lattice still shows long-range order. Energy transfer from electrons to the lattice heats leads to melting on a few picosecond timescale and the amorphization is achieved by thermal processes on longer timescales.

DS 38.5 Thu 16:00 H 0111

**Static and dynamic THz spectroscopy of epitaxially grown GeTe-Sb<sub>2</sub>Te<sub>3</sub> alloys** — ●VALERIA BRAGAGLIA<sup>1</sup>, KARSTEN HOLLDACK<sup>2</sup>, and RAFFAELLA CALARCO<sup>1</sup> — <sup>1</sup>Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — <sup>2</sup>Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany

In the last few years, the number of investigations on the dynamics of photo induced effects in GeTe-Sb<sub>2</sub>Te<sub>3</sub> alloys increased. Full optical measurements were mostly employed in order to get information on both, the electronic and structural response upon excitation. The films investigated are typically grown by sputtering and result in a polycrystalline structure [1].

In our study we focus on epitaxially grown GST which presents a high degree of structural quality. Static measurements were performed in transmittance and reflectance configuration on crystalline and amorphous GST employing Fourier transform Infrared spectroscopy (THz) which allows to access the spectral range of 20-700 cm<sup>-1</sup>. Epitaxial crystalline GST shows both free carrier and phonon absorption contributions. In particular, employing a multilayer structure model, we conclude that a Drude model convolved with several Lorentzian contributions arising from soft phonon modes simulate well the experimental data. Ultrafast dynamic measurements of amorphous and crystalline GST under laser excitation are ongoing employing 800 nm fs-laser pump and ps-THz probe in the same spectral range in order to investigate time resolved electronic response upon excitation.

[1] M.J. Shu et al., Appl. Phys. Lett. 102, 201903 (2013).

DS 38.6 Thu 16:15 H 0111

**Memristive Hebbian Plasticity: Device requirements for the emulation of Hebbian plasticity based on memristive devices** — ●MARTIN ZIEGLER<sup>1</sup>, MIRKO HANSEN<sup>1</sup>, MARINA IGNATOV<sup>1</sup>, THORSTEN BARTSCH<sup>2</sup>, and HERMANN KOHLSTEDT<sup>1</sup> — <sup>1</sup>Nanoelektronik, Technische Fakultät, Christian-Albrechts-Universität zu Kiel — <sup>2</sup>Klinik für Neurologie, Universitätsklinikum Schleswig-Holstein, Christian-Albrechts-Universität zu Kiel

Essential requirements of individual memristive devices for the emulation of Hebbian plasticity in neuromorphic circuits are defined and discussed. Memristive devices based on ionic and exclusively electronic mechanisms are explored. The ionic devices consist of the layer sequence metal/isolator/metal and represent today's most popular devices. The electronic device is a MemFlash-cell. The MemFlash-cell is based on a conventional floating gate transistor with a diode configuration wiring scheme exhibiting a memristive (pinched) I-V characteristic. The electric characteristics of both types of devices are experimentally and theoretically explored with a focus on artificial synaptic plasticity mechanisms. A phenomenological plasticity model

suitable for memristive devices is presented, based on advanced novel learning rules, which provide Hebbian plasticity in accordance to the Bienenstock-Cooper-Munro (BCM) rule.

DS 38.7 Thu 16:30 H 0111

**Memristive Tunnel Junctions** — ●MIRKO HANSEN<sup>1</sup>, MARTIN ZIEGLER<sup>1</sup>, THOMAS MUSSENBRÖCK<sup>2</sup>, SVEN DIRKMANN<sup>2</sup>, and HERMANN KOHLSTEDT<sup>1</sup> — <sup>1</sup>AG Nanoelektronik, Technische Fakultät, Christian-Albrechts-Universität zu Kiel, Germany — <sup>2</sup>Lehrstuhl für Theoretische Elektrotechnik, Fakultät für Elektrotechnik und Informationstechnik, Ruhr-Universität Bochum, Germany

We present results on a device which consists of a tunnel barrier and a thin niobium oxide layer in between two metal electrodes.

By using the well established niobium/aluminium technology to fabricate aluminium oxide tunnel junctions with a smooth interface, we are able to fabricate very thin (<3 nm) and highly resistive niobium oxides layers. The homogeneous change in resistance ( $R_{off}/R_{on} > 100$ ) and  $R_{xA}$  vs.  $A$  plots suggest an area-dependent and non-filamentary switching mechanism, which is explained by taking the interface effects at the tunnel barrier and the top electrode into account.

The memristive tunnel junctions were optimized for the use in neuromorphic circuits and were fabricated on 4" wafers using standard optical lithography, (reactive) DC sputtering and wet etching.

DS 38.8 Thu 16:45 H 0111

**Emulation of neuronal functionality by using a VO<sub>2</sub>-based oscillator circuit** — ●MARINA IGNATOV, MARTIN ZIEGLER, MIRKO HANSEN, ADRIAN PETRARU, and HERMANN KOHLSTEDT — Nanoelektronik, Technische Fakultät, Christian-Albrechts-Universität zu Kiel, Germany

A negative-differential oscillator circuit based on a vanadium dioxide (VO<sub>2</sub>) device is presented. The oscillator circuit allows to emulate basic neuronal functionalities, including spike coding. The obtained results are compared to common spiking neuron models. Additionally, a theoretical analysis of the oscillator circuit is used to gain insight into the functionality of the circuit and to give advice for the device development and the implementation of the circuit. In this respect, important requirements for the strongly correlated electron material VO<sub>2</sub> are presented and discussed in detail. Further, possible modifications of the oscillator circuit model for a better agreement with neuronal spikes are presented.

15 min. break.

DS 38.9 Thu 17:15 H 0111

**Effect of oxygen engineering and doping on resistive switching in HfO<sub>2</sub> based RRAM devices grown by MBE** — ●S.U. SHARATH<sup>1</sup>, JOSE KURIAN<sup>1</sup>, ERWIN HILDEBRANDT<sup>1</sup>, PHILIPP KOMISSINSKIY<sup>1</sup>, THOMAS BERTAUD<sup>2</sup>, CHRISTIAN WALCZYK<sup>2</sup>, PAULINE CALKA<sup>2</sup>, THOMAS SCHROEDER<sup>2</sup>, and LAMBERT ALFF<sup>1</sup> — <sup>1</sup>Materialwissenschaft, Technische Universität Darmstadt, Germany — <sup>2</sup>IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany

Thin films of titanium nitride (TiN, electrode) and hafnium oxide (HfO<sub>2</sub>) were grown using molecular beam epitaxy (MBE). Oxygen engineering using strongly oxygen deficient growth parameters and trivalent doping of HfO<sub>2</sub> thin films has been utilized to stabilize oxygen vacancy concentrations far beyond the thermodynamical equilibrium. Thin films of hafnium oxide grown at 320 °C on TiN crystallize in a monoclinic symmetry (*m*-HfO<sub>2</sub>) at higher oxidation conditions, whereas the oxygen deficient hafnium oxide films showed oxygen vacancy stabilized tetragonal like phase of hafnium oxide (*t*-HfO<sub>2-x</sub>) which was verified by X-ray diffraction [1]. A large concentration of oxygen vacancies lead to a defect band at the Fermi-level as observed by X-ray photoelectron spectroscopy (XPS). The electrical switching measurements show that the forming voltage is reduced for oxygen deficient films paving the way for low power devices in future. In oxygen deficient HfO<sub>2-x</sub> thin films grown on TiN/Si(001), the thickness dependence of the forming voltage is strongly suppressed [2].

[1] S. U. Sharath et al., Appl. Phys. Lett., 104, 063502 (2014).

[2] S. U. Sharath et al., Appl. Phys. Lett., 105, 073505 (2014).

DS 38.10 Thu 17:30 H 0111

**BiFeO<sub>3</sub>-based resistive switching cells with flexible rectifying contact** — ●TIANGUI YOU<sup>1</sup>, NAN DU<sup>1</sup>, STEFAN SLESAZECK<sup>2</sup>, THOMAS MIKOLAJICK<sup>2,3</sup>, GUODONG LI<sup>4</sup>, DANILO BÜRGER<sup>1</sup>, ILONA SKORUPA<sup>1</sup>, HARTMUT STÖCKER<sup>5</sup>, BARBARA ABENDROTH<sup>5</sup>, ANDREAS

BEYER<sup>6</sup>, KERSTIN VOLZ<sup>6</sup>, OLIVER G. SCHMIDT<sup>1,4</sup>, and HEIDEMARIE SCHMIDT<sup>1</sup> — <sup>1</sup>TU Chemnitz — <sup>2</sup>NaMLab gGmbH Dresden — <sup>3</sup>TU Dresden — <sup>4</sup>IFW Dresden — <sup>5</sup>TU Bergakademie Freiberg — <sup>6</sup>Philipps-Universität Marburg

Nonvolatile resistive switching in BiFeO<sub>3</sub> (BFO) has attracted increasing attention. However, the underlying resistive switching mechanism is still controversial which restricts its application in nonvolatile memory[1] and logics[2]. Here we develop a model on modifiable Schottky barrier height and elucidate the physical origin underlying resistive switching in Au-BFO-Pt/Ti resistive switching cells containing mobile oxygen vacancies.[3] Increased switching speed is possible by applying a large amplitude writing pulse as the migration of mobile oxygen vacancies is tunable by both the amplitude and length of the writing pulse. The local resistive switching has been investigated by conductive atomic force microscopy and exhibits the capability of down-scaling the resistive switching cell to the grain size.

[1] Y. Shuai, et al., J. Appl. Phys. 2011, 109, 124117

[2] T. You, et al., Adv. Funct. Mater. 2014, 24, 3357

[3] T. You, et al., ACS Appl. Mater. Interfaces 2014, 6, 19758

DS 38.11 Thu 17:45 H 0111

**Reversible Changes Induced by Liquid Electrolyte Gating in the WO<sub>3</sub> Electronic Structure** — ●CARLOS E. VIOLBARBOSA<sup>1</sup>, JULIE KAREL<sup>1</sup>, SIMONE G. ALTENDORF<sup>2</sup>, JANOS KISS<sup>1</sup>, YUKI UTSUMI<sup>1</sup>, MAHESH G. SAMANT<sup>2</sup>, LIU HAO TJENG<sup>1</sup>, CLAUDIA FELSER<sup>1</sup>, and STUART S. P. PARKIN<sup>2</sup> — <sup>1</sup>Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany 01187 — <sup>2</sup>IBM Almaden Research Center, San Jose, California, USA 95120

Tungsten trioxide (WO<sub>3</sub>) is a d0 transition metal oxide that has attracted broad interest due its optical and electrical properties. WO<sub>3-x</sub> has a rich phase diagram. Many of the studies in this material make use of modifications in the carrier concentration by chemical doping or creation of oxygen deficiencies. In this work, we utilize ionic liquid electrolyte gating in a electric-double-layer transistor device to induce a metallic state in WO<sub>3</sub> films, a process we will show is reversible.

The modifications in the electronic structure (core levels and valance band) resulting from the gating are probed by hard X-ray photoelectron spectroscopy. Electrolyte gating leads to a significant population of W 5d states in the conduction band and an enormous change in the W 4f core levels. Ab initio density functional theory are used to help describe the origin of these modifications in the electronic structure.

DS 38.12 Thu 18:00 H 0111

**Resistive switching of polycrystalline, multiferroic YMnO<sub>3</sub> thin films** — ●AGNIESZKA BOGUSZ<sup>1,2</sup>, SŁAWOMIR PRUCNAL<sup>1</sup>, DANIEL BLASCHKE<sup>1</sup>, ILONA SKORUPA<sup>1</sup>, DANILO BÜRGER<sup>2</sup>, OLIVER G. SCHMIDT<sup>2,3</sup>, and HEIDEMARIE SCHMIDT<sup>2</sup> — <sup>1</sup>Institute Of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf — <sup>2</sup>Department of Materials for Nanoelectronics, Chemnitz University of Technology — <sup>3</sup>Institute for Integrative Nanosciences, IFW-Dresden

Resistive switching (RS) phenomena have been widely investigated in the field of materials science, physics, and electrical engineering in the past decade. Recently, multiferroics have been considered as promising candidates for memristive switches. Specific properties of multiferroics might bring additional and/or new functionalities into the memristive switches. This work investigates the RS properties of multiferroic YMnO<sub>3</sub> thin films reported as a unipolar resistive switch [1]. YMnO<sub>3</sub> was grown at 400°C on Pt/Ti/SiO<sub>2</sub>/Si substrates by pulsed laser deposition (PLD) and crystallized by flash lamp annealing (FLA). Film thickness and the concentration of point defects were controlled during the PLD process. Transport and RS properties of Au/YMnO<sub>3</sub>/Pt/Ti/SiO<sub>2</sub> structures were determined by two-point probe measurements in a top-bottom configuration. Results imply that the filamentary, unipolar RS in YMnO<sub>3</sub> originates from the electro-redox reactions induced by the Joule heating. [1] A. Bogusz et al., AIP Advances 4, 107135 (2014)

DS 38.13 Thu 18:15 H 0111

**Kinetic Monte-Carlo simulations of resistive switching in silver doped titanium dioxide thin films** — SVEN DIRKMANN<sup>1</sup>, JAN TRIESCHMANN<sup>1</sup>, MIRKO HANSEN<sup>2</sup>, MARTIN ZIEGLER<sup>2</sup>, HERMANN KOHLSTEDT<sup>2</sup>, and ●THOMAS MUSSENBRÖCK<sup>2</sup> — <sup>1</sup>Ruhr-Universität Bochum, Lehrstuhl für Theoretische Elektrotechnik, 44780 Bochum — <sup>2</sup>Christian-Albrechts Universität zu Kiel, AG Nanoelektronik, 24143 Kiel

Low power consumption, low fabrication costs, fast write and read cycles, and scalability into the nanometer range make resistive switching devices attractive for future non-volatile memory applications and neuromorphic circuits. The majority of devices rely on nano-ionic mechanisms – one of which is electrochemical metallization, where the change in resistance is due to the formation and re-formation of conducting filaments. This contribution is devoted to demonstrate and discuss the formation and re-formation of Ag filaments in an Ag/TiO<sub>2</sub>/Pt sandwich-like thin film system at experimental time-scales by means of kinetic Monte-Carlo simulations. It is shown that filamentary electrochemical metalization devices provide distinct and reliable “on” and “off” states, but their dynamic range is limited.

DS 38.14 Thu 18:30 H 0111

**Tailoring the electrical properties of a TiO<sub>2</sub> layer by ion-beam irradiation for memristive applications** — ●DANIEL BLASCHKE<sup>1</sup>, AGNIESZKA BOGUSZ<sup>1</sup>, RENÉ HÜBNER<sup>1</sup>, FRANZISKA NIEROBISCH<sup>1</sup>, VIKAS RANA<sup>3</sup>, ANDREA SCHOLZ<sup>1</sup>, SIBYLLE GEMMING<sup>1,2</sup>, and PETER ZAHN<sup>1</sup> — <sup>1</sup>Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf — <sup>2</sup>Chair of Scale-bridging

Materials Modeling, Physics Department, TU Chemnitz — <sup>3</sup>Peter Grünberg Institut, Forschungszentrum Jülich

Reactively sputtered TiO<sub>2</sub> thin films on Pt/Ti/SiO<sub>2</sub>/Si substrates were irradiated with low energy Ar<sup>+</sup> ions of different energies to create surface or bulk modifications in the material. Furthermore, the fluence was varied to optimize the level of the modifications, which are e.g. amorphization, surface smoothing, and preferential sputtering of oxygen. These effects were detected by TEM, AFM and supported by TRIDYN simulations, respectively. The impact of these changes on the electrical properties of the TiO<sub>2</sub> layers was monitored by I-V and C-V measurements in top-bottom geometry with Pt, as well as Ti/Pt top contacts. The results indicate a transition from a Schottky-like behavior of the Pt/TiO<sub>2</sub> interface to an ohmic one with increasing fluence, which is very similar to the behavior of a Ti/TiO<sub>2</sub> interface. Furthermore, the capacity of the complete MIM stack increases with fluence, which points to a reduced effective thickness of the dielectric TiO<sub>2</sub> layer after irradiation.

The project is funded by the Initiative and Networking Fund of the Helmholtz Association (Virtual Institute Memriox, VH-VI-422).

## DS 39: Poster Session II

Time: Thursday 16:00–18:30

Location: Poster F

DS 39.1 Thu 16:00 Poster F

**Charge transfer effects in binary mixtures of organic semiconductors: DIP:F6-TCNNQ as a case study** — ●GIULIANO DUVA<sup>1</sup>, VALENTINA BELOVA<sup>1</sup>, ALEXANDER HINDERHOFER<sup>1</sup>, ALEXANDER GERLACH<sup>1</sup>, ANDREAS OPITZ<sup>2</sup>, PAUL BEYER<sup>2</sup>, and FRANK SCHREIBER<sup>1</sup> — <sup>1</sup>Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen (Germany) — <sup>2</sup>Humboldt-Universität zu Berlin, Department of Physics, Brook-Taylor-Str. 6, 12489 Berlin (Germany)

Binary mixtures of organic semiconductors have been studied in planar and bulk heterojunction architectures [1], and a correlation between the structural and optical properties has been found [2]. The orientation of the molecular components of donor-acceptor type binary mixtures has been recently shown to have a dramatic impact on charge-transfer efficiency [3]. However, charge transfer effects in donor-acceptor organic systems have not been fully understood yet. We use several experimental techniques to characterize the structure and molecular orientation and identify charge-transfer effects within systems of DIP as the donor and F6-TCNNQ as the acceptor, namely in bulk heterojunction architecture. Remarkably, charge transfer effects studied by means of IR spectroscopy, UV-vis and spectroscopic ellipsometry, and PL are related to structural properties of the films obtained by means of XRR and GIXD together with morphological characterization by means of AFM. [1]A. Hinderhofer and F. Schreiber, Chem. Phys. Chem. 13 (2012); [2]K. Broch et al., J. Chem. Phys. 139 (2013); [3]G. Aghamohammadi et al., J. Phys. Chem. C 118 (2014).

DS 39.2 Thu 16:00 Poster F

**Orientation controlled growth of metal phthalocyanines and their optical characterization** — JAN KUHNERT, ●MICHAEL KOTHE, WOLFRAM HEIMBRODT, and GREGOR WITTE — Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany

Phthalocyanines in combination with metal oxides are promising materials for future electronic devices such as organic solar cells (OPV). Despite their technological importance a microscopic understanding of optoelectronic excitations in such hybrid systems has yet not been achieved. To gain deeper insight ordered model systems with well-defined interfaces are mandatory. In this contribution we have studied the interrelation of structural and optical properties of Phthalocyanine thin films that were grown onto various substrates. Their structure were studied by means of XRD, AFM while the optical properties were analyzed by continuous wave and time-resolved photoluminescence spectroscopy and absorption measurements.

DS 39.3 Thu 16:00 Poster F

**Preparation and Characterisation of Crystalline C<sub>60</sub> and Pentacene Interfaces** — ●ANDREA KARTHÄUSER, TOBIAS BREUER, and GREGOR WITTE — Molekulare Festkörperphysik, Philipps-Universität Marburg, Renthof 7, D-35032 Marburg, Germany

Their tunable electronic properties as well as their high photon cross-sections have resulted in increased research efforts in organic semiconductors. However, the complex nature of their interface characteristics concerning the correlation between structural and electronic properties, has not yet been entirely elucidated, mostly due to the lack of appropriate model systems. Here we report on the preparation of such a model system of the donor-acceptor pair Pentacene (PEN, C<sub>22</sub>H<sub>14</sub>) and Buckminster-Fullerene (C<sub>60</sub>). Two strikingly different interfaces can be realised between these two compounds, due to their different molecular geometry, which have been theoretically predicted to strongly influence the stability of the interface formation [1] and the electronic properties [2]. Depositing C<sub>60</sub> on upright oriented PEN grown on SiO<sub>2</sub>, causes pronounced step decoration and yields non-crystalline C<sub>60</sub> adlayers [3]. Here we reserved the system and deposited PEN onto single crystalline C<sub>60</sub> films that were grown on NaCl(100). The resulting morphology and molecular orientation have been analysed by AFM, XRD and - after successfully transferring the films to conducting substrates - also by NEXAFS spectroscopy.

[1] Fu, Y. T. et al. Adv. Mater. (2013), 25, 878. [2] Yi, Y. P. et al. J. Am. Chem. Soc. (2009), 131, 15777. [3] Breuer, T. et al. ACS Appl. Mater. Interfaces (2013), 5, 9740.

DS 39.4 Thu 16:00 Poster F

**Reactive Metal/Organic Interfaces Studied with HAXPES and Nanojoule Calorimetry** — ●HAN ZHOU<sup>1</sup>, HANS-JÖRG DRESCHER<sup>1</sup>, MIN CHEN<sup>1</sup>, BENEDIKT KLEIN<sup>1</sup>, CLAUDIO KRUG<sup>1</sup>, MALTE ZUGERMEIER<sup>1</sup>, MALTE SACHS<sup>1</sup>, STEFAN KACHEL<sup>1</sup>, MIHAELA GORGOI<sup>2</sup>, and J. MICHAEL GOTTFRIED<sup>1</sup> — <sup>1</sup>Fachbereich Chemie, Philipps Universität Marburg, Hans-Meerwein-Straße 4, 35032 Marburg, Germany — <sup>2</sup>Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Metal/organic interfaces are of the critical importance to the performance of modern organic semiconductor devices. Besides the idealized model systems with an atomically abrupt and chemically inert interface, more realistic systems with the formation of extended diffusion and reaction zones between metal and organic phase must be considered. These extended interfaces required bulk sensitive methods such as Hard X-ray Photoelectron Spectroscopy (HAXPES) and Nanojoule Calorimetry for investigation. Here, we report on the interfaces between (a) Ca and sexithiophene (6T) and (b) Co and tetraphenylporphyrin (2HTPP), two model systems in which interface reactions were observed. Ca in contact to 6T forms CaS, resulting in massive structural changes of the organic semiconductor. In contrast, the reaction of Co with 2HTPP is much more specific and leads to the formation of the complex CoTPP as a well-define product. Depth profiling with HAXPES and complementary studies provide a comprehensive picture of the chemical and electronic structure of the interfaces.

DS 39.5 Thu 16:00 Poster F

**Investigation of organic thin films of DIP and C<sub>60</sub> mixtures**

using *in situ* X-ray diffraction techniques — ●HEIKO FRANK, CHRISTOPHER LORCH, RUPAK BANERJEE, ALEXANDER HINDERHOFER, ALEXANDER GERLACH, and FRANK SCHREIBER — Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen

Mixtures of organic semiconductors offer a variety of applications, including devices such as photovoltaic cells [1]. The optical and electrical properties of such devices depend *inter alia* on the structure of these mixtures and therefore on the preparation conditions [2,3]. Thus, understanding the structure of organic thin films is a key point for the optimization of such systems.

In this work, we investigate organic thin films consisting of mixtures of DIP and C<sub>60</sub> with a molecular ratio of 1:1 on SiO<sub>x</sub> substrates. The films are prepared using organic molecular beam deposition (OMBD) and characterized *in situ* and in real-time [4] using X-ray reflectivity (XRR) and grazing incidence X-ray diffraction (GIXD). Our results indicate that the structural ordering of the mixed films has a strong dependence on the kinetics of the growth, which can be influenced by parameters like the temperature of the substrate, the total deposition rate and the growth type (continuous vs. interrupted growth).

[1] J. Wagner *et al.*, Adv. Funct. Mater. **20**, 4295 (2010) [2] A. Hinderhofer and F. Schreiber, ChemPhysChem **13**, 628 (2012) [3] R. Banerjee *et al.*, Phys. Rev. Lett. **110**, 185506 (2013) [4] S. Kowarik *et al.*, Europ. Phys. J. - Special Topics **167**, 11 (2009)

DS 39.6 Thu 16:00 Poster F

**Electron-impact induced HF elimination in fluorinated PAHs: Molecular building blocks for new carbon nanostructures** — ●JÜRGEN WEIPPERT<sup>1</sup>, SEYITHAN ULAS<sup>1</sup>, PATRICK WEIS<sup>1</sup>, JEAN-FRANCOIS GREISCH<sup>2</sup>, KONSTANTIN Y. AMSHAROV<sup>3</sup>, ARTUR BÖTTCHER<sup>1</sup>, and MANFRED M. KAPPES<sup>1,2</sup> — <sup>1</sup>Institute of Physical Chemistry, Karlsruhe Institute of Technology (KIT), Fritz-Haber-Weg 2, 76131 Karlsruhe, Germany — <sup>2</sup>Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — <sup>3</sup>University Erlangen-Nürnberg, Institut für Organische Chemie, Henkestr. 42, 91054, Germany

Electron-impact induced HF-elimination (EIIHF) from fluorinated PAHs (F-PAHs) has been used to create curved molecular carbon structures which cannot be accessed synthetically. We have studied this process using three F-PAHs: C<sub>26</sub>H<sub>14</sub>F<sub>2</sub>, C<sub>36</sub>H<sub>15</sub>F<sub>3</sub> and C<sub>60</sub>H<sub>21</sub>F<sub>9</sub>. The products of the sequential EIIHF (C<sub>26</sub>H<sub>12</sub><sup>+</sup>, C<sub>36</sub>H<sub>12</sub><sup>+</sup> and C<sub>60</sub>H<sub>12</sub><sup>+</sup>) have been deposited mass-selectively onto HOPG substrate and their electronic, thermodynamic and vibrational properties analysed by means of UPS, XPS, AFM, TDS and Raman spectroscopy. For all studied molecules HF-elimination is the major fragmentation channel. In contrast to large planar C<sub>60</sub>H<sub>21</sub>F<sub>9</sub> molecules, the smaller precursors were found to be entirely dehydrofluorinated upon 70 eV e<sup>-</sup> impact. The hydrodefluorination of C<sub>60</sub>H<sub>21</sub>F<sub>9</sub> molecules stops after the sixth EIIHF-step and the resulting products exhibit molecular structures (caps) of relevance for further (n,m)-selective growth of SWCNT.

DS 39.7 Thu 16:00 Poster F

**CHARGE TRANSFER IN ORGANIC MIXED FILMS OF DIINDENOPERYLENE AND PDIR-CN2** — ●VALENTINA BELOVA<sup>1</sup>, GIULIANO DUVA<sup>1</sup>, PAUL BEYER<sup>2</sup>, ALEXANDER HINDERHOFER<sup>1</sup>, ALEXANDER GERLACH<sup>1</sup>, FRANK SCHREIBER<sup>1</sup>, and ANDREAS OPITZ<sup>2</sup> — <sup>1</sup>Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany — <sup>2</sup>Department of Physics, Humboldt-Universität zu Berlin, Brook-Taylor-Straße 6, 12489 Berlin, Germany

Interface doping by molecular charge transfer is a promising approach to tune the electronic properties of organic semiconductors without changing their molecular arrangement [1]. DIP (diindenoperylene) was chosen as a prototypical donor with good charge transport properties and optical contrast [2]. Since DIP (C<sub>32</sub>H<sub>14</sub>) possesses relatively high ionization energy (5.35 eV) it requires strong acceptor like PDIR-CN2 (C<sub>x</sub>H<sub>y</sub>O<sub>4</sub>N<sub>4</sub>) with electron affinity 4.3 eV. We studied thin blended (co-evaporated) films by structural and optical methods in order to investigate charge transfer effect between the HOMO of DIP and the LUMO of PDIR-CN2. Optical studies involved FTIR spectroscopy, spectroscopic ellipsometry, UV-VIS absorption, as well as photoluminescence (temperature dependent) and Raman spectroscopy. Structural and morphological characterisation of the mixed films was carried out by X-ray diffraction and atomic force microscopy. Signatures of

intermolecular interaction in DIP:PDIR-CN2 mixtures are discussed.

[1] A. Hinderhofer/F. Schreiber, ChemPhysChem, **13**, 628 (2012) [2] J. Wagner *et al.*, Adv. Funct. Mater. **20**, 4295 (2010)

DS 39.8 Thu 16:00 Poster F

**Epitaxial TTF-TCNQ Thin Films on KCl(100): New Preparation Methods and Observation of Interface-Mediated Thin Film Polymorph** — ●ALEXANDER MÄNZ, TOBIAS BREUER, and GREGOR WITTE — Molekulare Festkörperphysik, Fachbereich Physik, Philipps-Universität Marburg, Renthof 7, 35032 Marburg

Though the bulk properties of the prototypical organic charge-transfer complex Tetrathiafulvalene-Tetracyanoquinodimethane (TTF-TCNQ) have been studied in detail, the influence of defects and crystallite size on resulting electronic properties as well as an integration of these materials in organic thin film devices is barely explored. One important requirement for such a comprehension is the precise control over crystallite size and quality. In this study, we report on different strategies to prepare crystalline TTF-TCNQ thin films and compare their structural quality. While conventional organic molecular beam deposition of TTF-TCNQ onto KCl(100) substrates enables the growth of epitaxial thin films with grain dimensions of up to 2 μm, further enhancement of the crystallite dimensions by raising the growth temperature is thermally limited by vanishing sticking and onset of vaporization. Using more sophisticated methods like hot wall evaporation, however, allows to overcome these limitations and yields crystalline islands with extensions enhanced by two orders of magnitude. Furthermore, we identify and provide a full structure solution of a yet unknown interface-mediated thin film polymorph of TTF-TCNQ, which is adopted in films of thicknesses below 1 μm.

DS 39.9 Thu 16:00 Poster F

**Influence of graphene interlayer on CoPc/Pt(111) interface** — ●MALGORZATA POLEK<sup>1</sup>, HILMAR ADLER<sup>1</sup>, ALEXANDER GENERALOV<sup>2</sup>, MATHIAS GLASER<sup>1</sup>, MILUTIN IVANOVIC<sup>1</sup>, ALEXEI PREOBRAJENSKI<sup>2</sup>, JOHANNES UHLEIN<sup>1</sup>, HEIKO PEISERT<sup>1</sup>, and THOMAS CHASSÉ<sup>1</sup> — <sup>1</sup>University of Tübingen, Institute of Physical and Theoretical Chemistry, Auf der Morgenstelle 18, 72076 Tübingen, Germany — <sup>2</sup>MAX IV Laboratory, Ole Römers väg 1, 22363 Lund, Sweden

In optoelectronic devices based on organic semiconductors such as transition metal phthalocyanines (TMPcs), interactions at interfaces between organic molecules and metal substrates can significantly affect the device performance. The introduction of graphene as an additional buffer layer can help to tune these interactions and thus the electron transport across the interface as recently shown for TMPcs on graphene/Ni(111) [1]. Due to the interfacial doping effect, graphene on Ni(111) is however a rather specific system. We compare therefore CoPc on graphene/Ni(111) to CoPc on graphene/Pt(111). The system was studied using synchrotron radiation based techniques: Photoemission and X-ray absorption spectroscopies (PES, XAS). Thin films of CoPc on Pt(111) and graphene/Pt(111) are composed of well-ordered, flat lying molecules on the substrate surface. Similar to Ni(111), a charge transfer to the central metal atom of CoPc was observed at the interface between CoPc and Pt(111). In contrast to Ni(111) however, the introduction of graphene as an interlayer prevents the charge transfer completely.

[1] J. Uihlein *et al.*, J. Chem. Phys. **2013**, 138, 081101.

DS 39.10 Thu 16:00 Poster F

**Strong Interaction of MnPc on Ni(111): Influence of Graphene Buffer Layer** — ●JOHANNES UHLEIN<sup>1</sup>, HEIKO PEISERT<sup>1</sup>, HILMAR ADLER<sup>1</sup>, MATHIAS GLASER<sup>1</sup>, MALGORZATA POLEK<sup>1</sup>, RUSLAN OVSYANNIKOV<sup>2</sup>, MAXIMILIAN BAUER<sup>2</sup>, and THOMAS CHASSÉ<sup>1</sup> — <sup>1</sup>Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Tübingen, Germany. — <sup>2</sup>Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany.

The interactions at interfaces of transition metal phthalocyanines (TMPcs) on metal substrates strongly influence the charge transport across these interfaces, which may become important for possible future organic electronic and spintronic devices. Molecule-substrate interactions may influence the local charge and thus the spin state of the central metal atom within the first molecular layer. This will be especially important for metal atoms possessing an open shell structure. For CoPc and FePc it was shown that with insertion of a graphene buffer-layer these interactions can be modified, depending on the central metal atom.[1][2] In contrast to CoPc and FePc, MnPc suffers serious damage to its molecular structure on Ni(111) with impact on the electronic structure. The insertion of graphene prevents the chemical

reaction and an interfacial charge transfer is observed.[3] The studies were carried out using X-ray absorption and photoemission spectroscopies.

- [1] J. Uihlein et al., *J. Chem. Phys.* 2013, 138, 081101.  
 [2] J. Uihlein et al., *J. Phys. Chem. C* 2014, 118, 10106.  
 [3] J. Uihlein et al., *J. Phys. Chem. C* 2014, accepted.

DS 39.11 Thu 16:00 Poster F

**The adsorption and DBD-plasma-polymerization of thiophene on titania** — ●SEBASTIAN DAHLE<sup>1,2</sup>, MARIA SONNENBERG<sup>2</sup>, MARCEL MARSCHEWSKI<sup>2</sup>, EIKE HÜBNER<sup>3</sup>, and WOLFGANG MAUS-FRIEDRICHS<sup>1,2</sup> — <sup>1</sup>Clausthaler Zentrum für Materialtechnik, Technische Universität Clausthal, Agricolastraße 2, D-38678 Clausthal-Zellerfeld, Germany — <sup>2</sup>Institut für Energieforschung und Physikalische Technologien, Technische Universität Clausthal, Leibnizstraße 4, D-38678 Clausthal-Zellerfeld, Germany — <sup>3</sup>Institut für Organische Chemie, Technische Universität Clausthal, Leibnizstraße 6, D-38678 Clausthal-Zellerfeld, Germany

The adsorption of thiophene from the gas phase onto clean and oxidized titanium foils as well as onto perchloric acid or bromine pre-treated titanium foils did not yield any chemical interaction or even stable adsorption. Especially the oxidative polymerization as classical approach for the synthesis and deposition of polythiophene cannot be employed for titania substrates. Using a dielectric barrier discharge plasma during the thiophene gas dosage results in the deposition of plasma-polymerized thiophene films at quite large deposition rates. The deposition mode, however, changes from a Frank-van-der-Merwetype growth within the first seconds towards the deposition of two different classes of particles presumably originating from gas phase agglomeration.

DS 39.12 Thu 16:00 Poster F

**Real-time observation of superlattice formation in co-evaporated binary mixtures of Picene and Perfluoropentacene** — ●JOHANNES DIETERLE<sup>1</sup>, KATHARINA BROCH<sup>2</sup>, ALEXANDER HINDERHOFER<sup>1</sup>, HEIKO FRANK<sup>1</sup>, JIRI NOVAK<sup>3</sup>, RUPAK BANERJEE<sup>1</sup>, ALEXANDER GERLACH<sup>1</sup>, and FRANK SCHREIBER<sup>1</sup> — <sup>1</sup>Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen — <sup>2</sup>Cavendish Laboratory, University of Cambridge, Cambridge, UK — <sup>3</sup>Central European Institute of Technology, Masaryk University, Kamenice 5, CZ-62500 Brno, Czech Republic

Studies of the mixing and ordering behaviour of binary organic semiconductor blends are not only relevant for applications, where blends are often used as the active layer, but also interesting for fundamental research, as new, mixing induced, ordering schemes may evolve [1,2]. For a detailed understanding of the mechanisms of structure formation during growth of binary blends, controlled growth and full structural characterization is crucial. For binary blends of Picene (C<sub>22</sub>H<sub>14</sub>) ('high gap') and Perfluoropentacene (C<sub>22</sub>F<sub>14</sub>) ('low gap') we observe the formation of a superlattice during co-evaporation. To study the dynamics of the superlattice formation and possible transient effects we perform real-time x-ray scattering and optical spectroscopy during growth of the blends.

- [1] A. Hinderhofer and F. Schreiber, *ChemPhysChem* 13, 628 (2012)  
 [2] A. Auferderheide et al., *Phys. Rev. Lett.* 109, 156102 (2012)

DS 39.13 Thu 16:00 Poster F

**Indium-Tin-Oxide (ITO) Surface Functionalization with Organic Self-Assembled-Monolayers** — ●JULIA RITTICH, SEBASTIAN MÄDER, BEATE SCHULZ, and MATTHIAS WUTTIG — I. Institute of Physics (IA), RWTH Aachen University, Germany

In recent years optoelectronic devices based on organic thin-films have gained considerable interest. The performance of devices such as organic light emitting diodes (OLED) or organic solar cells (OSC) depends critically on the interfaces between the different layers, e.g. the organic layer and the transparent conductive oxide (TCO) electrode. The most common material for such a transparent anode is Tin doped Indium-Oxide (ITO). In order to improve the device functionality the electronic alignment at the interface between the anode and the organic layer became the focus of interest. One way to change the electronic properties of the contact is given by the application of self-assembled monolayers (SAM).

In this study, self-assembled monolayers with high nano-dipoles were used to tailor the work function of the ITO anode. The used molecules are based on functional groups of phosphonic and carboxylic acid to anchor to the surface. In order to investigate the change in work function alignment to the organic layer and the coverage and arrangement

of the surface dipoles, ultraviolet and X-ray photoelectron spectroscopy (UPS/XPS) measurements were performed.

DS 39.14 Thu 16:00 Poster F

**Recombination of charge carriers on nano-interfaces** — ●JĘDRZEJ SZMYTKOWSKI — Faculty of Applied Physics and Mathematics, Gdańsk University of Technology, Gdańsk, Poland

It is well known that the recombination of charge carriers plays a key role in the decreasing of efficiency for photovoltaic cells. The interfaces between nanostructures can be considered as the recombination centers. In this work, the role of tail and deep states on the process of interface recombination has been demonstrated. In order to analyze this effect, the disordered materials described by the double-exponential density of states (DOS) have been assumed. The studies of concentration effect on the time of recombination have been performed. Additionally, we report on the influence of temperature on the increasing of recombination order.

DS 39.15 Thu 16:00 Poster F

**Tailoring Surface Properties of Metals and Metal-Oxides Using Self-Assembled-Monolayers** — ●SEBASTIAN MÄDER, JULIA RITTICH, DOMINIK MEYER, and MATTHIAS WUTTIG — I. Physikalisches Institut IA, RWTH Aachen

Due to the high demand of power and of efficient lightning, the field of optoelectronic devices based on organic thin-films has gained considerable interest. Organic films offer a way of producing lightweight, flexible, inexpensive and eco-friendly light emitting diodes (OLED) and solar cells (OSC). Since the device functionality depends critically on the interface between the active organic layer and the cathode or the anode, an alignment of the electronic charge transport levels is a crucial step towards efficient charge transfer at this interface. One way to achieve this aim is given by the application of self-assembled monolayers (SAM).

In this work, we present a method to achieve a universal work function for noble metals using self-assembled monolayers with high interface-dipoles. Furthermore, we transferred the concepts and methods learned from the metal surfaces in order to achieve a tailored work function of transparent conductive oxides (TCOs) suited as an anode to contact organic active layers. The alignment of the work function as well as the surface coverage was examined using ultraviolet and X-ray photoelectron spectroscopy (UPS/XPS).

DS 39.16 Thu 16:00 Poster F

**Investigation of the metallization of P(VDF-TrFE) with gold by RF-sputter deposition** — ●ALEXANDER HINZ<sup>1</sup>, OLEKSANDR POLONSKYI<sup>1</sup>, MATTHIAS SCHWARTZKOPF<sup>2</sup>, GONZALO SANTORO<sup>2</sup>, EZZELDIN METWALLI<sup>3</sup>, YUAN YAO<sup>3</sup>, THOMAS STRUNSKUS<sup>1</sup>, FRANZ FAUPEL<sup>1</sup>, STEPHAN V. ROTH<sup>2</sup>, and PETER MÜLLER-BUSCHBAUM<sup>3</sup> — <sup>1</sup>CAU zu Kiel, Kaiserstr. 2, 24143 Kiel — <sup>2</sup>DESY, Notkestr. 85, 22607 Hamburg — <sup>3</sup>TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching

Although it is well established in industry and important for many applications the sputter deposition of metals onto organic surfaces is yet to be completely understood. Due to the inherent complexity (e.g. bombardment of the organic surfaces by energetic ions) of the sputtering process the basic mechanisms determining the final microstructure are still to be identified. The complexity of sputter deposition and the post-deposition changes which are to be expected necessitate the use of in-situ methods. In-situ grazing incidence small angle scattering (GISAXS) has been used to extract structural information with high spatial and temporal resolution from a growing Au-film deposited via RF-sputter deposition onto a P(VDF-TrFE)-film. The Au-P(VDF-TrFE) system has been chosen as a model system of a relatively inert metal-polymer pair. Analysis of the GISAXS data yields information about the morphology of the growing Au-film. Comparing these results to simulated scattering data provides further information about the basic growth mechanisms acting at different stages of the growth of the metal film.

DS 39.17 Thu 16:00 Poster F

**Copper Phthalocyanine as Contact Primer for Organic Semiconductor Films on Metal Substrates** — ●ALEXANDER MÄNZ and GREGOR WITTE — Molekulare Festkörperphysik, Fachbereich Physik, Philipps-Universität Marburg, Renthof 7, 35032 Marburg

Organic self assembled monolayers can be utilized as contact primer for the growth of organic semiconductors on metal surfaces. In order to

avoid involved charge transport limitations of SAMs, flat lying PAHs such as Phthalocyanines can be used alternatively. In our study we exemplarily used Copper Phthalocyanine (CuPc) as contact primer for the growth of the organic semiconductor Pentacene (PEN) on coinage metals. The initial stage of growth was investigated by means of AFM and NEXAFS, which give insight into the morphology and the molecular orientation of submonolayer coverages. Additionally, films with thicknesses up to 30 nm were analyzed by means of XRD. In all cases we observed PEN to grow in upright orientation, adopting the thin film polymorph as known for PEN on inert substrates. This observation is in contrast to the thin film growth of other planar PAHs like PTCDAs on CuPc monolayers.

DS 39.18 Thu 16:00 Poster F

**Temperature Induced Phase Transition in Pentacene Thin Films** — ●LEONARD VON HELDEN, TOBIAS BREUER, and GREGOR WITTE — Molekulare Festkörperphysik, Philipps Universität Marburg, Renthof 7, D-35032 Marburg, Germany

Pentacene ( $C_{22}H_{14}$ ) is a widely investigated organic semiconductor and serves as model system for organic thin film growth. It is known to form crystalline thin films in two slightly different, consecutively growing polymorphs on  $SiO_2$ : the "thin film phase" (TFP) and the "Campbell phase" (CP), i.e. bulk phase.<sup>1</sup> Here we report a study on high temperature dynamics, which was realized by mounting a metal cap on top of the sample under vacuum conditions, providing an unmodified surface of the organic thin film. XRD and AFM measurements prove a phase transition of the TFP into the energetically favored CP, when heated about 40 K beyond its usual desorption point. Moreover we found, that sample contact to ambient air has a tremendous influence on the desorption and transition process.

[1] C. Ambrosch-Draxl et al., New Journal of Physics, 11, 125010, (2009)

DS 39.19 Thu 16:00 Poster F

**Spectroscopic and transport properties of a novel charge transfer salts** — ●TORSTEN HAHN<sup>1</sup>, FLORIAN RÜCKERL<sup>2</sup>, and SIMON LIEBING<sup>1</sup> — <sup>1</sup>Institut für Theoretische Physik, Leipziger Str. 23, TU Freiberg, D-09599 Freiberg — <sup>2</sup>IFW Dresden, Helmholtzstraße 20, D-01069 Dresden

The recently synthesized Picene/F4TCNQ charge transfer salt [1] shows promising physical properties for the application in molecular electronics. Based on theoretical calculation within the density functional theory framework we predict the material to act as a molecular diode with high rectification ratio [2]. We further conclude that the hybrid states formed by the donor / acceptor system are playing the key role to determine the spectroscopic and quantum transport properties. Additionally we extend our investigation to other novel charge transfer salts like Chrysene/F4TCNQ or Tetracene/F4TCNQ. We will show that the tuning of spectroscopic and transport properties through intramolecular charge transfer is a general concept which opens a new route towards functional materials for molecular electronics.

[1] Mahns, B. et. al., Cryst. Growth and Design 14, 1338-1346 (2014). [2] T. Hahn, S. Liebing, and J. Kortus, Nanoscale 6, 14508 (2014).

DS 39.20 Thu 16:00 Poster F

**The Role of Chemical Defects for Charge Injection Barriers at Metal / Organic Semiconductor Interfaces** — ●HERMANN EDLBAUER, SHASHANK S. HARIVYASI, EGBERT ZOJER, and OLIVER T. HOFMANN — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, 8010 Graz, Austria

The efficiency of organic electronic devices is strongly determined by the contact resistance caused by the interface of the organic semiconductor and the metal electrode. One approach for its reduction is modifying the work function of the metal contact by adsorbing a monolayer of deliberately chosen molecules onto the metal surface. Our density functional theory (DFT) calculations for instance show that a monolayer of the electron acceptor tetrafluoro-benzoquinone adsorbed on Cu(111) causes a work function increase of about 0.5 eV. However, imperfections and chemical defects, e.g., through hydrogen adsorption, can mitigate this effect. Within this work, we investigate how sensitively the injection barrier depends on the formation of chemical defects. In particular, the corrugation of the electrostatic potential above the surface and the implications for the formation of "hot spots" are discussed. This is studied by a gradual hydrogenation of parts of the molecules in a supercell. Using ab initio thermodynamics, further we show how the number of chemical defects and hence the work func-

tion change can be linked to the partial pressures of the participating molecules in a surrounding gas phase.

DS 39.21 Thu 16:00 Poster F

**Characterization of surface contaminants of medical devices by means of Synchrotron Radiation-based FTIR microspectroscopy and X-Ray spectrometry** — BEATRIX POLLAKOWSKI<sup>1</sup>, ●ANDREA HORNEMANN<sup>1</sup>, BONNIE TYLER<sup>2</sup>, RORY STEVEN<sup>2</sup>, PEGGY EMMER<sup>1</sup>, and BURKHARD BECKHOFF<sup>1</sup> — <sup>1</sup>Physikalisch-Technische Bundesanstalt, Berlin, Germany — <sup>2</sup>National Physics Laboratory, London, United Kingdom

It is an emerging topic to develop metrology tools for a traceable characterization of advance biomaterials for the medical device industry. One aspect concerns the detection and identification of defect structures and contaminants, which may lead to delamination, cracking and spalling of the coating and ultimately lead to the device failure. This work deals with analysis of contaminants dedicatedly deposited on relevant substrates. Bis-steramide is a surface contamination originating from the production and packing process. Employing both vacuum-based and ambient techniques, represented here by X-ray fluorescence analysis under grazing incidence condition (GIXRF) and FTIR spectroscopic techniques, it allows for a traceable and reliable analysis of mass deposition and the chemical species of the contaminants. The combination of GIXRF and XAFS offers a non-destructive access to depth-resolving analysis with respect to both, the chemical speciation and the depth-dependent elemental composition. The results on different bis-steramide samples with varying layer thicknesses show that the combination of complementary methods substantially supports the development of a metrology for complex biomaterial for medical devices.

DS 39.22 Thu 16:00 Poster F

**Epitaxial Growth and Photoluminescence of  $\alpha$ -Sexithiophene on KCl- and Si/SiO<sub>2</sub>-Substrates** — ●FRIEDER LENNART MÜNTZE<sup>1,2</sup>, HISAO YANAGI<sup>2</sup>, and DERCK SCHLETTWEIN<sup>1</sup> — <sup>1</sup>Institute of Applied Physics, Justus-Liebig-University Gießen, D-35390 Giessen — <sup>2</sup>Graduate School of Materials Science, Nara Institute of Science and Technology, Nara 630-0192, Japan

$\alpha$ -Sexithiophene ( $\alpha - 6T$ ) is a well-known organic semiconductor with possible applications in organic electronics. Different crystalline phases of  $\alpha - 6T$  have been established. Either nanofibers or 3D islands can be formed. This has an influence on the photoluminescence (PL)-properties of the materials. In this work, three differently coloured domains of  $\alpha - 6T$  were obtained in sublimation studies. These samples were analysed with UV-vis, PL-spectroscopy and XRD to determine the respective crystal phase. Thin films were studied which proved to be of the LT-structure established in the literature for films grown on  $KCl(001)$  or onto  $Si/SiO_2$  substrates for temperatures up to 150 °C. On the  $KCl$ , we found nanofibers while on the  $Si/SiO_2$  substrates, islands were formed. When excited by UV the islands emitted in the green part of the spectrum while the needles on  $KCl$  emitted orange. For films grown on  $KCl$  at 180 °C, however, needles were formed that emitted in the green part of the spectrum. Based on these findings, based on the polarization dependence of the emission intensity and based on the orientation of the needles relative to the substrate the orientation of  $\alpha - 6T$  relative to the different substrate surfaces is discussed.

DS 39.23 Thu 16:00 Poster F

**Organic light emitting diode (OLED) on Silicon for Biomedical Sensor Applications** — ●MATTHIAS JAHNEL<sup>1</sup>, MICHAEL THOMSCHKE<sup>1</sup>, BEATRICE BEYER<sup>1</sup>, KARSTEN FEHSE<sup>1</sup>, KARL LEO<sup>2</sup>, and VOLKER KIRCHHOFF<sup>1</sup> — <sup>1</sup>Fraunhofer Institute for Organic Electronics, Electron Beam and Plasma Technology FEP, Maria-Reiche-Strasse 2, 01109 Dresden, Germany — <sup>2</sup>Institut für Angewandte Photophysik, Technische Universität Dresden (TUD), 01062 Dresden, Germany

Organic thin film devices like light emitting diodes (OLED) or organic photo diodes (OPD) integrated on silicon backplanes could be one promising way to achieve low cost sensors. We present two types of top emitting OLED devices that are suitable for lab-on-a-chip applications. Both include optically filtered green light emission, 1st case by a single titanium dioxide (TiO<sub>2</sub>) layer in 2nd case using a distributed-Bragg-reflector (DBR) based on TiO<sub>2</sub> and silicon oxide (SiO<sub>2</sub>). These OLED devices are covered with a thin film encapsulation. We investigated the influence of the substrate surface temperature during the deposition on the performance of the devices and compared them to

reference devices without TiO<sub>2</sub> layers. Further, we achieved a narrow emission spectrum with a Full Width at Half Maximum (FWHM) of 20 nm and additionally a minimized angular dependency of the electroluminescence peak. Both device architectures can be used for large area deposition as well as integration onto Silicon-CMOS backplanes and resultingly, a combination of optical functional dielectric layers with organic electronic devices in bio and medical sensor applications.

DS 39.24 Thu 16:00 Poster F

**Investigation of Stearates as Solution-Processable Electron Injection Layers in Organic Light-Emitting Diodes** — ●FLORIAN ULLRICH<sup>1,2,3</sup>, SEBASTIAN STOLZ<sup>1,3</sup>, NORMAN MECHAU<sup>1,3,4</sup>, GERARDO HERNANDEZ-SOSA<sup>1,3,4</sup>, MALTE JESPER<sup>5</sup>, MANUEL HAMBURGER<sup>1,5</sup>, and ERIC MANKEL<sup>1,6</sup> — <sup>1</sup>InnovationLab GmbH, Heidelberg, Germany — <sup>2</sup>University of Heidelberg, Kirchhoff-Institute for Physics, Germany — <sup>3</sup>Karlsruhe Institute of Technology, Light Technology Institute, Germany — <sup>4</sup>Karlsruhe Institute of Technology, Institute of Microstructure Technology, Germany — <sup>5</sup>University of Heidelberg, Organisch-Chemisches Institut, Germany — <sup>6</sup>TU Darmstadt, Material-Wissenschaft, Surface Science, Germany

One crucial obstacle which has to be overcome for the production of efficient organic light-emitting diodes (OLEDs) by high-throughput printing techniques is the injection of electrons into the device, since typical cathode layers with low work-functions like calcium or barium are highly reactive and cannot be solution-processed.

In this work, we investigate alkalimetal stearates as solution processable electron injection layers in OLEDs. Therefore yellow emitting OLEDs with different concentrations of Cs, Rb, K and Na stearate were fabricated and the influence on device performance, such as efficiency, efficacy and operational lifetime, was studied. For the various stearates, significantly different current efficiencies were observed with a maximum value of about 9 cd/A which equals that of reference devices. Photoelectron spectroscopy in comparison to Kelvin probe measurements as well as layer thickness characterization are in progress.

DS 39.25 Thu 16:00 Poster F

**Enhanced Infrared Spectroscopy of Organic Field Effect Transistor (OFET) Materials for an In-Line Production Control** — ●MICHAEL SENDNER<sup>1,2</sup>, ANTON HASENKAMPF<sup>1</sup>, and ANEMARIE PUCCI<sup>1,2,3</sup> — <sup>1</sup>Kirchhoff-Institut für Physik, Universität Heidelberg — <sup>2</sup>InnovationLab GmbH, Heidelberg — <sup>3</sup>Centre for Advanced Materials, Universität Heidelberg

For a mass production of flexible organic devices, such as Organic Field Effect Transistors (OFETs), printing in a roll-to-roll-process becomes of increasing importance. For the realization of an in-line production control a fast characterization of the organic semiconductors is needed. Infrared spectroscopy enables the possibility of controlling contaminations of the organic semiconductors and at the same time the determination of film thickness of the used materials. A reduction of the measurement time is possible if one uses metal nanostructures which enhance the vibrational signals of the materials due to collectively excited conduction electrons (plasmons). We show that metal nanostructures are a possible tool for in-line control of organic semiconductors on a flexible organic substrate by means of enhancement and measurement time.

DS 39.26 Thu 16:00 Poster F

**Nanospectroscopic studies in organic thin film devices** — ●XIAOYAN DU<sup>1</sup>, BENEDIKT RÖSNER<sup>1</sup>, PETER WARNICKE<sup>2</sup>, XUECHEN JIAO<sup>3</sup>, TAYEBEH AMERI<sup>4</sup>, and RAINER FINK<sup>1</sup> — <sup>1</sup>Physikalische Chemie II, FAU Erlangen-Nürnberg, 91058 Erlangen, Germany — <sup>2</sup>Paul-Scherrer-Institut, Villigen, Schweiz — <sup>3</sup>Department of Physics, NCSU, Raleigh, North Carolina 27695-8202, USA — <sup>4</sup>FAU Erlangen-Nürnberg, Institute of Materials for Electronics and Energy Technology (I-MEET), Germany

The performance of organic thin film devices are greatly dependent on the morphology of the active layer. Combining Atomic Force Microscopy (AFM), Transmission Electron Microscopy (TEM) and chemical sensitive methods like Scanning Transmission X-ray Microscopy (STXM) and Resonant Soft X-ray Scattering (RSoXS) can enable us to gain a better understanding of the structure-performance relationship on the nanometer scale. Combining these techniques, we were able to correlate the organic field effect transistor properties of thin films of 6,13-Dihydro-6,13-diazapentacene (DHDAP) with the film morphology which is influenced by the deposition temperature. While STXM is particularly suited to monitor the molecular orientations locally, AFM indicates crystallinity smaller than the oriented domains. STXM,

RSoXS and TEM were combined to study active layer morphology of ternary organic solar cells. Our results clearly showed that the miscibility between polymers and fullerenes is a key factor in determining the functionality of ternary solar cells. The structure findings correlate with the device performance.

DS 39.27 Thu 16:00 Poster F

**Accurate measurement of the exciton diffusion length based on a single solar cell** — ●BERNHARD SIEGMUND, JOHANNES BENDUHN, KOEN VANDEWAL, CHRISTIAN KÖRNER, and KARL LEO — Institut für Angewandte Photophysik, Dresden, Germany

The photo-current of organic solar cells is the result of a multi-step process. It includes the generation and diffusion of excitons as well as their separation into free charge carriers, their transport to the electrodes, and their final extraction.

Cascade structures of neat absorber layers have recently proven to be a convincing concept for efficient exciton harvesting with power conversion efficiencies comparable to those of tandem devices. Enhanced diffusion lengths of excitons would provide further improvements in terms of higher short-circuit currents. Bulk heterojunction devices would also profit from a longer diffusion length, since this would require less interface area for charge generation, which in turn inhibits free carrier recombination, improving both fill factor and open-circuit voltage.

In this work, we introduce an accurate as well as elegant way to determine the diffusion length of organic thin films based on the evaluation of the photo-current produced by an organic bilayer solar cell. In this context, a non-unity conversion probability of interfacial excitons into extracted charge carriers might complicate data analysis. Applying varying gradients of optical fields, we demonstrate how to determine both this conversion probability and the diffusion length independently by means of a single device measurement.

DS 39.28 Thu 16:00 Poster F

**Electrodeposited Al-doped ZnO used in Hybrid Organic-Inorganic Solar Cells** — ●NADINE DANNEHL<sup>1,2</sup>, JENNIFER T. DAMASCO TY<sup>1</sup>, HISAO YANAGI<sup>1</sup>, and DERCK SCHLETTWEIN<sup>2</sup> — <sup>1</sup>Graduate School of Materials Science, Nara Institute of Science and Technology, Nara 630-0192, Japan — <sup>2</sup>Institute of Applied Physics, Justus-Liebig-University Gießen, D-35390 Giessen

Hybrid organic-inorganic solar cells which use dyes as absorbers, polymers as donors and inorganic nanostructures as acceptors combine the advantages of organic and inorganic materials. In our study, we investigate hybrid solar cells fabricated with Al-doped zinc oxide (AZO) grown by electrochemical deposition using AlCl<sub>3</sub> as aluminum source. The AZO films with different Al : Zn molar ratios (0.5%, 2.5%, 5.0%) were grown on ZnO- and AZO-seeded Indium-Tin-Oxide (ITO) substrates. The seed layers were deposited by spin-coating methanolic precursor solutions of the respective metal salts onto ITO-substrates followed by annealing. To fabricate the cells a solution of 1:1 poly(3-hexylthiophen) (P3HT) and [6,6]-Phenyl C61 butyric acid methyl ester (PCBM) in 1:1 chlorobenzene and trichlorobenzene was spin-coated onto the electrodeposited AZO layer. A MoO<sub>3</sub> electron-blocking layer and a Au electrode were vapor-deposited on top of the organic layer to complete the cells. Nanorods with diameters of about 40 nm and high vertical orientation were obtained from electrolyte solutions with 0.5% Al : Zn molar ratios. The solar cells fabricated from these nanorod array structures achieved efficiencies up to 1.1% showing the principle applicability of such layers.

DS 39.29 Thu 16:00 Poster F

**Analytical Transmission Electron Microscopy on Small Molecule Bulk Heterojunction Organic Solar Cells** — DIANA NANOVA<sup>1,2,4</sup>, ●LARS MÜLLER<sup>1,2,4</sup>, FELIX SCHELL<sup>2,4</sup>, MICHAEL SCHERER<sup>1,2,4</sup>, ANNE K. KAST<sup>3,4</sup>, PIRMIN KÜKELHAHN<sup>2,3</sup>, RASMUS R. SCHRÖDER<sup>3,4</sup>, ROBERT LOVRINCIC<sup>1,4</sup>, and WOLFGANG KOWALSKY<sup>1,4</sup> — <sup>1</sup>Institute for High-Frequency Technology, TU Braunschweig, Germany — <sup>2</sup>Kirchhoff-Institute for Physics, Heidelberg University, Germany — <sup>3</sup>CellNetworks, BioQuant, Heidelberg University, Germany — <sup>4</sup>InnovationLab GmbH, Heidelberg, Germany

Understanding the interplay of morphology, material crystallinity and device performance in organic bulk heterojunction (BHJ) solar cells is crucial for the development of efficient devices. The application of electron energy loss spectroscopy (EELS), electron diffraction, and electron tomography in a transmission electron microscope (TEM) allows for a detailed analysis of the BHJ. Here, we investigate the influence of substrate composition and temperature during deposition on fluorinated

zinc phthalocyanine / fullerene BHJs. Combined with device performance data, the influence of these two separately varied parameters is studied in terms of 3D-morphology and long range order within the materials. With additional EELS measurements that reveal electronic and even dielectric properties of the materials by application of the Kramers-Kronig relations, a diversified description of the investigated layer can be given.

DS 39.30 Thu 16:00 Poster F

**Highly conductive polythiophene brushes and its application for Organic Solar Cell** — ●RAVI-KUMAR DIVAKAR<sup>1,2</sup>, JI-LING HOU<sup>2</sup>, RENE SCHUBEL<sup>1</sup>, TAO ZHANG<sup>1</sup>, LARS MÜLLER-MESKAMP<sup>2</sup>, KARL LEO<sup>2,3</sup>, RAINER JORDAN<sup>1,3</sup>, and IHSAN AMIN<sup>1,3</sup> — <sup>1</sup>Makromolekulare Chemie, Technische Universität Dresden, 01069 Dresden, Germany — <sup>2</sup>Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany — <sup>3</sup>Centre for Advancing Electronics Dresden, Technische Universität Dresden, George-Schumannstrasse 11, 01187 Dresden, Germany

Conductive polymers, especially polythiophene (PT) and its derivatives have attracted intensive interest both in research and industry due to its potential application for optoelectronic devices such as organic field effect transistors (OFETs), organic light emitting devices (OLEDs) and organic solar cells (OSCs). For most applications, PT is dissolved in a good solvent such as chlorobenzene, and then spin-coated onto dielectric substrates such as SiO<sub>2</sub>. However, the spin-coated PT film may form a wrongly oriented polymer chains which may result in a low conductivity of the film. Here, we report on fabrication of PT brushes via direct photografting on aminofunctionalized surfaces. The resulted polymer brush chains have “out of plane” orientations and thus show a high conductivity. We foresee the highly conductive polythiophene brushes would have potential applications in OLEDs, OFETs and OSCs.

DS 39.31 Thu 16:00 Poster F

**Growth of pinholes in metal electrodes of organic photovoltaic cells** — ●DANIEL FLUHR, ROLAND RÖSCH, BURHAN MUHSIN, MARCO SEELAND, and HARALD HOPPE — Institute of Physics, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Lifetime is still a major problem of organic photovoltaic (OPV) cells. There are many reasons for solar cell degradation varying from shunts induced by impurities or electromigration over photoinduced oxidation of active layer materials to corrosion and delamination of the metal contact both induced by oxygen or water ingress.

One issue concerns so-called pinholes through the metal back electrode of the device. These pinholes offer pathways for ingress of water and oxygen which may attack the metal-organic interface by introducing delamination through formation of insulating metal oxides or hydrogen evolution. As charge injection and extraction is suppressed at delaminated areas, the active area taking part in power conversion - and hence the overall efficiency - becomes reduced.

We investigated the influence of different environmental conditions on the reduction of the active area of the OPV cell. Spatially resolved measurements give information on location and size of insulated areas induced by pinholes in the metal back contact. Time resolved measurements during degradation of the devices revealed the dynamics and rate of growth of these individual defects. Looking at different device structures provides conclusions for increasing the lifetime of organic photovoltaic cells.

DS 39.32 Thu 16:00 Poster F

**Identification of the weakest mechanical point in OPV devices** — ●AURÉLIE TOURNEBIZE<sup>1</sup>, ALBERTO GREGORI<sup>2</sup>, STEFAN SCHUMANN<sup>3</sup>, ANDREAS ELSCHNER<sup>3</sup>, CHRISTINE DAGRON-LARTIGAU<sup>2</sup>, ROGER C. HIORN<sup>4</sup>, AHMED ALLAL<sup>2</sup>, HEIKO PEISERT<sup>1</sup>, and THOMAS CHASSÉ<sup>1</sup> — <sup>1</sup>Institut für Physikalische und Theoretische Chemie, Tübingen, Germany — <sup>2</sup>EPCP, IPREM (UMR-5254), Université de Pau et des Pays de l'Adour, France — <sup>3</sup>Heraeus Precious Metals GmbH & Co. KG, Electronic Materials Division, Leverkusen, Germany — <sup>4</sup>CNRS, EPCP, IPREM (UMR-5254), Pau, France

While the electrical failure mechanisms in organic photovoltaic (OPV) devices have been thoroughly investigated, little is known about their mechanical stability, which is as important and critical to ensure long term reliability. In this study, a new set-up has been developed for the so-called probe using an inverted structure glass/ITO/ZnO/P3HT:PCBM/PEDOT:PSS/Ag. The technique has been extended varying low bandgap polymers for the active layer in combination with two different PEDOT:PSS formulations. After me-

chanical tests, the upper and lower surfaces have been characterized by AFM and XPS to locate the fracture point. A difference in the stress at break for devices made with different combinations of active and hole transporting layers is visible, suggesting different fracture paths. Acknowledgments The research leading to these results has received funding from the European Union Seventh Framework Programme (FP7/2011 under grant agreement ESTABLIS n° 290022).

DS 39.33 Thu 16:00 Poster F

**Multilayer Aluminum Thin Films as Effective Encapsulation for Flexible Organic Devices** — ●FELIX DOLLINGER, FREDERIK NEHM, KARL LEO, and LARS MÜLLER-MESKAMP — Institut für Angewandte Photophysik, Technische Universität Dresden, Deutschland

Thin film organic devices like organic solar cells require encapsulation against water vapor. Depending on the device, water vapor transmission rates (WVTR) in the range of  $10^{-5} \frac{g}{m^2 \cdot day}$  are needed for lifetimes of at least five years. In this work we aim at improving the encapsulation properties of opaque vacuum-evaporated aluminum back-electrodes to fulfill these barrier requirements.

Water diffusion through aluminum layers is defect-driven. To reduce defect densities, the growth behavior of the aluminum layer is modified by underlying metallic seed-layers which have shown improved performance in transparent metal thin-film electrodes.

Significant improvement of WVTR can be achieved with multilayer structures. Thin interlayers that decouple the defect positions in consecutive aluminum layers provide long and tortuous diffusion-paths for water-molecules. In our study, we use the electrical calcium-test to investigate stacks of aluminum layers with various interlayers with respect to steady-state WVTR and lag-time. The interlayers consist of different planarizing, diffusion-limiting, or getter materials that absorb water-molecules as they diffuse through the barrier.

These optimized aluminum multilayers are promising candidates for organic thin-film encapsulation.

DS 39.34 Thu 16:00 Poster F

**Calculation of hopping based electronic transport through donor-acceptor polymeric systems** — ●FLORIAN GÜNTHER<sup>1,2</sup>, SIBYLLE GEMMING<sup>1,3</sup>, and GOTTHARD SEIFERT<sup>2</sup> — <sup>1</sup>Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — <sup>2</sup>Physical Chemistry and Electrochemistry, TU Dresden, Germany — <sup>3</sup>Institute of Physics, TU Chemnitz, Germany

In order to design high performance organic transistors, semiconducting materials exhibiting high charge carrier mobility are needed. Current record hole as well as electron mobilities have been achieved by diketopyrrolopyrrole (DPP) based donor-acceptor polymers.

Our study addresses the influence of the molecular structure on the electronic transport properties of such systems. Thereby, we focus on intermolecular hopping since it plays the major role in the limitation of the charge transport. For this aim, we consider a model based on Marcus transfer theory. Here, we focus on the coupling matrix elements and their dependence on the stacking configuration. Using a Boltzmann-like approach for evaluating an average value of this quantity, we obtain good agreements to experimental trends. Especially the dominating transport type is nicely reproduced by our approach.

Our calculations are based on density functional based tight binding (DFTB), because it is a well appropriate method for our aim and computational most efficient compared to other first-principle approaches.

DS 39.35 Thu 16:00 Poster F

**Semitransparente leitfähige und flüssigprozessierbare Elektroden für die Optoelektronik** — ●PETER FISCHER, HARALD HOPPE und EDDA RÄDLEIN — TU Ilmenau

Diese Arbeit befasst sich mit der Lösung des Problems der Herstellung kostengünstiger leitfähiger semitransparenter flüssig-prozessierter Metalloxidschichten. Ein erster Ansatz hierzu in die Dotierung von Titandioxid mit Niob. In einem ersten Schritt wurde hierzu die Durchleitfähigkeit mit bestimmten Bauelementen getestet. Dabei galt es insbesondere homogene und engmaschig dichte Schichten zu erzeugen.

Das Thema ist für die kostengünstige Produktion von verschiedenen Optoelektronikbauteilen, wie z.B. Bildschirmen, Touch-Panels, organischen Solarzellen und Leuchtdioden bedeutend, aber auch in Bezug auf fundamentale physikalische Eigenschaften sehr interessant. Die zur Zeit als Standard verwendete Elektrode in der organischen Photovoltaik, Indiumzinnoxid (ITO), ist trotz ihrer hohen Leitfähigkeit und Transparenz für eine wirtschaftliche Verwendung auf Grund der hohen Kosten von Indium, die zur Zeit mehr als 50% des Preises einer organischen Solarzelle ausmachen, nicht geeignet.

## DS 40: Metallic nanowires on the atomic scale (joint session with O)

Time: Friday 9:30–13:15

Location: H 2032

## Invited Talk

DS 40.1 Fri 9:30 H 2032

**From 2D to 1D: Honeycomb crystals and their nanoribbons** — ●FRIEDHELM BECHSTEDT — Friedrich-Schiller-Universität Jena, Germany

Metal-induced quantum wires are usually prepared on Si and Ge surfaces. Novel two-dimensional (2D) sheet crystals silicene, germanene and stanene as well as their functionalized counterparts are prototypes to study such atomically-thin layer systems.

Their exotic properties are studied using modern electronic-structure methods and discussed in the light of available experiments:

(i) Despite partial  $sp^3$ -bonding Dirac cones appear in their band structure similar to the  $sp^2$ -bonded graphene.

(ii) The infrared absorbance is given by the Sommerfeld fine-structure constant.

(iii) Chemical functionalization opens significant fundamental gaps. Excitons occur with giant binding energies.

(iv) A quantum spin Hall phase is due to spin-orbit interaction.

According to recent predictions one-dimensional structures, i.e., nanoribbons, should conduct electricity with 100% efficiency at room temperature with zero resistance along their edges. The predictions are critically discussed. The influence of magnetic ordering of edge states and external electric fields are investigated.

DS 40.2 Fri 10:00 H 2032

**Impurity-mediated early condensation of an atomic layer electronic crystal: oxygen-adsorbed In/Si(111)-(4x1)/(8x2)**

— ●STEFAN WIPPERMANN<sup>1</sup>, WOLF GERO SCHMIDT<sup>2</sup>, DEOK MAHN OH<sup>3</sup>, and HAN WOONG YEOM<sup>3</sup> — <sup>1</sup>Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany — <sup>2</sup>Universität Paderborn, D-33098 Paderborn, Germany — <sup>3</sup>Pohang University of Science and Technology, Pohang 790-784, Korea

While impurities have been widely known to affect phase transitions, the atomistic mechanisms have rarely been elucidated. The self-assembled In/Si(111)-(4x1) nanowire array is an extremely popular model system for one-dimensional electronic systems and features a reversible temperature-induced phase transition into a charge density wave (CDW) ordered state, a representative electronic phase.

We present a joint experimental and *first principles* study, demonstrating oxygen impurity atoms to condense the In/Si(111) nanowire array locally into its CDW ordered ground state, even above the transition temperature. Interestingly, CDW ordering is not induced by single impurities, but instead by the cooperation of multiple impurities. The mechanism is explained as a coherent superposition of the local impurity-induced lattice strain, stressing the coupled electronic and lattice degrees of freedom for CDW ordered phases.

DS 40.3 Fri 10:15 H 2032

**Transport in spatially confined anisotropic systems** — ●FREDERIK EDLER<sup>1</sup>, ILIO MICCOLI<sup>1,2</sup>, HERBERT PFNÜR<sup>1</sup>, and CHRISTOPH TEGENKAMP<sup>1</sup> — <sup>1</sup>Institut für Festkörperphysik, Univ. Hannover, DE — <sup>2</sup>Dept. Innovation Engineering, Univ. Salento, IT

Atomic chain ensembles are 1D-prototype systems with intriguing electronic properties, e.g. Peierls driven metal-insulator transitions (MIT). While such inherent instabilities can be probed smartly by surface transport, details of the phase transitions depend crucially on atom-sized imperfections. In order to correlate such imperfections (including finite size effects) with transport properties, a spatial constriction of the electron paths is mandatory, e.g. by using appropriately designed templates.

The In/Si(111) system reveals a strong anisotropy and has been comprehensively studied of the last years. We used it here as a benchmark system to investigate systematically the effects of confinement as well as of different contact geometries which is finally important to deduce correctly the resistivity components from resistance measurements. While spatial constrictions were achieved using Si(111)-mesas structures, various 4-point probe geometries could be realized by means of a 4-tip STM/SEM system. The anisotropy of the In-4 × 1 has been quantified by rotating the tips gradually in squared configuration. Indeed, the sensitivity was increased by one order of magnitude by performing the transport experiments on confined areas. Furthermore, first studies of the MIT tuned by adsorption of, e.g. oxygen, have been performed and will be discussed.

DS 40.4 Fri 10:30 H 2032

**Ultrafast dynamics of (quasi-1D) Pb overlayers grown on flat and vicinal Si(111)** — ●ABDUL SAMAD SYED<sup>1</sup>, VESNA MIKŠIĆ TRONTL<sup>1</sup>, MANUEL LIGGES<sup>1</sup>, MATHIAS SANDHOFER<sup>1</sup>, ISHITA AGARWAL<sup>1</sup>, ISABELLA AVIGO<sup>1</sup>, DANIEL LÜKERMANN<sup>2</sup>, CHRISTOPH TEGENKAMP<sup>2</sup>, HERBERT PFNÜR<sup>2</sup>, and UWE BOVENSIEPEN<sup>1</sup> — <sup>1</sup>Fakultät für Physik, Universität Duisburg-Essen — <sup>2</sup>Institut für Festkörperphysik, Leibniz Universität Hannover

Due to real space anisotropy of the vicinal Si(111) surfaces, hot electrons can be expected to exhibit different dynamics along and perpendicular to the steps [1] as compare to the Si(111) flat surface. We made a comparative study of Pb overlayer structures grown on vicinal Si (557) and flat Si (111) using femtosecond time- and angle-resolved two-photon photoemission. We mapped the unoccupied electronic band structure near  $\Gamma$  and find that both systems have two unoccupied states at  $E - E_F = 3.3$  and 3.5 eV. In pump-probe experiments combined with a position sensitive electron time of flight spectrometer we analyze the ultrafast momentum dependent electron dynamics along two in plane directions. On vicinal surfaces we observe a specific, momentum dependent population dynamics which are absent on the flat surface. This signature shows a delay in population build up of 5 fs as a function of angle with respect to the terrace direction. We assign this behavior to step-induced scattering. We gratefully acknowledge funding by the DFG through FOR1700.

[1] Roth et al., Phys. Rev. Lett. 88, 096802 (2002)

DS 40.5 Fri 10:45 H 2032

**Observation of correlated spin-orbit order in a strongly anisotropic quantum wire system** — ●CHRISTIAN BRAND<sup>1</sup>, MONIKA JÄGER<sup>1</sup>, HERBERT PFNÜR<sup>1</sup>, GABRIEL LANDOLT<sup>2,3</sup>, HUGO DIL<sup>2,4</sup>, STEFAN MUFF<sup>2,4</sup>, TANMOY DAS<sup>5</sup>, and CHRISTOPH TEGENKAMP<sup>1</sup> — <sup>1</sup>Institut für Festkörperphysik, Leibniz Universität Hannover, Germany — <sup>2</sup>Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland — <sup>3</sup>Physik-Institut, Universität Zürich, Switzerland — <sup>4</sup>Institute of Condensed Matter Physics, École Polytechnique Fédérale de Lausanne, Switzerland — <sup>5</sup>Theoretical Division, Los Alamos National Laboratory, USA

The surface of 1.31 ML Pb on Si(557) reveals a highly anisotropic wire ensemble structure becoming insulating in the direction across the wires when cooling below 78 K (2D/1D transition) as seen by surface transport. The delicate interplay between the superlattice structure, band filling, and extremely large Rashba type spin-orbit interaction results in a highly correlated entangled spin- and charge-state. The spin texture close to the Fermi surface is found to be alternating and equidistant, thus Fermi nesting occurs in between bands with the opposite helicity. Furthermore, the interwire coupling has been gradually changed by adsorption of excess Pb nucleating preferentially at the step edges. The analysis of spin-resolved momentum distribution curves shows that Fermi nesting is preserved up to 0.2 ML. Both the spin-dephasing seen in ARPES as well as the increase of the spin-orbit scattering rates from former magneto transport measurements is quantitatively explained in the framework of a spin-orbit density wave.

DS 40.6 Fri 11:00 H 2032

**Tuning the Playground for Spin-Polarization in Au-Induced Atom Chains on High-Index Silicon Surfaces** — ●JULIAN AULBACH<sup>1</sup>, JOERG SCHAEFER<sup>1</sup>, STEVEN C. ERWIN<sup>2</sup>, and RALPH CLAESSEN<sup>1</sup> — <sup>1</sup>Physikalisches Institut und Röntgen Center for Complex Materials Systems (RCCM), Universität Würzburg, Germany — <sup>2</sup>Naval Research Laboratory, Washington DC, USA

Atomic wires on semiconductor substrates allow direct access to spectroscopic studies of the low-temperature ground state of quasi-one-dimensional systems, such as a charge density wave or a Tomonaga-Luttinger liquid. A particularly intriguing concept is the use of high-index silicon surfaces of the type Si(hhk), providing tunability with respect to terrace width and adatom coverage. As a specific representative, stabilization of the Si(553) surface by Au adsorption results in two different atomically defined chain types, one made of Au atoms and one of Si. The latter, situated at the step edges, forms a honeycomb nanoribbon. At low temperature these silicene-like ribbons develop a period tripling, previously attributed to a Peierls instability. Here we report evidence from scanning tunneling microscopy that

rules out this interpretation [1]. On the contrary, our results are in excellent agreement with density functional calculations [2], which reveal an antiferromagnetic ordered state, where every third Si atom at the step edge hosts a single electron [1]. Additionally we will also address the consequences for this spin ordering by varying the high index substrate.

[1] J. Aulbach et al., Phys. Rev. Lett. 111, 137203 (2013).

[2] S. C. Erwin and F. J. Himpsel, Nature Commun. 1, 58 (2010).

DS 40.7 Fri 11:15 H 2032

**Vibrational properties and optical anisotropy of lead nanowires on Si(557)** — ●EUGEN SPEISER<sup>1</sup>, ARNE BAUMANN<sup>1</sup>, SANDHYA CHANDOLA<sup>1</sup>, JOCHEN RÄTHEL<sup>1</sup>, DANIEL LÜKERMANN<sup>2</sup>, CHRISTOPH TEGEKAMP<sup>2</sup>, and NORBERT ESSER<sup>1</sup> — <sup>1</sup>Leibniz-Institut für Analytische Wissenschaften - ISAS - e. V., Department Berlin, Schwarzschildstrasse 8, 12489 Berlin, Germany — <sup>2</sup>Institut für Festkörperphysik, Appelstraße 2, 30167 Hannover, Leibniz Universität Hannover, Germany

We use Raman spectroscopy and Reflectance Anisotropy Spectroscopy (RAS) to investigate the vibrational properties and anisotropic optical response of Pb nanowires on Si(557). This model system, which shows quasi-1D conductance below 78 K, consists of 1.31 ML of Pb on the Si(557) surface. The adsorption of Pb induces a refaceting of the surface into evenly stepped (223) facets, decorated by one Pb nanowire each. Above 78 K the 2D coupling between the individual wires increases and allows conductivity perpendicular to them. RAS measurements of the Si(557) surface before and after Pb deposition show that the adsorption of Pb clearly induces a reorganization of the surface. Both phases exhibit a strongly anisotropic optical conductance behavior and anisotropic optical transitions which can be associated with the Pb induced reformation of the surface. The Raman spectra show surface vibrational modes which are only present after Pb deposition. With theoretical calculations it is possible to elucidate the relation of the surface vibrational modes with atomic structure and propose structural models for the high and low temperature phases.

15 min. break.

DS 40.8 Fri 11:45 H 2032

**Doping Induced 1D Plasmons in Ag Monolayer Stripes on Si(557)** — ●TIMO LICHTENSTEIN, ULRICH KRIEG, CHRISTOPH TEGEKAMP, and HERBERT PFNÜR — Leibniz Universität Hannover, Institut für Festkörperphysik, 30167 Hannover, Germany

We demonstrate here by testing the plasmonic properties for the system Ag/Si(557) that the interaction between adsorbate layers of transition metal atoms and strongly anisotropic surfaces can lead to various quasi-1D signatures, which, however, are not all necessarily metallic. Using low energy electron diffraction in combination with scanning tunneling microscopy and electron energy loss spectroscopy, we correlate the structure with the properties of low dimensional collective excitations, as measured with momentum and energy resolving electron loss spectroscopy. Semiconducting structures with double periodicity along the chains are formed for Ag coverages below 0.3 ML. At higher coverages, coupled with the onset of  $\sqrt{3} \times \sqrt{3}$  order, metallic wires are formed. This is evident from the appearance of plasmonic losses, which show 1D dispersion only along the wires. This 1D property even persists up to 1 ML, where a densely packed array of metallic  $\sqrt{3} \times \sqrt{3}$  stripes is formed. We show evidence that the metallic property is induced by an extrinsic doping process of excess Ag atoms localized at the step edges, which can be reversibly removed and added. With this system we were able to explicitly show that the 1D plasmon frequency depends on the electron density proportional to  $\sqrt{n_e}$  also in the 1D case, and that the confinement of the electrons on the wires is also dependent on doping concentration.

DS 40.9 Fri 12:00 H 2032

**Optical and electronic properties of quasi-1D gold nanowires on Si(553) surfaces** — ●SANDHYA CHANDOLA<sup>1</sup>, EUGEN SPEISER<sup>1</sup>, CONOR HOGAN<sup>2</sup>, SVETLANA SUCHKOVA<sup>1</sup>, JOCHEN RÄTHEL<sup>1</sup>, JULIAN PLAICKNER<sup>1</sup>, and NORBERT ESSER<sup>1</sup> — <sup>1</sup>Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Department Berlin, Schwarzschildstrasse 8, 12489 Berlin, Germany — <sup>2</sup>Institute for Structure of Matter, CNR-ISM, Via Fosso del Cavaliere, 00133 Rome, Italy

The structures of many 1D metallic nanowire systems have not yet been sufficiently clarified, such as gold nanowires on vicinal Si surfaces. Such structures are intrinsically anisotropic and can be investi-

gated by Reflection anisotropy spectroscopy (RAS) which is a powerful optical technique for probing electronic states of surfaces. The optical response of the Si(553)-Au and hydrogenated Si(553)-Au surfaces are measured with RAS and compared with density functional theory simulations. Good agreement between experiment and theory is obtained. Local structural elements such as the Si honeycomb chains and the gold atomic wires, yield distinctive features in the optical spectra. By comparing the optical response of the freshly prepared and hydrogenated Si(553)-Au surfaces, the spectral features can be directly attributed to particular structural elements on the surface. This combination of experiment and theory is very useful in identifying specific structural sites on the surface, which generate distinctive features in the optical response. The surface will be used to attach molecules such as 3,4-toluenedithiol. The ordered array of the molecules could act as a template for further functionalization.

DS 40.10 Fri 12:15 H 2032

**Vibrational properties of Au nanowires on Si(553) and Si(111) surfaces** — ●SERGEJ NEUFELD<sup>1</sup>, SIMONE SANNA<sup>1</sup>, JOCHEN RÄTHEL<sup>2</sup>, NORBERT ESSER<sup>2</sup>, and WOLF-GERO SCHMIDT<sup>1</sup> — <sup>1</sup>Lehrstuhl für Theoretische Physik, Universität Paderborn — <sup>2</sup>Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Berlin

Metallic nanowires on semiconducting substrates such as silicon and germanium have been attracting considerable interest in the last decade. Besides various potential applications as non ohmic conductors, they are candidate systems for the demonstration of the basic concepts of one-dimensional physics such as electron correlation and Luttinger liquid behavior. In particular, the phase transitions observed on these systems have been controversially discussed and are still poorly understood. Self organizing gold chains at vicinal surfaces such as the Si(553) and Si(111) are of particular interest, as the use of stepped templates allows to vary the geometric parameters and, thus, tune the inter-chain coupling. While well-established microscopic structural models of Au nanowires on various Si surfaces based on density functional theory are available in the literature, few is known about their vibrational properties. In this work, the phonon eigenmodes and eigenfrequencies of the Au/Si(553) and Au/Si(111) wires are calculated from first-principles at the center of the Brillouin zone. Several surface localized phonon modes are found, whose phonon frequencies can be directly compared with the spectra obtained by Raman measurements. Raman scattering efficiencies are calculated in order to facilitate the comparison between experiment and theory.

DS 40.11 Fri 12:30 H 2032

**Plasmonic excitations in Au/Si(553) and Au/Si(775)** — ●TIMO LICHTENSTEIN<sup>1</sup>, JULIAN AULBACH<sup>1</sup>, JÖRG SCHÄFER<sup>2</sup>, CHRISTOPH TEGEKAMP<sup>1</sup>, and HERBERT PFNÜR<sup>1</sup> — <sup>1</sup>Leibniz Universität Hannover, Institut für Festkörperphysik, 30167 Hannover, Germany — <sup>2</sup>Physikalisches Institut und Röntgen Center for Complex Materials Systems (RCCM), Universität Würzburg, 97074 Würzburg, Germany

Si(553) and Si(775) surfaces are highly stabilized by Au adsorption resulting in chain reconstructions of Au and Si atoms. For low temperatures the chains develop a change in periodicity not because of a Peierl's transition but because of frozen spin-polarization. Therefore, they remain metallic at low temperature. Here we study the metallicity of these systems by investigating the plasmons of the spin-split bands.

The sample quality was controlled with SPA-LEED. The plasmon dispersion was then investigated via a combination of EELS and SPA-LEED setup providing both high energy and momentum resolution. Measurements were carried out at room temperature and at 77 K.

Similar to Au/Si(557) [1], the dispersion for Au/Si(553) and Au/Si(775) is also linear for  $k_{\parallel} > 0.07 \text{ \AA}^{-1}$ , a typical signature in 1D. Compared to Au/Si(557) the slope is decreased by a factor of about 2, reflecting the lower electron density of  $1 \times 10^7 \text{ cm}^{-1}$ . For lower  $k_{\parallel}$  the dispersion relations saturate at 200 meV (150 meV) for Au/Si(553) (Au/Si(775)), indicative of quantum well states perpendicular to the steps expected for electronically well separated wires [2].

[1] T. Nagao et al., Phys. Rev. Lett. 97(11), 116802 (2006).

[2] U. Krieg et al., J. Phys.: Condens. Matter 25(1), 14013 (2013)

DS 40.12 Fri 12:45 H 2032

**Structural Fluctuations on Si(553)-Au** — ●INGO BARKE<sup>1</sup>, STEFAN POLEI<sup>1</sup>, PAUL C. SNIJDERS<sup>2</sup>, and KARL-HEINZ MEIWES-BROER<sup>1</sup> — <sup>1</sup>University of Rostock, Institute of Physics, 18051 Rostock, Germany — <sup>2</sup>Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA

The (1x3) reconstruction on Si(553)-Au can be excited to a (1x2) structure by charge injection from the tip of a scanning tunneling microscope [1,2]. Time-resolved measurements enable access to the system's dynamics revealing rapid fluctuations due to a competition between excitation and decay. In this contribution we focus on the time-dependent response to the specific charge injection site. Two distinct locations of high excitation efficiency are identified. This site specific behavior is also found in spatially resolved current-distance curves which are further employed for a quantitative analysis of the current-dependent structural transition of this system. The results are discussed in view of structural and electronic ground state properties of Si(553)-Au.

[1] S. Polei, P.C. Snijders, S.C. Erwin, F.J. Himpsel, K.-H. Meiwes-Broer, and I. Barke, Phys. Rev. Lett. 111, 156801 (2013).

[2] S. Polei, P.C. Snijders, K.-H. Meiwes-Broer, and I. Barke, Phys. Rev. B 89, 205420 (2014).

DS 40.13 Fri 13:00 H 2032

**Tb silicide nanowires on Si(001) - a one-dimensional metal?**  
— ●STEPHAN APPELFELLER, MARTIN FRANZ, CHRISTOPHER PROHL, JAN GROSSE, ZENO DIEMER, and MARIO DÄHNE — Inst. f. Festkör-

perphysik, TU Berlin, Hardenbergstr. 36, 10623 Berlin

Rare earth metals are well known for their formation of metallic bulk silicides with low Schottky-barrier heights to *n*-type Si. Using appropriate preparation conditions, some rare earth metals, e.g. Tb, are forming silicide nanowires on Si(001) by self-assembly, which have widths of only a few nanometers and lengths of several hundred nanometers. Here, the structural and electrical properties of Tb silicide nanowires are elucidated.

The structural information gained by scanning tunneling microscopy indicates that the Tb silicide nanowires consist of metallic hexagonal TbSi<sub>2</sub>. Scanning tunneling spectroscopy confirms this finding by showing metallic behavior. Furthermore, angle resolved photoemission data obtained at the UE56/2 PGM1 beamline of BESSY clearly reveal a one-dimensional metallic band structure without dispersion perpendicular to the nanowire main axis. Thus, Tb silicide nanowires are promising for future investigations of unique phenomena of one-dimensional metals, such as the Peierls transition.

This work was supported by the DFG, FOR 1700, project E2. We kindly acknowledge the support of K. Horn and coworkers and of BESSY.

## DS 41: Semiconductor substrates: structure, epitaxy and growth (joint session with O)

Time: Friday 10:30–12:45

Location: MA 042

DS 41.1 Fri 10:30 MA 042

**Surface and step conductivities at Si(111)-(7×7) surfaces investigated by multi-tip STM** — ●SVEN JUST<sup>1</sup>, MARCUS BLAB<sup>1</sup>, STEFAN KORTE<sup>1</sup>, VASILY CHEREPANOV<sup>1</sup>, HELMUT SOLTNER<sup>2</sup>, and BERT VOIGTLÄNDER<sup>1</sup> — <sup>1</sup>Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, and JARA-Fundamentals of Future Information Technology — <sup>2</sup>Central Institute for Engineering, Electronics and Analytics (ZEA-1), Forschungszentrum Jülich

Four point measurements using a multi-tip scanning tunneling microscope (STM) are carried out to determine surface and step conductivities at Si(111)-(7×7) reconstructed surfaces. In a first step, distance dependent linear four point measurements are used to disentangle the 2D surface conductivity from bulk and space charge layer contributions. In order to further disentangle the surface conductivity of the step free surface from the contribution due to steps, the four probe method is applied in a quadratic configuration as function of the rotation angle. In total this combined approach allows to uniquely determine the surface conductivity, as well as the step conductivity at silicon surfaces.

DS 41.2 Fri 10:45 MA 042

**Atomic structure of terbium-induced nanostructures on Si(111)** — ●MARTIN FRANZ, JAN GROSSE, ROBERT KOHLHAAS, and MARIO DÄHNE — Technische Universität Berlin, Institut für Festkörperphysik, Berlin

Rare earth metals are known to form a variety of very interesting self-assembled nanostructures on silicon surfaces. Examples are the metallic nanowires that form on the Si(001) and the Si(557) surface. On the planar Si(111) surface, the formation of two- and three-dimensional layers is observed.

Here, we report on a detailed scanning tunneling microscopy study on the growth and the atomic structure of terbium-induced nanostructures growing on the Si(111)7×7 surface for different terbium coverage. At extremely low coverage, the 7×7 substrate acts as a template for the growth of terbium-induced magic clusters. In the submonolayer regime, a 2√3×2√3 superstructure, a chain-like 5×2 superstructure, and elongated islands with a 2×1 reconstruction on top are found. The 5×2 phase consists of alternating silicon Seiwatz and honeycomb chains with terbium rows in between. The observed different configurations can be explained by registry shifts between neighboring terbium rows or defects within one row. At higher coverage, the two-dimensional TbSi<sub>2</sub> monolayer forming a 1×1 reconstruction and the three-dimensional Tb<sub>3</sub>Si<sub>5</sub> multilayer forming a √3×√3 reconstruction are found.

This work was supported by the DFG through FOR 1282 project D.

DS 41.3 Fri 11:00 MA 042

**Tailoring Si(100) substrate surfaces for GaP growth by Ga predeposition** — ●MICHAEL HÄBERLE, BENJAMIN BORKENHAGEN,

GERHARD LILIENKAMP, and WINFRIED DAUM — Clausthal University of Technology, Institute of Energy Research and Physical Technologies, Leibnizstraße 4, 38678 Clausthal-Zellerfeld, Germany

For GaP-on-Si(100) heteroepitaxy, currently considered as a model system for monolithic integration of III-V semiconductors on Si(100), the surface steps of Si(100) have a major impact on the quality of the GaP film. Monoatomic steps cause antiphase domains in GaP with detrimental electrical properties. A viable route is to grow the III-V epilayer on single-domain Si(100) with biatomic steps, but preferably not at the expense of reduced terrace widths introduced by miscut substrates [1]. We have performed in situ investigations of the influence of Ga deposition on the surface terrace dynamics of Si(100) at elevated substrate temperatures by low-energy electron microscopy (LEEM). Starting from nearly equally distributed T<sub>A</sub>- and T<sub>B</sub>-terraces of a two-domain Si(100) surface, submonolayer deposition of Ga resulted in a transformation into a surface with prevailing T<sub>A</sub>-terraces. By increasing deposition rate or decreasing temperature, we induced restructuring of Si(100) into a surface dominated by T<sub>B</sub>-terraces as reported by Hara et al. [2]. The occurrence and mutual transformations of surface structures with different terrace and step structures in a narrow range of temperatures and Ga deposition rates are discussed.

[1] K. Volz et al., J. Cryst. Growth 315, 37 (2011)

[2] S. Hara et al., J. Appl. Phys. 98, 083513 (2005)

DS 41.4 Fri 11:15 MA 042

**Calculated formation energies of charged defects at surfaces from the repeated-slab approach** — ●CHRISTOPH FREYSOLDT and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Defects play an important role for the electrical, optical, and chemical properties of semiconductor surfaces under realistic conditions. In theory, the relevant structures, i.e., surfaces and point defects, are often simulated in the supercell approach. Yet, supercell calculations suffer from artificial interactions between the repeated images that are absent in the physical situation of interest. This is particularly problematic for formally charged defects because of the slow 1/*r* decay of the Coulomb interaction. In this contribution, we suggest a correction for the effect from an analysis of the underlying electrostatics. Screening is taken into account right from the beginning to account for potentially complex screening mechanisms. Yet, the universal long-range behavior limits the complexity to a finite range, allowing for simplified screening models in the end. By using a formulation based on charges and screened potentials, direct contact is made to electronic-structure calculations. The approach will be demonstrated for a model defect at the H-terminated Si(111) surface. The analysis reveals that the electric behavior of defects at surfaces depends on *two* macroscopic parameters (e.g. potential and field far from the surface), rather than *one* as for bulk point defects. Different choices of boundary conditions in charged surface calculations and extrapolation to arbitrary surface

charges will be discussed.

DS 41.5 Fri 11:30 MA 042

**Nanoscale Structure of Si/SiO<sub>2</sub>/Organics Interfaces** — ●HANS-GEORG STEINRÜCK<sup>1</sup>, ANDREAS SCHIENER<sup>1</sup>, TORBEN SCHINDLER<sup>1</sup>, JOHANNES WILL<sup>1</sup>, ANDREAS MAGERL<sup>1</sup>, OLEG KONOVALOV<sup>2</sup>, GIOVANNI LI DESTRI<sup>2</sup>, OLIVER H. SEECK<sup>3</sup>, MARKUS MEZGER<sup>4</sup>, JULIA HADDAD<sup>5</sup>, MOSHE DEUTSCH<sup>5</sup>, ANTONIO CHECCO<sup>6</sup>, and BENJAMIN M. OCKO<sup>6</sup> — <sup>1</sup>FAU, Germany — <sup>2</sup>ESRF, France — <sup>3</sup>DESY, Germany — <sup>4</sup>MPI Mainz, Germany — <sup>5</sup>Bar-Ilan University, Israel — <sup>6</sup>BNL, USA

Single-crystal silicon is by far the most widely used substrate for the deposition of organic thin films. Its surface is invariably terminated by a few nanometer-thick amorphous native SiO<sub>2</sub> layer. The structure of the transition layer between the silicon and its oxide is neither well characterized nor well understood at present.

Using high-resolution x-ray reflectivity measurements of increasingly more complex interfaces involving silicon (001) substrates, we reveal the existence of a low-density, few-angstrom-thick, transition layer at the Si/SiO<sub>2</sub> interface [1]. The importance of accounting for this layer in modeling silicon/liquid interfaces and silicon-supported monolayers is demonstrated by comparing fits of reflectivity curves by models including this layer and the widely used Tidswell model [2], which excludes this layer. The 6-8 missing electrons per silicon unit cell area found here support previous theoretical models and simulations of the Si/SiO<sub>2</sub> interface [3].

[1] H.-G. Steinrück *et al.*, ACS Nano (2014), DOI: 10.1021/nn5056223.

[2] I. M. Tidswell *et al.*, Phys. Rev. B **41**, 1111 (1990).

[3] Y. Tu and J. Tersoff, Phys. Rev. Lett. **84**, 4393 (2000).

DS 41.6 Fri 11:45 MA 042

**Comparative study of Co and Ni germanides growth on Ge(001) substrates** — ●TOMASZ GRZELA<sup>1</sup>, WOJCIECH KOCZOROWSKI<sup>2</sup>, GIOVANNI CAPELLINI<sup>1,3</sup>, RYSZARD CZAJKA<sup>2</sup>, NEIL CURSON<sup>4,5</sup>, and THOMAS SCHROEDER<sup>1,6</sup> — <sup>1</sup>IHP, Im Technologiepark 25, Frankfurt (Oder), 15236, Germany — <sup>2</sup>Institute of Physics, PUT, Piotrowo 3, Poznan, Poland — <sup>3</sup>Dipartimento di Scienze, Università degli Studi Roma Tre, Roma, Italy — <sup>4</sup>London Centre for Nanotechnology, UCL, London, UK — <sup>5</sup>Department of Electronic and Electrical Engineering, UCL, London, UK — <sup>6</sup>BTU Cottbus, Konrad-Zuse Str. 1, 03046 Cottbus

Extending the performance of existing Si microelectronics beyond the limits faced by either miniaturization ("More Moore") or available functions ("More than Moore") requires the integration of new materials. Germanium, due to its superior physical properties with respect to Si in terms of optoelectronics and its CMOS processing compatibility, is one of the most promising materials to further develop the existing Si platform. However, there are challenges to the formation of low resistance metallic contacts to Ge. Different metal/Ge systems present promising electrical properties, but given wide-spread use in Si CMOS technologies in form of their respective silicides-, cobalt- and nickel- germanides are of special importance. In this contribution we focus our attention on the systematic and comparative growth studies of Co- and Ni- germanides on Ge(001) substrates, by means of STM technique. In addition, other measurement technique like TEM-EDX, XPS and LEED were applied to corroborate these STM results.

DS 41.7 Fri 12:00 MA 042

**Investigation of the surface termination of BiTeI by combined STM/AFM** — ●JULIAN BERWANGER, FLORIAN PIELMEIER, and FRANZ J. GIESSBL — Institut für Experimentelle und Angewandte Physik der Universität Regensburg, 93053 Regensburg, Deutschland

Cleaved BiTeI surfaces consist of domains which are either terminated by Te or I [1-3]. The size of these domains depends on the bulk crystallinity of the sample and ranges from 100 μm [1] to 100 nm [3]. The samples investigated here by a combination of scanning tunneling microscopy (STM) and atomic force microscopy (AFM) also consist

of domains with smaller size. We find a similar surface structure as reported in Ref. 3 at 4.5K with plain STM in our room and low temperature STM/AFM experiments. Two different step heights are observed by STM in Ref. 3 and our experiments: 0.7 nm and 0.2 nm. The larger step height corresponds to the height of a -Bi-Te-I-stack. The smaller step height was also suggested to be a structural step caused by a stacking fault [3]. In contrast, the atomically resolved STM/AFM data of the smaller "step" suggests that this is indeed an atomically flat layer. The observed step height in STM is a purely electronic effect due to the different density of states at the Fermi-level of Te- and I-terminated surfaces. [1] Crepaldi *et al.* Phys. Rev. Letters 109, 096803 (2012) [2] Landolt *et al.* Phys. Rev. Letters 109, 116403 (2012) [3] Butler *et al.* Nat. Com. 5, 4066 (2014)

DS 41.8 Fri 12:15 MA 042

**Morphology of ultra-thin ZnO on Ag(111)** — ●BJOERN BIENIEK<sup>1</sup>, PATRICK RINKE<sup>1,2</sup>, TAKASHI KUMAGAI<sup>1</sup>, SHAMIL SHAIKHUTDINOV<sup>1</sup>, BO HONG LIU<sup>1</sup>, and MATTHIAS SCHEFFLER<sup>1</sup> — <sup>1</sup>Fritz Haber Institut der MPG, Berlin, Germany — <sup>2</sup>Aalto University, Helsinki, Finland

In the context of catalysis and hybrid inorganic/organic systems, metal supported ultra-thin ZnO can be used as model systems. However, the atomic morphology of these films is not well understood [1,2,3]. To investigate the thickness and termination of ZnO adsorbed on Ag we combine experimental techniques with all-electron density-functional theory calculations performed with the FHI-aims code and the PBE functional. PBE *ab initio* thermodynamics calculations predict H terminated 2x1-H structures to be most stable for all film thickness and H<sub>2</sub> pressures from low to ultra-high vacuum. However, a comparison of relative apparent height differences in calculated and measured scanning tunnelling microscopy (STM) images gives the best agreement for H- and OH-free two layer ZnO films. Further evidence for H- and OH-free unreconstructed ZnO films comes from the absence of OH peaks in infra-red spectroscopy and the comparison of measured and simulated field effect resonances (FER). We attribute this discrepancy to the *ab initio* thermodynamics prediction to kinetic effects such as energy barriers for the dissociation of H<sub>2</sub> and H<sub>2</sub>O. [1] C. Tusche *et al.* PRL **99**, 026102 (2007) [2] Y. Martynova *et al.*, J. Cat., **301**, 227-223 (2013) [3] G. Weirum *et al.* J. Phys. Chem. C, 114 (2010)

DS 41.9 Fri 12:30 MA 042

**Adding 3D to conventional SEM or FIB surface imaging information - In situ Surface Sensing and Nanoprofilometry for Focused Electron and Ion Beam Induced Processes Verification** — ●FRANK NOUVERTNE<sup>1</sup>, AXEL RUDZINSKI<sup>1</sup>, TORSTEN MICHAEL<sup>1</sup>, MARC LEVERMANN<sup>1</sup>, and EVA MAYNICKE<sup>2,3</sup> — <sup>1</sup>Raith GmbH, Konrad-Adenauer-Allee 8, Dortmund, 44263, Germany — <sup>2</sup>RWTH Aachen, 2. Phys. Inst., Otto-Blumenthal-Str. 28, 52074 Aachen, Germany — <sup>3</sup>Klocke Nanotechnik GmbH, Pascalstr.17, 52076 Aachen, Germany

Recently, the bandwidth of nanofabrication applications for dedicated nanopatterning tools using Electron Beam Lithography (EBL) or FIB has significantly broadened. Some few latest generation professional and multi-technique electron and ion beam nanolithography tools even facilitate additional resistless, focused electron or ion beam induced in situ processes such as material deposition or gas enhanced etching. The number of variable parameters for such complex processes is nearly "infinite", so that an efficient in situ characterization of e.g. material deposition, milling or etching rates becomes crucial for most effective understanding and subsequent optimization of such processes.

We have implemented a nanomanipulator with nanoprofilometric capabilities, which allows efficient in situ characterization of nanostructures in 3D by collecting topographic sample surface information via line scans with approx. 10nm height resolution.

First results of direct in situ growth rate determination of focused electron beam induced material deposition (FEBID) will be presented.