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-SiO2 nanocomposite as photovoltaic absorber: Synthesis by solid vs liquid state decomposition of SiOx — •Erik Schumann[1], Karl-Heinz Heinig[1], René Hübner[1], Verónica Carcelen[2], Matthias Krause[1], and Sibylle Gemming[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstr. 400, 01328 Dresden, Germany — [2]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-SiO2 nanocomposites with sponge-like Si embedded in SiO2 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 SiOx films (x<1), which leads to phase separation into a percolated network of Si nanowires embedded in SiO2, tentatively accompanied by crystallization of the Si. SiOx layers have been grown by ion beam sputter deposition as well as by reactive magnetron sputtering. Phase separation into Si-SiO2 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. Compositional and structural characterization has been performed by Rutherford backscattering spectroscopy, energy filtered transmission electron microscopy, and Raman spectroscopy. The two sputter techniques of SiOx 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 (Cu2ZnSnS4 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 Cu2-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[2], •Alexander von Hoegen[1], Aaron Lindenberg[2], and Matthias Wuttig[1] — [1]1. Physikalisches Institut (IA), RWTH Aachen University, 52066 Aachen, Germany — [2]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 $Ag_4In_3Sb_{67}Te_{26}$ (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 $Sn_1Bi_2Te_4$ via UHV DC Magnetron Sputter Deposition — •Juri Banchewski[1], Felix R.L. Lange[1], Tobias Schäfer[1], Jonas Huyeng[1], Stefan Jakobs[1], and Matthias Wuttig[1,2] — [1]1.Physikalisches Institut (IA), RWTH Aachen University, Germany — [2]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 $Ge_1Sb_2Te_4$ with an additive $Sn_1Bi_2Te_4$ 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 $Sn_1Bi_2Te_4$ 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 $Ge_1Sb_2Te_4$ — •Matthias M. Dück[1], Felix R. L. Lange[1], Tobias Schäfer[1], Sebastian Mäder[1], Hanno Volker[1], and Matthias Wuttig[1,2] — [1]I. Physikalisches Institut (IA), RWTH Aachen University, D-52056 Aachen, Germany — [2]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_2Te_3 [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[1], Julia Benke[1], Manuel Bornhöfft[2], Joachim Mayer[2,3,4], and Matthias Wuttig[1,3] — [1]1. Physikalisches Institut IA, RWTH Aachen University, 52074 Aachen, Germany — [2]GFE, RWTH Aachen University, 52074 Aachen, Germany — [3]JARA-FIT, RWTH Aachen University, 52056 Aachen, Germany — [4]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 $GeSb_2Te_4$ — •Enno Bröring[1], Tobias Schäfer[1], Felix R. L. Lange[1], Hanno Volker[1], and Matthias Wuttig[1,2] — [1]1. Physikalisches Institut (IA), RWTH Aachen University, Germany — [2]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 $GeSb_2Te_4$ 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 diffractrometry. The influence of texture on the electrical properties is determined via low temperature transport measurments.

DS 36.8 Thu 9:30 Poster A

Chalcogenide Superlattices (CSL) for Energy Efficient Data Storage by Magnetron Sputtering — •Felix Lange[1], Jamo Momand[2], Henning Hollermann[1], Juri Banchewski[1], Stefan Jakobs[1], Andrea Redaelli[3], Enrico Varesi[3], Bart J. Kooi[2], and Matthias Wuttig[1,4] — [1]1.Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands — [3]Micron Semiconductor Italia, Process R&D, Agrate Brianza, Italy — [4]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_2Te_3 instead of just bulk $(Sb_2Te_3)_x(GeTe)_y$ (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_2Te_3 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 $Ge_2Sb_2Te_5$ 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 $Ge_2Sb_2Te_5$ (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 SiO2/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 Ge2Sb2Te5 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 Ge2Sb2Te5 (GST), which is interesting for industrial point of view.

Thin films of Ge2Sb2Te5 (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) orientated 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 Ge2Sb2Te5 to Ge1Sb2Te4. 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 TiO2 Nanoparticles and Sb2Te3 Hexagonal Platelets — •Tobias Saltzmann[1], Dirk Oliver Schmidt[1], Hehe Zhang[2], Manuel Bornhöfft[3], Michael Noyong[1], Susanne Hoffmann-Eifert[2], Joachim Mayer[3], and Ulrich Simon[1] — [1]IAC, RWTH Aachen University and JARA - FIT, 52074 Aachen, Germany — [2]Forschungszentrum Juelich GmbH, PGI 7 and JARA - FIT, 52425 Juelich, Germany — [3]GFE, RWTH Aachen University, Aachen, 52074, Germany

We chemically synthesized TiO2 nanoparticles (NPs) and Sb2Te3 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 Sb2Te3 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 TiO2 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 TiOx 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 $([SnSe]_{1.15})_1(VSe_2)_n$ with $n = 1, 2, 3, 4$ — •Andreas Fiedler[1], Matthias Falmbigl[2], David C. Johnson[2], and Saskia F. Fischer[1] — [1]Novel Materials, Department of Physics, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Department of Chemistry, University of Oregon, Eugene OR 97401-3753, USA

The compounds, $([SnSe]_{1.15})_1(VSe_2)_n$ with $n = 1, 2, 3$, and 4, were prepared using designed precursors in order to investigate the influence of the thickness of the VSe_2 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 $([SnSe]_{1.15})_1(VSe_2)_1$ was confirmed and is suppressed as the layer thickness of the VSe_2 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 temper-

ature 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_2 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 H2S-Sensors based on Cu2O deposited by RF-sputtering — •Christian Kandzia[1], Philipp Hering[1], Jörg Henemann[2], Angelika Polity[1], Bruno Meyer[1], and Brend Smarsly[2] — [1]1.Physikalisches Institut, Justus Liebig Universität Gießen, Heinrich-Buff-Ring 16 — [2]Physikalisch-Chemisches Institut, Justus-Liebig Universität Gießen, Heinrich-Buff-Ring 58

Cuprite (Cu2O) 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_2S-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_2S. After exposure the material reacts to Cu_xS 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_2O_5 and $BaTiO_3$-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 $BaTiO_3$ and Ta_2O_5. 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 hystereses loops, which is found for Ta_2O_5 and $BaTiO_3$, 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[1], Savio Fabretti[1], Lauritz Schnatmann[1], Alessia Niesen[1], Markus Schäfers[1], Karsten Rott[1], Andy Thomas[1], and Elisabetta Chicca[2] — [1]Center for Spinelectronic Materials and Devices, Physics Department, Bielefeld University, Germany — [2]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 $Pt/Nb_2O_5/Ti/Pt$ crossbar structures obtained from amorphous Nb_2O_5 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_2O_5 is an insulator allowing for VCM-type resistive switching while NbO_2 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 used as a highly non-linear selector. $Pt/Nb_2O_5/Ti/Pt$ crossbar structures are fabricated from amorphous Nb_2O_5 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_2 thin films by low-oxygen MAD: influence of O_2-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_2 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_2O_3, VO_2, V_2O_5, ... [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_2 and V_2O_3 thin films on Al_2O_3 substrates by controlling the chamber pressure with LO-MAD technique. The thin films were characterised by x-ray diffraction and by scanning tunneling microscopy. Resistivity measurements reflect the influence of the O_2-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_2 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_2) nanostructures show an extremely sharp metal-insulator phase transition (MIT) at a critical temperature of 68 °C. Phase pure VO_2 has a narrow existence region in the V-O-phase diagram, thus mixed vanadium oxides (VO_x) are easily obtained by thermal annealing of VO_2 in either reducing or oxidizing environment. In this work free-standing, single-crystalline VO_2 nanowires were grown on SiO_2 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_2 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_2 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_2 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_2 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_2 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_2 films for application in resistive switching memory cells. Thin HfO_2 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_2 films are integrated into metal/HfO_2/metal crossbar structures of about 2 μm^2 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^+ irradiated TiO_2 thin films — •Daniel Blaschke[1], Agnieszka Bogusz[1], René Hübner[1], Frans Munnik[1], René Heller[1], Andrea Scholz[1], Franziska Nierobisch[1], Vikas Rana[3], Sibylle Gemming[1,2], and Peter Zahn[1] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf — [2]Chair of Scale-bridging Materials Modeling, Physics Department, TU Chemnitz — [3]Peter Grünberg Institut, Forschungszentrum Jülich

Transition metal oxide thin films, like TiO_2, 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_{2-x} layer can act as a reservoir for oxygen vacancies and improves the switching characteristics. Such a layer was introduced into the virgin TiO_2 film by low energy Ar^+ 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^+ irradiation.

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DS 36.23 Thu 9:30 Poster A

Introducing band gap states in MoS_2 monolayers by triangular defects — Tommy Lorenz[1,2], Peter Zahn[1], •Sibylle Gemming[1,3], Artur Erbe[1], and Gotthard Seifert[2] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden - Rossendorf e.V., 01314 Dresden, Germany. — [2]Theoretical Chemistry, TU Dresden, 01062 Dresden, Germany. — [3]Theoretical Physics, Faculty of Sciences, TU Chemnitz, 09107 Chemnitz, Germany.

Triangular defects in MoS_2 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_2 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_2 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_2, 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 $([SnSe]_{1+\delta})_m(NbSe_2)_1$ misfit layer compounds — •Georg Hoffmann[1], Corinna Grosse[1], Andreas Fiedler[1], Matti B. Alemayehu[2], David C. Johnson[2], and Saskia F. Fischer[1] — [1]Neue Materialien, Institut für Physik, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Department of Chemistry and Materials Science Institute, University of Oregon, Eugene, Oregon 97403, United States

The control of material properties by combining layers with differ-

ent 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 $([SnSe]_{1+\delta})_m(NbSe_2)_1$ between 2 K and 300 K. The Hall coefficient and the resistivity increase with increasing m (number of SnSe layers between each $NbSe_2$ layer). While the temperature dependence of $([SnSe]_{1+\delta})_1(NbSe_2)_1$ 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_2CoMnO_6 (LCMO) and Pr_2CoMnO_6 (PCMO) with monoclinic $P12_1/n_1$ structure can be derived from a single perovskite by alternating layers of Co^{2+} and Mn^{4+} 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 $SrTiO_3(100)$ and $SrTiO_3(111)$ substrates, grown by metalorganic aerosol deposition (MAD), was performed. The spectra exhibit a strong A_g mode in the $600-700\ cm^{-1}$ range, indicating B-site cation ordering. Applying TERS, the spectra reveal anenhancement 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 $CaMnO_3$ thin films with intensity enhancement and an emergence of a new phonon mode at 650 cm^{-1}.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 $BaTiO_3$-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 $SrTiO_3$ substrates with metallic $La_{0.7}Sr_{0.3}MnO_3$, ferroelectric $Ba_{0.5}Sr_{0.5}TiO_3$ and paralectric $SrTiO_3$ 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 $LaMnO_3$ and $SrMnO_3$ interlayers and heterostructures with lattice matched $Ba_{1-x}Ca_xTiO_3$ 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_x) 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_x 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_x. Cyclic voltammetry (CV) was then applied to LiPON/WO_x- and to raw WO_x-samples in order to investigate the colouration efficiency of WO_x 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_x 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 $\mu S\ cm^{-1}$.

DS 36.29 Thu 9:30 Poster A

Alternative transparent electrode for inorganic solar cells based on amorphous silicon — •Daniel Rosenkranz[1], Alex Neumüller[2], Matin Vehese[2], Jürgen Parisi[1], and Manuela Schiek[1] — [1]Department of Physics, University of Oldenburg, 26111 Oldenburg, Germany — [2]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[1,2], Rüdiger Mitdank[1], Justus Just[2], Segej Levcenco[2], Thomas Unold[2], and and Saskia F. Fischer[1] — [1]AG Neue Materialien, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 14109 Berlin, Germany

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_{Cu}/n_{Zn+Sn}) to low copper amount (0.47 n_{Cu}/n_{Zn+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[1], LN Leonat[2], J Patek[1], D Roth[3], P Bauer[3], MC Scharber[2], NS Sariciftci[2], and JD Pedarnig[1] — [1]Institute of Applied Physics, Johannes Kepler University Linz, A-4040 Linz, Austria — [2]Linz Institute for Organic Solar Cells (LIOS) / Institute

of Physical Chemistry, Johannes Kepler University Linz, A-4040 Linz, Austria — [3]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 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[1,2], Manuela Junghähnel[2], Stephanie Weller[2], and Edda Rädlein[1] — [1]Technische Universität Ilmenau, Department of Inorganic-Nonmetallic Materials, Ilmenau, Germany — [2]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 TiO2- and SnO2-based transparent conductive oxides — •Frank Lungwitz[1], Erik Schumann[1], Marcel Neubert[2], Matthias Krause[1], and Sibylle Gemming[1,3] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstraße 400, 01328 Dresden — [2]DTF Technology GmbH, Am Promigberg 16, 01108 Dresden — [3]Chemnitz University of Technology, Institute of Physics, Reichenhainer Straße 70, 09107 Chemnitz

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 TiO2 and SnO2 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[1], •Karsten Henkel[2], and Dieter Schmeisser[2] — [1]Organic Nano-piezoelectric Device Laboratory, Department of Physics, Jadavpur University, Kolkata 700032, India — [2]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 (La2/3Sr1/3)xMnyOz thin film growth — •Alexandra Steffen[1], Sabine Pütter[1], Jürgen Schubert[3], Stefan Mattauch[1], Willi Zander[3], Stefan Geprägs[4], and Thomas Brückel[1,2] — [1]Jülich Centre for Neutron Science JCNS, Forschungszentrum Jülich GmbH, Outstation at MLZ, Lichtenbergstr. 1, 85748 Garching — [2]Jülich Centre for Neutron Science JCNS und Peter Grünberg Institut PGI, JCNS-2, PGI-4: Scattering Methods, Forschungszentrum Jülich GmbH, 52425 Jülich — [3]Peter Grünberg Institut PGI, PGI-9: Semiconductor Nanoelectronics, Forschungszentrum Jülich GmbH, 52425 Jülich — [4]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 $(La_{2/3}Sr_{1/3})_xMn_yO_z$. 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 Mg2Fe based thin films — •Thu Trang Trinh[1], Oscar Liedke[1], Wolfgang Anwand[1], Andreas Wagner[1], Oguz Yilidirim[2], Steffen Cornelius[2], Bernard Dam[3], Kohta Asano[4], and Kay Potzger[2] — [1]Institute of Radiation Physics, Helmholtz-Zentrum Dresden-Rossendorf e.V. , D-01328 Dresden, Germany — [2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf e.V. , D-01328 Dresden, Germany — [3]Chemical Engineering, Delft University of Technology, 2628 BL Delft, Netherlands — [4]Energy Technology Research Institute, National Institute of Advanced Industrial Science and Technology, Ibaraki 305-8565, Japan

Due to chemochromism, Mg2MeHx (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 Mg2FeH6 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 nanonlayers 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 monocapillary [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 Ll- and Lα-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].

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*corresponding author: rainer.unterumsberger@ptb.de

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[1], •Tim Wiegmann[1], Martin Ruge[1], Jochim Stettner[1], and Olaf Magnussen[1,2] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Germany — [2]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 oxidisation 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 $Mn_5Ge_3C_x$ films — •Maximilian Kauth[1], Christoph Sürgers[1], and Hilbert v. Löhneysen[1,2] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, D-76049 Karlsruhe — [2]Institut für Festkörperphysik, Karlsruher Institut für Technologie, D-76021 Karlsruhe

Ferromagnetic $Mn_5Ge_3C_x$ 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 $Mn_5Ge_3C_x$ (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. $Mn_5Ge_3C_x$ 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 Mn_5Ge_3 seed layer on Ge(111). The films show a lower corrugation, lower resistivity, higher residual resistance ratio, and a 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 $Bi_2Te_{3-x}Se_x$ layers — •Karl Brunner[1], Steffen Schreyeck[1], Adrian Kirchner[1], Claus Schumacher[1], Jean Geurts[1], Grzegorz Karczewski[2], and Laurens W. Molenkamp[1] — [1]Universität Würzburg, Exp. Physik III, Würzburg, Germany — [2]Institute of Physics, Polish Academy of Sciences, Warsaw, Poland

Layers of $Bi_2Te_{3-x}Se_x$, 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. $Bi_2Te_{3-x}Se_x$ 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 Bi_2Te_2Se.

The Raman-active phonon modes E_{2g}, A^1_{1g} and A^2_{1g} 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 Bansen, 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 different 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 allow 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 allowing, 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 SiNx/SiO2 hetero-superlattices — •Anastasiya Zelenina[1], Andrey Sarikov[2], Denis Zhigunov[3], and Margit Zacharias[1] — [1]Georges-Koehler-Allee 103, Freiburg 79110, Germany — [2]45 Nauki Avenue, Kiev 03028, Ukraine — [3]Leninskie Gory 1, Moscow 119991, Russia

SiNx/SiO2 hetero-superlattices with SiNx sublayer thickness of 3 nm and SiO2 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 leaded 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 SiO2 barrier. The increasing of SiO2 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 SiO2 barriers into SiNx 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[1], Petr Formanek[2], Markus Löffler[1], and Ehrenfried Zschech[1,3] — [1]Dresden Center for Nanoanalysis, Technische Universität Dresden, Dresden, Germany — [2]Leibniz-Institut für Polymerforschung Dresden, Dresden, Germany — [3]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 production 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[1], •Rupak Banerjee[1], Martin Oettel[1], Alexander Gerlach[1], Jiří Novák[1,2], Gonzalo Santoro[3], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany — [2]Central European Institute of Technology, Masaryk University, Kamenice 5, CZ-62500 Brno, Czech Republic — [3]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 — •Zhengbang Wang[1], Hikmet Sezen[1], Jinxuan Liu[1], Chengwu Yang[1], Stephanie Roggenbuck[2], Katharina Peikert[2], Michael Fröba[2], Andreas Mavrantonakis[3], Barbara Supronowicz[3], Thomas Heine[3], Hartmut Gliemann[1], and Christof Wöll[1] — [1]Institute of Functional Interfaces, Karlsruhe Institute of Technology — [2]Institute of Inorganic and Applied Chemistry, Department of Chemistry, University of Hamburg — [3]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 photoelectron 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 TiO_2 Thin Films by Doping — •Anton Neumann[1], Sebastian Mäder[1], Roland Sittner[1], Rüdiger Schmidt[1], and Matthias Wuttig[1,2] — [1]I. Physikalisches Institut (IA), RWTH Aachen University, Germany — [2]JARA - Fundamentals of Information Technology, RWTH Aachen University, Germany

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 TiO_2 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 TiO_2 thin films.

In this study, we show that by adjusting the cationic dopant concentration in the TiO_2 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 — •Gregor Becker, Konrad Ritter, Emanuel Schmidt, and Elke Wendler — Institut für Festkörperphysik, Jena, Deutschland

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 where 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,α_0)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[1], Daniel Hanf[1], Frank Lungwitz[1], René Heller[1], René Hübner[1], Sibylle Gemming[1,2], and Matthias Krause[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Technische Universität Chemnitz, Chemnitz, Germany

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[1], Saša Bajt[2], Victor Soltwisch[1], Christian Laubis[1], and Frank Scholze[1] — [1]Physikalisch-Technische Bundestanstalt, Abbestr. 2-12, 10587 Berlin, Germany — [2]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 distored-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[1], Michael Störmer[1], Hans-Werner Becker[2], Christian Horstmann[1], Reinhard Kampmann[1], Daniel Höche[1], Martin Haese-Seiller[1], Jean-Francois Moulin[1], Christian Randau[3], Uwe Lorenz[1], Richard Hall-Wilton[4], Martin Müller[1], and Andreas Schreyer[1] — [1]Helmholtz-Zentrum Geesthacht, 21502 Geesthacht, Germany — [2]RUBION - Zentrale Einrichtung für Ionenstrahlen und Radionuklide, Ruhr-Universität Bochum, 44780 Bochum, Germany — [3]Georg-August Universität Göttingen, 37077 Göttingen, Germany — [4]European Spallation Source ESS AB, 221 00 Lund, Sweden

Due to the present shortage of 3He, the supply of large neutron detection systems becomes unaffordable. Alternative neutron detection concepts based on solid 10B 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 10B4C 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 10B4C 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 10B 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 3He-monitor.

DS 36.54 Thu 9:30 Poster A

critical current density scaling of FeSe0.5Te0.5 thin films on different substrates — •Feifei Yuan[1,2], Kazumasa Iida[2,3], Marco Langer[2], Jens Hänisch[2], Ataru Ichinose[4], Ichiro Tsukada[4], Alberto Sala[5], Marina Putti[5], Ruben Hühne[2], Ludwing Schultz[2], and Zhixiang Shi[1] — [1]Department of Physics and Key Laboratory of MEMS of the Ministry of Education, Southeast University, Nanjing, China — [2]Institute for Metallic Materials, IFW Dresden, Dresden, Germany — [3]Department of Crystalline Materials Science Graduate School of Engineering, Nagoya University, Nagoya, Japan — [4]Central Research Institute of Electric Power Industry, 2-6-1 Nagasaka, Yokosuka, Kanagawa, Japan — [5]Dipartimento di Fisica, Università di Genova, Via Dodecaneso, Genova, ItalyI

FeSe0.5Te0.5 thin films grown by pulsed laser deposition on CaF2, LaAlO3 (LAO) and MgO substrates were structurally and electromagnetically characterized. The in-plane lattice mismatch between FeSe0.5Te0.5 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 Jc at θ=180°, which arises from c-axis defects as confirmed by transmission election microscopy. In contrast, no c-axis Jc(θ) peaks were observed in films on CaF2 and LAO. A successful scaling of the Jc(θ) can be realized for both films without c-axis correlated defects by the anisotropy ginzburg-landau (AGL)approach with appropriate anisotropy ratio γ.the AGL scaling parameter γ is decreasing with decreasing temperature.

DS 36.55 Thu 9:30 Poster A

Structural and magnetic properties of ultrathin epitaxial Fe_3O_4/NiO bilayers and Fe_3O_4 films grown on $SrTiO_3$(001) — •Olga Schuckmann[1], Tobias Schemme[1], Nico Pathé[1], Frederic Timmer[1], Ralph Bus[1], Timo Kuschel[2], Karsten Kuepper[1], and Joachim Wollschläger[1] — [1]Physics Department, Osnabrück University, Germany — [2]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_3O_4 films was investigated. Epitaxial Fe_3O_4/NiO bilayers and Fe_3O_4 films were grown on niobium doped $SrTiO_3(001)$ 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 magnetooptic 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 $SrTiO_3(001)$ — •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_3O_4 films could be influenced by the difference of the strain, stoichiometry or defect states, e.g., using $SrTiO_3(001)$ as substrate [3,4]. In this study structural properties of ultrathin magnetite films grown on $SrTiO_3(001)$ were investigated. The films were deposited at different temperatures on single crystalline niobium doped $SrTiO_3(100)$ substrates by reactive molecular beam epitaxy (RMBE, Fe evaporation in O_2 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-SiO2 nano-composite coating on Aluminum — •Sahar Salehi[1], Sina Sadreddini[2], and Mohsen Ahmadi[3] — [1]Metallurgical & Materials Engineering Department, School of Chemical & Materials Engineering, Islamic Azad university, Shiraz, Iran. — [2]Department of Materials Science and Engineering, Science and Research Branch, Islamic Azad University, Tehran, Iran. — [3]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 SiO2 nano sized particles in the bath on deposition rate, surface morphology and wear behavior of Ni-P-SiO2 Composite coatings were investigated. The deposition rate of coating was influenced by incorporation of SiO2 Particles. The microstructural observations were performed with field emission scanning electron microscopy (FESEM). The amount of SiO2 was examined by Energy Dispersive Analysis of X-Ray (EDX). Results showed that for the coating produced at 12.5 g/l of nano SiO2 in the bath, the amount of SiO2nanoparticles 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. Nanocomposite 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/dm2. 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 Newberyite structure was formed in the coating structure and at a current density of 5mA/cm2, 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[1], Hida Rassaie[2], and Sina Sadreddini[2] — [1]Department of engineering management,upm university, Malaysia. — [2]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 SiO2 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-SiO2 nanocomposite coating — •Sina Sadreddini[1], Hida Rassaie[1], and Mohsen Ahmadi[2] — [1]Department of Materials Science and Engineering, Science and Research Branch, Islamic Azad University, Tehran, Iran. — [2]Department of Mining and Metallurgical Engineering, Amir kabir University of Technology, Hafez Ave., Tehran, Iran.

In this study, the surface morphology of Ni-P-SiO2 composite coating was investigated with field emission scanning electron microscopy (FESEM). The amount of SiO2 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-SiO2 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 (LiNbO3) 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 LiNbO3 by standard etching technologies is difficult due to its chemical 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, LiNbO3 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 Hofsäss — 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 Bradly-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.

[1] S. Habenicht, Phys. Rev. B 63,125419 (2001).
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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 Hofsäss — 2. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Microelectromechanical systems (MEMS) combine electrial 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 dimenstional structures by varying only the fluence of the proton irradiation on a p-GaAs sample, followed by electrochemical etching [4].

High precision and reproducability 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.

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[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
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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 Hofsäss — 2. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Microelectromechanical systems (MEMS) are micrometer scale systems that combine electrial and mechanical functionality for applications like energy harvesters, accelerometers and pressure sensors [1,2].

Proton beam writing (PBW) is a relatively new, maskless lithographic 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.

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DS 36.70 Thu 9:30 Poster A

Noble gas ion-induced ripple pattern formation on carbon surfaces — •Omar Bobes, Kun Zhang, and Hans Hofsäss — 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 hat 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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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^{-1} at room temperature which shifts to 822 cm^{-1} upon cooling down to 20 K. The signal can be attributed 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 refacetting 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].

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DS 36.74 Thu 9:30 Poster A

Electronic Structure and Doping of quasi-1D Ag Nanowires — •Chris Nicholson[1], Claude Monney[1], Ulrich Krieg[2], Karsten Horn[1], and Martin Wolf[1] — [1]Abteilung PC, Fritz-Haber-Institut der MPG, Faradayweg 4-6, 10825 Berlin — [2]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.

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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 collective "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[1], Michael Marz[1], Christoph Sürgers[1], Hilbert v. Löhneysen[1,2], and Regina Hoffmann-Vogel[1] — [1]Karlsruher Institut für Technologie, Physikalisches Institut, D-76131 Karlsruhe — [2]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 signifcant incluence 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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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].

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DS 36.78 Thu 9:30 Poster A

Manipulation of atomic chains on Ge(001) surface — •Deniz 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[1], Eugen Speiser[1], Sandhya Chandola[1], Conor Hogan[2], Julian Plaickner[1], and Norbert Esser[1] — [1]Leibnitz-Institut für Analytische Wissenschaften - ISAS - e.V., Department Berlin, Schwarzschildstr. 8-10, 12489 Berlin, Germany — [2]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 $Fe_xCo_{1-x}Sb_3$ Skutterudite Thin Films — •Felix Timmermann[1], Marcus V. Daniel[2], Ayham Dalla[2], and Manfred Albrecht[1] — [1]Institute of Physics, University of Augsburg, Universitätsstr. 1, 86159 Augsburg, Germany — [2]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 $CoSb_3$, are materials that meet those criteria well. Substituting Fe with Co gradually could improve the properties further.

In this work, the transport parameters of $Fe_xCo_{1-x}Sb_3$ 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 $CoSb_3$, the electrical conductivity and the Seebeck coefficient were simulated for different values of the Fermi level.

For comparison 30 nm thick thin $Fe_xCo_{1-x}Sb_3$-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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DS 36.82 Thu 9:30 Poster A

Calculation of Thermal Conductivity across an Interface using Beam Matching — Debanjan Basu[1], •Peter Blöchl[1], Cynthia Volkert[2], and Christian Jooss[2] — [1]Institute for Theoretical Physics,Clausthal University of Technology — [2]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[1,2] and Rossitza Pentcheva[2,1] — [1]Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), Technische Universität München, Lichtenbergstraße 1, 85748 Garching, Germany — [2]Faculty of Physics and Center for Nanointegration, CENIDE, University of Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany

The hexagonal delafossites $PdCoO_2$ and $PtCoO_2$ exhibit highly anisotropic transport properties and have been identified as potential themoelectric materials. For instance, along the hexagonal a-b-plane

the thermopower S_{xx} exhibits positive values characterisitic 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 $PdCoO_2$ 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 semiconducting material systems have been investigated in the search for new high performance TE-materials. It has been demonstrated that doping of Bi_2S_3 and Bi_2S_3-Bi_2Se_3 alloys can increase their thermoelectric performance significantly. In this study we have synthesized Bi_2S_3 and Bi_2S_3-Bi_2Se_3 alloys using sealed quarz 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: σ,κ and α) on commercial equipment. The chemical composition and crystal structure are also examined. We observed a larger powerfactor ($\alpha^2\sigma$) in rapidly cooled melts of Chlorine doped Bi_2S_3 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 SrTiO3 films grown on DyScO3 are examined. The anisotropic lattice mismatch between the SrTiO3 film and DyScO3 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 Tmax=258 K and Tmax=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 NaNbO3 films grown on NdGaO3 — •Biya Cai[1], Jutta Schwarzkopf[2], Eugen Hollmann[1], Dorothee Braun[2], Martin Schmidbauer[2], and Roger Wördenweber[1] — [1]1Peter Grünberg Institute (PGI) Jülich, D-52425 Jülich, Germany — [2]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-plain strain can be imposed to an epitaxially grown film. NaNbO3 films are epitaxially deposited on (110) NdGaO3 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 NaNbO3 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)TiO3). For this purpose a series of Ba0.5Sr0.5TiO3 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 ϵeff of 600 at low frequency to ϵeff 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[1,5], Nicole Köhler[2], Sven Zimmermann[1,2], Tobias Fischer[2], Christian Wagner[2], Jörg Schuster[1], Sibylle Gemming[3,4], Stefan Schulz[1,2], and Thomas Gessner[1,2] — [1]Fraunhofer ENAS, Chemnitz — [2]Center for Microtechnologies, TU Chemnitz, Chemnitz — [3]Institute of Physics, TU Chemnitz, Chemnitz — [4]Helmholtz-Zentrum Dresden-Rossendorf, Dresden — [5]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 TiO_2 by noble gas ion implantation — •Solveig Rentrop[1], Barbara Abendroth[1], Wolfram Münchgesang[1], Juliane Walter[1], Jura Rensberg[2], Hartmut Stöcker[1], and Dirk C. Meyer[1] — [1]TU Bergakademie Freiberg, Deutschland — [2]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 TiO_2-based MIM devices, as TiO_2 is one of the most studied and well known binary dielectric for resistive switching.

Here, we used TiN-TiO_2-Au devices with oxide layer thickness ranging from 16-44 nm. TiO_2 layers are deposited by atomic layer deposition and are either amorphous or crystalline in the anatase phase. Ion implantation of Kr^+ 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 x 10^{15} ions/cm^2. We demonstrate stable and reproducible non-volatile switching behaviour for as deposited amorphous TiO_2 and the change in resistive switching parameters such as $R_{ON/OFF}$ ratio and current compliance induced by ion implantation and in dependence on the ion fluence. Volatile switching with a very high $R_{ON/OFF}$ ratio of 946 was found for anatase layers after ion implantation using small fluences of F = 1 x 10^{13} ions/cm^2.

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 Hofsäss — 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 Fe_xSi_{1-x} surface layer is a dominant contribution to self-organized pattern formation [1,2,3]. Isotopically enriched ^{57}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 ^{57}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 Fe_xSi_{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.

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DS 36.91 Thu 9:30 Poster A

Formation of hybrid Ge:Mn structures during flashlamp annealing — •Danilo Bürger[1], Stefan Baunack[2], Jürgen Thomas[2], Daniel Blaschke[3], Thomas Schumann[3], Shengqiang Zhou[3], Oliver G. Schmidt[1,2], and Heidemarie Schmidt[1] — [1]Material Systems for Nanoelectronics, Chemnitz University of Technology — [2]Institute for Integrative Nanosciences, IFW Dresden — [3]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 homogenous 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 inhomogenous 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[1], Torsten Boeck[1], Berit Heidmann[2], Martina Schmid[2], Christian Symietz[3], Jörn Bonse[3], and Jörg Krüger[3] — [1]IKZ, Max-Born-Straße 2, 12489 Berlin — [2]HZB, Hahn-Meitner-Platz 1, 14109 Berlin — [3]BAM, Unter den Eichen 44-46, 12203 Berlin

Cu(In,Ga)Se2 (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[1], Christian Eberl[1], Sinja Pagel[1], Christina Klamt[1], Anna Major[1], Henning Ulrichs[2], Maria Mansurova[2], Markus Münzenberg[3], and Hans-Ulrich Krebs[1] — [1]Institute for Materials Physics, University of Göttingen — [2]1st Institute of Physics, University of Göttingen — [3]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. ZrO2, MgO, or Ta2O5) 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 ferrimagnetism 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 expo-

nential 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 — •Huaihai Pan[1,2,3], Christian Späth[1,3], Alexander Guggenmos[1,3], SooHoon Chew[1,3], Jürgen Schmidt[1,3], Quanzhong Zhao[2], and Ulf Kleineberg[1,3] — [1]Ludwig-Maximilians-Universität München, Fakultät für Physik, Am Coulombwall 1, 85748 Garching, Germany — [2]State Key Laboratory of High Field Laser Physics, Shanghai Institute of Optics and Fine Mechanics, ChineseAcademy of Sciences, Shanghai 201800, China — [3]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[1], Olga Lohse[1], Muhammad Bashouti[1], Lubomir Spahel[3], and Silke Christiansen[1,2] — [1]Max Planck Institute for the Science of Light — [2]Helmholz-Center Berlin — [3]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 TiO2/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[1], Joshua McNeur[1], Ang Li[1], Kenneth Leedle[2], Jonas Hammer[1], Norbert Schönenberger[1], Peyman Yousefi[1], James Harris[2], and Peter Hommelhoff[1] — [1]Department of Laserphysics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]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.

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[2] K. Leedle et al., to be published.

DS 36.99 Thu 9:30 Poster A

A memristor-based hardware cryptography — •N. Du[1], N. Manjunath[1], Y. Shuai[2], D. Buerger[1], I. Skorupa[1], R. Schueffny[3], C. Mayr[4], D. N. Basov[5], M. Di Ventra[5], O. G. Schmidt[1,6], and H. Schmidt[1] — [1]TU Chemnitz — [2]UESTC — [3]TU Dresden — [4]University of Zurich and ETH Zurich — [5]University of California — [6]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 $BiFeO_3$ 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 $BiFeO_3$ 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 $BiFeO_3$ memristor (LRS, HRS) shows that the encoded data distribute randomly.

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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_2O_3 and Y_2O_3, are promising candidates as tritium permeation barrier layers. In this contribution magnetron sputtered Y_2O_3 thin films on Si-wafers are presented. They are annealed at 600 °C to achieve a plenary cubic phase of the Y_2O_3 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_2O_3 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 constrains. 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-amperommetry in liquid (EC:DEC 1M LiClO4) 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 et 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 photo-

catalytic 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 BiFeO3/Si3N4 gate — •Kefeng Li[1], Tiangui You[1], Tim Kaspar[1], Nan Du[1], Danilo Bürger[1], Ilona Skorupa[1], Thomas Mikolajick[2], Oliver G. Schmidt[1,3], and Heidemarie Schmidt[1] — [1]Material Systems for Nanoelectronics, Chemnitz University of Technology, Reichenhainer Strasse 70, D-09107 Chemnitz, Germany — [2]Namlab gGmbH, Noethnitzer Strasse 64, 01187 Dresden, Germany — [3]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 BiFeO3 (BFO) has attracted much attention [3] and has been attributed to flexible barriers [4]. In this work, field effect transistors with a BFO/Si3N4 gate stack have been fabricated and the output characteristics are discussed in dependence on the nonvolatile capacitive switching in the BFO/Si3N4 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. Slesazeck, 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[1] and Gerhard Wilde[2] — [1]Department of Physics, College of Science, Al-Mustansiriyah University, Baghdad, IRAQ — [2]Institute of Material Physics, Westfalisch 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 oC 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, Huaihai 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 ~ 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 HfO2 thin films — •Silma Alberton Corrêa, Simone Brizzi, Massimo Tallarida, and Dieter Schmeisser — Department of Applied Physics and Sensors, Brandenburg University of Technology, 03046 Cottbus, Germany

HfO2 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 HfO2 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 $SrO(SrTiO_3)_n$ films, prepared by means of Atomic Layer Epitaxy with Metalorganic Aerosol Deposition — •Fryderyk Lyzwa[1], Markus Jungbauer[1], Sebastian Hühn[1], Ricardo Egoavil[2], Haiyan Tan[2], Jo Verbeeck[2], Gustaaf Van Tendeloo[2], and Vasile Moshnyaga[1] — [1]1. Physikalisches Institut, Universität Göttingen — [2]EMAT, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerp, Belgium

The Ruddlesden-Popper(RP) films represent a material system, in which perovskite layers of $(SrTiO_3)_n$ are separated by SrO layers. Those dielectrics are promissing due to low-loss for microwave frequencies. We report RP thin films of $SrO(SrTiO_3)_n$ with $n = 2, 3, 4$ using metalorganic aerosol deposition (MAD) in the atomic layer epitaxial mode (ALE). The films were grown on $SrTiO_3$(100) by sequential deposition of Sr-O/Ti-O_2 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 $DyScO_3$(110). Financial support from EU FP 7 Project IFOX (interfacing oxides) is acknowledged.

DS 36.108 Thu 9:30 Poster A

Synthesis of TiS_2 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_2 thin films is gaining attention because of their promising thermoelectric properties. In the future TiS_2 could become a very important material choice to replace already existing and popular materials such as Bi_2Te_3, Sb_2Te_3, and Bi_2Se_3.

Two different synthesis approaches of TiS_2 are explored: First, TiO_2 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_2 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_2. 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[1], Michael Latzel[1,2], and Silke Christiansen[1,3] — [1]Max Planck Institute for the Science of Light, Günther-Scharowsky-Straße 1, Erlangen, Germany — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg, Institut of Optic, Information and Photonics, Staudstr. 7, Erlangen, Germany — [3]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/champer setup which easily can be combined with an optical microscope or Raman, due to the thin and smal 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 smoth 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 sucessful a mean field model of sphericalnoble metal gluster 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].

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