

## DS 43: Poster II: Organic thin films; Atomic layer deposition, Thin film characterization: Structure analysis and composition (XRD, TEM, XPS, SIMS, RBS, ...)

Time: Thursday 16:00–19:00

Location: P1

DS 43.1 Thu 16:00 P1

### Influence of surface energetics on perylene thin film growth —

•CATHY JODOCY, DANIEL MOKROS, MATHIAS CORNELISSEN, CHRISTIAN EFFERTZ, CAROLIN C. JACOBI, and MATTHIAS WUTTIG — I. Institute of Physics (IA), RWTH Aachen University, D-52056 Aachen, Germany

In recent years, organic semiconductors have received considerable interest. Promising applications include organic field effect transistors (OFETs), organic light-emitting devices (OLEDs) and photovoltaic cells. These devices have in common that they are based on organic thin films, and that they are very sensitive to the order of these films. An understanding of thin film growth is crucial to tailor surface morphologies and organic film properties suitable for specific applications.

The molecule-substrate interaction plays a significant role for resulting film structure. Therefore, the evolution of the growth of perylene thin-films on substrates, which were deposited on self-assembled monolayers (SAMs), was investigated.

In this study, perylene has been used as an organic semiconductor material, which has been deposited both on surfaces treated with SAMs and on clean silicon dioxide. Atomic Force Microscopy (AFM) has been employed to investigate the surface morphology and X-Ray Diffraction (XRD) has been used to determine the crystalline structure of the thin perylene films.

DS 43.2 Thu 16:00 P1

### Growth Study of Organic Thin Films - Perylene derivatives on DTC-modified noble metals —

•JANINA FELTER, DANIEL MOKROS, DOMINIK MEYER, INGOLF SEGGER, and MATTHIAS WUTTIG — I. Institute of Physics (IA), RWTH Aachen University, D-52056 Aachen, Germany

Perylene derivatives, such as N,N'-dimethyl-3,4,9,10-perylenetetracarboxylic diimide (DiMe-PTCDI), are high potential organic semiconductors for thin film applications like organic solar cells (OSC), organic light emitting diodes (OLED) and organic thin film transistors (OTFT). In order to access the full potential of these molecules the structural and electronic thin film properties have to be optimized. To achieve this goal, an in-depth understanding of the molecular ordering is necessary. In recent works, it has been shown that the application of self-assembling monolayers of Dithiocarbamate (DTC) molecules leads to a significant downshift of the work function of Au by 2 eV, which enhances the electron injection from the metal to the active organic layer of an OTFT. In this work, films of perylene derivatives have been deposited by molecular beam deposition (MBD) on smooth noble metal surfaces, which are modified by DTC monolayers. Additionally to their influence on the electronic structure examined by Ultraviolet and X-ray Photoemission Spectroscopy (XPS/UPS), we investigate the molecular orientation by Fourier Transform Infrared Spectroscopy (FTIR). The surface morphology is investigated by Atomic Force Microscopy (AFM), while crystallinity and texture are determined by X-ray Diffractometry (XRD).

DS 43.3 Thu 16:00 P1

### Influence of Surface Energetics on Thin Film Evolution —

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The evolution of the growth of perylene thin-films on substrates, which were energetically modified by polymeric dielectrics such as PDMS and PMMA, was investigated by atomic force microscopy (AFM). Thin-film evolution from a few monolayers to thick films in the case of perylene is a three step process: Initial growth is dominated by the formation of high isolated islands, which show an average height significantly higher than the nominal film thickness. This growth phase is influenced by a significant post-growth behavior. In the second step, the evolution of thin-films undergoes a transition to a more lateral growth mode. In the final growth phase, with increasing amount of deposited material the growing islands coalesce. At the contact point of two islands dislocations can occur. In the case of PDMS modified substrates, the regime of coalescence is accompanied by a pronounced spiral growth. Additionally the PDMS modified substrates show a high crystalline order, which was confirmed by x-ray diffraction (XRD) mea-

surements. By combining measurements of the surface free energy of the differently modified substrates with the scaling relationship of nucleation, we were able to predict a profound influence of the dielectric on thin-film growth kinetics.

DS 43.4 Thu 16:00 P1

### Manipulating the Electronic Properties of Manganese Phthalocyanine Thin Films by Potassium Intercalation —

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Manganese phthalocyanine (MnPc) presents great promise towards molecular spintronics due to its high spin state of  $S=3/2$  which can be lowered to  $S=1/2$  by reaction with molecular oxygen [1] or even increased to  $S=5/2$  by doping with alkali metals [2], which promotes 3 stable n-doped phases [3]. Within this work the changes of the occupied and unoccupied electronic states of K intercalated MnPc were investigated by combined UPS, IPS, XPS, and NEXAFS techniques. MnPc films of 10 nm thickness were prepared by organic molecular beam deposition onto Co foils and consecutively doped by K evaporation from a getter source in UHV conditions. The amount of K was determined by XPS while the NEXAFS Mn L edge branching ratio provides information on the spin states of  $S=3/2$  and  $S=5/2$  for pristine and fully doped MnPc, respectively. Finally, from the UP and IP spectra the evolution of the transport band gap upon K intercalation was revealed.

[1] R. Friedrich *et al.*, *J. Chem. Phys.* 136, 064704 (2012)[2] Y. Taguchi *et al.*, *J. Am. Chem. Soc.* 128, 3313 (2006)[3] B. Mahns *et al.*, *J. Chem. Phys.* 134, 194504 (2011)

DS 43.5 Thu 16:00 P1

### FePc and CoPc on Ni(111) and graphene/Ni(111): Influence of the central metal atom —

•JOHANNES UIHLEIN, HEIKO PEISERT, HILMAR ADLER, MATHIAS GLASER, MALGORZATA POLEK, and THOMAS CHASSÉ — Institut für Physikalische und Theoretische Chemie, Auf der Morgenstelle 18, 72076 Tübingen, Germany

The interactions at interfaces between transition metal phthalocyanines (TMPCs) and metal substrates play an important role for charge transport across the interfaces, which may become important for possible future spintronic devices. Molecule-substrate interactions may influence the local charge and thus the spin state of the central metal atom within the first molecular adlayer. This will be especially important for metal atoms possessing an open shell structure. For cobalt phthalocyanine (CoPc) on Ni(111) it has recently been shown, that a graphene buffer layer preserves a charge transfer from the Ni substrate to the molecules metal atom, but changes the detailed electronic situation at the molecule substrate interface [1]. To reveal the effect of the central metal atom of the Pc on interactions at these interfaces we studied iron phthalocyanine on Ni(111) and graphene/Ni(111) using X-ray absorption and photoemission spectroscopies. The comparison to CoPc reveals significant differences.

[1] J. Uihlein *et al.*, *J. Chem. Phys.* 2013, 138, 081101.

DS 43.6 Thu 16:00 P1

### Impact of plasmonic nanostructures on the optical properties of fluorinated ZnPc thin films —

•VERENA KOLB<sup>1</sup>, MICHAEL BRENDEL<sup>1</sup>, and JENS PFLAUM<sup>1,2</sup> — <sup>1</sup>Experimental Physics VI, Julius Maximilians University of Würzburg, 97074 Würzburg — <sup>2</sup>ZAE Bayern, 97074 Würzburg

By adjusting the localized surface plasmon resonance (LSPR) of defined metal nanostructures either the absorption or photoluminescence of organic layers can be enhanced and thus might be an interesting approach for improving both organic solar cells and LEDs. This enhancement is caused by an increase of the near-field component of the electromagnetic field and in the case of absorption the scattering of light. In this contribution gold nanostructures were fabricated via shadow nanosphere lithography and optically and morphologically characterized. Complementary, finite difference time domain simulations were used to determine their LSPR. Finally, their impact on the

optical properties of fluorinated Zn-Phthalocyanines (ZNPc), which prove to be interesting candidates for organic electronics, was investigated. Financial support by the Solar Technologies go Hybrid project is gratefully acknowledged.

DS 43.7 Thu 16:00 P1

**Growth Study of Thermally Evaporated Metal Thin Films on PTCDI-C13** — ●MATTHIAS M. DÜCK, CAROLIN C. JACOBI, JURI BANCHEWSKI, CATHY JODOCY, CHRISTIAN EFFERTZ, and MATTHIAS WUTTIG — I. Physikalisches Institut (IA), RWTH Aachen University, D-52056 Aachen, Germany

Optoelectronic devices based on organic thin films have gained more and more interest over the last few years. The performance of such devices depends critically on the interfaces between the different layers, e.g. the organic layer and the metal electrodes. Especially during the evaporation of metals onto organic thin films various effects can occur, such as thermally induced stress, or diffusion of metal atoms into the organic layer. This is our motivation to study the interface between organic and metallic thin films, in order to be able to optimize functionality of future devices.

Its high electron mobility makes N,N'-ditridecyl-3,4,9,10-perylene-tetracarboxylic diimide (PTCDI-C13) a promising n-type material for organic field effect transistors (OFETs). In this work, thin films of various metals have been deposited by thermal evaporation on 30 nm PTCDI-C13 films produced with Organic Molecular Beam Deposition (OMBD). The surface morphology has been investigated by atomic force microscopy (AFM) and scanning electron microscopy (SEM), whereas the crystallinity was determined by x-ray diffractometry (XRD).

DS 43.8 Thu 16:00 P1

**Investigation of electronic and structural properties of vanadyl phthalocyanine on graphene interlayers on Ni(111)** — ●HILMAR ADLER, HEIKO PEISERT, MATEUSZ PASZKIEWICZ, JOHANNES UIHLEIN, MALGORZATA POLEK, and THOMAS CHASSÉ — Institut für Physikalische und Theoretische Chemie, Auf der Morgenstelle 18, 72076 Tübingen, Germany

In previous years, transition metal phthalocyanines (TMPcs) gained increasing attention due to their tunable properties, resulting in various applications based on these materials such as light-emitting diodes, field-effect transistors and solar cells and, most recently, the interface between TMPcs and metal substrates raised additional interest due to their important role in spintronic nanodevices. In the case of TMPcs, molecule-substrate interactions can drastically influence both electronic and magnetic properties of the first layer of the organic semiconductor. The interface properties however can be tuned by the insertion of a buffer layer [1]. Graphene with its exciting electronic properties is an ideal candidate for such layers. Vanadyl phthalocyanine as a polar and non-planar TMPc is in particular suited for the tuning of electronic properties of interfaces. Charge transfer processes depending on the adsorption geometry on Ni(111) and graphene/Ni(111) were investigated using scanning tunneling microscopy, X-ray photoelectron spectroscopy and X-ray absorption spectroscopy.

[1] J. Uihlein, H. Peisert, M. Glaser, M. Polek, H. Adler, F. Petraki, R. Ovsyannikov, M. Bauer, T. Chassé *J.Chem.Phys.* 138 (2013) 081101.

DS 43.9 Thu 16:00 P1

**AlCIPc on silver: Influence of substrate surface.** — ●MALGORZATA POLEK<sup>1</sup>, TAMARA V. BASOVA<sup>2</sup>, FOTINI PETRAKI<sup>1</sup>, FLORIAN LATTEYER<sup>1</sup>, HEIKO PEISERT<sup>1</sup>, and THOMAS CHASSÉ<sup>1</sup> — <sup>1</sup>University of Tuebingen, Institute of Physical and Theoretical Chemistry, Auf der Morgenstelle 18, 72076 Tuebingen, Germany — <sup>2</sup>Nikolaev Institute of Inorganic Chemistry, Lavrentiev Pr. 3, Novosibirsk, 630090, Russia

Phthalocyanines (Pcs) are promising materials for various applications such as organic solar cells, field effect transistors and light emitting diodes. To improve the efficiency of the aforementioned opto-electronic devices, one needs to adjust the properties and understand better the interactions between the building blocks. Due to its permanent dipole moment and the chemical reactivity, AlCIPc is in particular suited for the tuning of the interface properties. We investigated electronic properties and chemical interactions of AlCIPc with polycrystalline Ag foil and Ag(100) using photoelectron spectroscopy (XPS, UPS) and low energy electron diffraction (LEED). Clear indications for a chemical interactions were found for both substrates. In addition, charge transfer processes to the macrocycle of the Pc were observed, indicated by the appearance of an interface-related peak at  $E_F$ , which can be

explained as a partial filling of the former LUMO at the interface.

DS 43.10 Thu 16:00 P1

**PS-b-PMMA block copolymer films: Self-assembly and dielectric properties on different substrates** — ●RIITTA SAVIKOSKI<sup>1,2</sup>, GUILLAUME FLEURY<sup>2</sup>, ANDREA GASSMANN<sup>1</sup>, GEORGES HADZIOANNOU<sup>2</sup>, and HEINZ VON SEGGERN<sup>1</sup> — <sup>1</sup>Electronic Materials Division, Institute of Materials Science, Technische Universität Darmstadt, Alarich-Weiss-Str. 2, 64287 Darmstadt, Germany — <sup>2</sup>Laboratoire de Chimie des Polymères Organiques, Université Bordeaux 1, Bât 8, Avenue des Facultés, 33405 Talence cedex, France

The self-assembly of block copolymers (BCPs) on Si-substrates has been widely investigated. The present work aims using self-assembled BCP films as gate dielectric in bottom gate organic field-effect transistors and evaluating in how far the morphology of the film influences the performance of the device. Nowadays silicon is not the material of choice for the gate electrode any more. Instead, metals or ITO are common materials. The BCP under investigation is polystyrene-block-poly(methyl methacrylate) (PS-b-PMMA). PS-b-PMMA, with molar ratios of 1:1 and 2:1, were self-assembled on different gate electrode materials, including gold, silver, ITO and Si-substrates as a reference. A vertical orientation of BCP films was achieved on oxidized Si-substrates by adding a brush layer of random BCP (PS-r-PMMA). However, this vertical orientation can also be achieved through a nanometer scale surface roughness. The success of self-assembly was studied for spin coated films using atomic force microscopy (AFM). Furthermore, dielectric properties of the films were investigated by impedance measurements.

DS 43.11 Thu 16:00 P1

**Influence of the short interaction range of C<sub>60</sub> on nucleation and step-edge barrier during growth** — ●SEBASTIAN BOMMEL<sup>1,2</sup>, NICOLA KLEPPMANN<sup>3</sup>, SABINE H.L. KLAPP<sup>3</sup>, and STEFAN KOWARIK<sup>2</sup> — <sup>1</sup>Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85, D-22607 Hamburg, Germany — <sup>2</sup>Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, D-12489 Berlin, Germany — <sup>3</sup>Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, D-10623 Berlin, Germany

Atoms, molecules and colloids show different growth phenomena attributed to their different phase diagrams, particle sizes and interaction ranges. Here, we report on the influence of the short interaction range of the fullerene C<sub>60</sub> on nucleation and step-edge barrier [1]. Quantitative agreement between real-time x-ray scattering experiments during molecular growth with kinetic Monte Carlo (KMC) simulations allow us to analyze the particle-resolved dynamics of C<sub>60</sub> on the surface. Compared to atoms, we find relatively long surface diffusion times before the molecules are immobilized at islands. We attribute these to the colloid-like, short-ranged character of C<sub>60</sub>-interactions [2]. However, the step-edge barrier of C<sub>60</sub> differs from colloids in that it is not a pseudo-step-edge barrier arising from lower diffusion probability at a step-edge, but a true energetic barrier as is observed for atoms. Thus, our findings will help to gain insight into nucleation and surface growth processes between the scales of atomic and colloidal systems.

[1] S. Bommel, N. Kleppmann et al., submitted [2] S. P. Tewari et al., *Int. J. Mod. Phys. B* 24, 4281 (2010)

DS 43.12 Thu 16:00 P1

**Theoretical analysis of the Anthracene NEXAFS signature** — ●MICHAEL KLUES<sup>1</sup>, KLAUS HERMANN<sup>2</sup>, and GREGOR WITE<sup>1</sup> — <sup>1</sup>Physics Department, Philipps Uni. Marburg, 35032 Marburg — <sup>2</sup>Theory Department, Fritz Haber Institute, 14195 Berlin

NEXAFS is a powerful technique that is experiencing a renewed interest owing to the recent success in the field of organic electronics, as it provides detailed information on electronic properties and orientational ordering in such molecular materials. However, to fully exploit the potential of this technique, a precise and reliable identification and assignment of spectral features within the NEXAFS spectra is needed. In the present work, we have calculated the NEXAFS spectra of Anthracene in the frame of density functional theory by using the StoBe code. Comparison to experimental data shows excellent agreement and points out the high precision StoBe reaches in predicting energies of excitations with errors less than 300meV. The key to such accurate values without any subsequent, empirical energy shift is to handle excited electronic configurations. By matching spectra resulting from excited states with different localized excitation centers we carve out the influence of chemical shifts and core hole effects. Furthermore it is possible to label the numerous resonances occurring in the NEXAFS spectrum.

The detailed calculation also enables a visualization of final states like for example Rydberg states using the fully relaxed excited electronic structure. These illustrations point out the influence of initial and final states on the intensity and energetic shift of the individual partial NEXAFS resonances of the various excitation centers.

DS 43.13 Thu 16:00 P1

**Optical anisotropy in picene thin films** — ●JOHANNES DIETERLE, KATHARINA BROCH, ALEXANDER GERLACH, and FRANK SCHREIBER — Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen

The organic semiconductor picene has attracted significant interest due to reports on its excellent charge-transport properties and O<sub>2</sub> gas sensing ability in organic field-effect transistors (OFETs) [1,2]. In thin films picene grows in high columnar islands depending on substrate temperature and growth rate and exhibits uniaxial anisotropic optical properties. For a complete characterization of the system a knowledge of the in-plane as well as the out-of-plane optical properties is fundamental [3,4]. We investigate thin picene films using optical spectroscopy including variable angle spectroscopic ellipsometry in an energy range of 1.5 to 5 eV at different preparation conditions. Due to the complexity of the system only the in-plane component of the system has been reported so far [5]. We discuss results of different growth conditions.

[1] R. Mitsuhashi et al., *Nature*, 464 (2010), [2] H. Okamoto. et al., *Am. Chem. Soc.*, 130 (2008), [3] T. Hosokai et al., *Chem. Phys. Lett.*, 544 (2012), [4] M. Dressel et al., *Opt Express.*, 16 (2008), [5] S. Fanetti et al. *J. Chem. Phys.*, 137 (2012)

DS 43.14 Thu 16:00 P1

**Hydration effects of chitosan on silicon.** — ●MARCELO CISTERNAS<sup>1</sup>, MARIA J. RETAMAL<sup>1</sup>, SEBASTIAN GUTIERREZ<sup>2</sup>, MARK BUSCH<sup>3</sup>, PATRICK HUBER<sup>3</sup>, TOMAS PEREZ-ACLE<sup>2</sup>, ULRICH VOLKMANN<sup>1</sup>, and MICHAEL KAPPL<sup>4</sup> — <sup>1</sup>P. Universidad Catolica de Chile, Santiago, Chile — <sup>2</sup>Fundacion Ciencia y Vida, Santiago, Chile — <sup>3</sup>Tech. Univ. Hamburg-Harburg, Hamburg, Germany — <sup>4</sup>MPI for Polymer Research, Mainz, Germany

Chitosan (CH) is a polysaccharide obtained by the deacetylation of chitin, a component of the exoskeleton of crustaceans. Among its most important features we can mention that it is biocompatible, non-toxic and biodegradable. Therefore, it has been used both in the field of agriculture, as well as in medicine. Chitosan appears to be very interesting for biological applications, both as a macro- and micro-scale material. We are interested in CH deposited on a planar silicon substrate (with a native SiO<sub>2</sub> surface) as a possible support for hydration of artificial biological membranes (phospholipids), which form the base for different biosensors. We prepare CH islands and layers of different thickness in a solvent free environment and control with high resolution ellipsometry the layer thickness during formation as well as before and after hydration. The film topography is studied with AFM at room temperature and during heating cycles. The CH-layer capability for water storing is tested with ellipsometry during heating cycles from room temperature to 370 K. We observed that CH does not wet the SiO<sub>2</sub> surface when deposited from the gas phase. It forms spontaneously semi-spheres. This behavior favors the capability of the structure for water storage.

DS 43.15 Thu 16:00 P1

**Growth of Gold on P(VDF-TrFE) During RF-Sputter Deposition** — ●ALEXANDER HINZ<sup>1</sup>, OLEKSANDR POLONSKYI<sup>1</sup>, THOMAS STRUNSKUS<sup>1</sup>, MATTHIAS SCHWARTZKOPF<sup>2</sup>, GONZALO SANTORO<sup>2</sup>, JAN PERLICH<sup>2</sup>, EZZELDIN METWALLI<sup>3</sup>, YUAN YAO<sup>3</sup>, FRANZ FAUPEL<sup>1</sup>, STEPHAN ROTH<sup>2</sup>, and PETER MÜLLER-BUSCHBAUM<sup>3</sup> — <sup>1</sup>CAU zu Kiel, Technische Fakultät, LS Materialverbunde, Kaiserstr. 2, 24143 Kiel — <sup>2</sup>Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85, 22607 Hamburg, — <sup>3</sup>TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching

Metallization of organic surfaces via sputtering is well established in industry and important for many applications. However, in contrast to metal evaporation, the basic mechanisms determining the final microstructure are not well understood due to the complex deposition process involving collisions with gas molecules and defect generation on the sensitive organic surface by energetic ions. The complex nature of the sputter process calls for in-situ measurements. Here we use in-situ grazing incidence small angle scattering (GISAXS) to obtain structural information with high spatial and temporal resolution. The growth of Au on P(VDF-TrFE) is chosen as a model system of inert metal and reactive polymer. The analysis of the GISAXS data yields

morphological information about the different stages of the growing metal film. These results will be compared to results of a parallel GISAXS-study on the growth of Au on PS and already published results on the growth of Au on Si [1].

[1] Schwarzkopf et al., *Nanoscale* 5, 5053-5062 (2013)

DS 43.16 Thu 16:00 P1

**Investigation of the thermal stability and structure of 4,4'-dimercaptostilbene on Au(111)** — ●JOHANNES VÖLKNER, ANDRE PICK, and GREGOR WITTE — Molekulare Festkörperphysik, Philipps-Universität Marburg, 35032 Marburg

Sensing devices for biological molecular species such as proteins or sugars in solution are receiving increasing interest because they enable monitoring of physiological parameters or can lead to bioelectronics. One approach is a photoelectrochemical biosensor which requires an efficient coupling of involved semiconductor nano-particles and the gold electrode to enable charge transfer from the NP towards the electrode without direct quenching the optical excitation with the NP. In a previous study it was shown that self-assembled monolayers of 4,4'-dimercaptostilbene provide a suitable linker that combines structural order and sufficient conductance [1]. However, the ordering and quality of this thiolate-bound interlayer critically depends on several preparation parameters, such as assembling temperature and the choice of solvent. Therefore we investigated the thermal stability and structural order of differently prepared 4,4'-dimercaptostilbene self-assembled monolayers on Au(111) surfaces by means of TDS, XPS and NEXAFS.

[1] W. Khalid et al. *ACS Nano*, 5, 9870 (2011).

DS 43.17 Thu 16:00 P1

**A comparison of dielectric elastomers and electrostrictive polymers for vibration energy harvesting applications** — ●KIRSTIN BORNHORST, CHRISTIAN SCHIRRMANN, ANDREAS WEDER, ANDREAS HEINIG, and FLORENTA COSTACHE — Fraunhofer Institute for Photonic Microsystems IPMS, Dresden, Germany

Harvesting energy from the surrounding environment and converting it into usable electrical energy has become an attractive approach to producing sustainable power sources for wireless sensors and low-power electronics.

In this paper, electroactive polymers (dielectric elastomers and electrostrictive polymers) are compared in terms of their potential for vibration energy harvesting applications. Stacks consisting of polymer thin films placed in between thin metallic electrodes were subjected to dynamic deformation by means of a pneumatic piston of variable frequency and pressure characteristics. A self-priming energy harvesting circuit was developed and used to harvest the generated energy. We investigated the polymer harvester performance, i.e. energy gained from the capacity change, when employing electroactive polymers of different elastic moduli, dielectric constants or electrostrictive constants. Furthermore, we studied the influence of the stack geometry. It is shown that for instance by using a polymer with high electromechanical coupling a harvested energy density of about 0.2 mJ/cm<sup>3</sup> at 15 Hz could be obtained. The harvested energy could be further increased by increasing the frequency of the induced deformation. Applications such as power generation for wireless sensors will be addressed.

DS 43.18 Thu 16:00 P1

**Crystalline phase formation during the atomic layer deposition of TiO<sub>2</sub>** — ●BARBARA ABENDROTH, SOLVEIG RENTROP, THERESA MOEBUS, HARTMUT STÖCKER, and DIRK C. MEYER — Institut für Experimentelle Physik, TU Bergakademie Freiberg, Germany

Titanium dioxide is a wide gap semiconductor and is, based on its optical and electronic properties, widely used in various applications. For its use as thin dielectric layer in microelectronic data storage or in electrochemical energy storage devices, TiO<sub>2</sub> is commonly produced by atomic layer deposition (ALD). In this work we present the deposition of TiO<sub>2</sub> thin films by ALD from tetrakis(dimethylamino) titanium and water on silicon and polycrystalline TiN substrates for the use in metal - insulator - metal resistive switching random access memory cells. For this application, amorphous TiO<sub>2</sub> layers are desirable to minimize leakage currents, however, other applications of TiO<sub>2</sub> layers, such as a high *k* dielectric or photocatalysis require crystalline structures of either rutile or anatase polymorph. For our ALD process, we find a dependence of crystallisation of anatase and rutile on deposition temperature and layer thickness. A survey of literature data on TiO<sub>2</sub> ALD based on various precursors, shows that our results are representative for thermal ALD of TiO<sub>2</sub> on silicon substrates and can be

summarized in a general thickness - temperature - phase diagram.

DS 43.19 Thu 16:00 P1

**In-situ gold cluster growth kinetics on polystyrene thin films during sputter deposition - Influence of molecular weight** — ●MATTHIAS SCHWARTZKOPF<sup>1</sup>, GONZALO SANTORO<sup>1</sup>, JAN PERLICH<sup>1</sup>, OLEKSANDR POLONSKYI<sup>2</sup>, ALEXANDER HINZ<sup>2</sup>, THOMAS STRUNSKUS<sup>2</sup>, EZZELDIN METWALLI<sup>3</sup>, YUAN YAO<sup>3</sup>, FRANZ FAUPEL<sup>2</sup>, PETER MÜLLER-BUSCHBAUM<sup>3</sup>, and STEPHAN V. ROTH<sup>1</sup> — <sup>1</sup>Deutsches Elektronen-Synchrotron, Notkestr. 85, 22607 Hamburg — <sup>2</sup>CAU Kiel, Institut für Materialwissenschaft, LS Materialverbünde, Kaiserstr.2, 24143 Kiel. — <sup>3</sup>TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching.

The adjustment of size-dependent catalytic, electrical and optical properties of gold cluster assemblies and to tailor their morphology with polymer templates is a very significant issue in modern applied nanotechnology. We investigate in situ the growth kinetics of gold nanostructures on polystyrene thin films with different molecular weights during RF-sputter deposition with high time resolution by means of GISAXS. The morphological parameters related to the metallic layer growth such as cluster size, correlation distance and surface coverage are deduced from a general model solely based on geometrical assumptions [1]. Our study opens up the opportunity to deduce the influence of polymer chain length on the wetting behaviour of gold films and provides a better understanding of the growth process kinetics at the polymer-metal interface during sputter deposition. [1] Schwartzkopf et al., *Nanoscale* 5, 5053-5062 (2013)

DS 43.20 Thu 16:00 P1

**Characterization of diamond-like carbon (DLC) coatings on industrial polyethylene and polyoxymethylene by SEM, AFM and NEXAFS** — ●LIZ M. RÖSKEN<sup>1</sup>, MAGDALENA ROHRBECK<sup>1</sup>, ALBERTO CATENA<sup>1</sup>, STEFAN WEHNER<sup>1</sup>, CHRISTIAN B. FISCHER<sup>1</sup>, MATTHIAS RICHTER<sup>2</sup>, MATTHIAS STÄDTER<sup>2</sup>, and DIETER SCHMEISSER<sup>2</sup> — <sup>1</sup>Department of Physics, University Koblenz-Landau, 56070 Koblenz, Germany — <sup>2</sup>Department of Applied Physics and Sensors, Brandenburg University of Technology, 03046 Cottbus, Germany

Diamond-like carbon (DLC) coatings are often utilized to change the base properties of raw materials, e. g. to gain robust or chemically inert surfaces. Here the deposition of hard DLC layers on soft polymers is tested. The common industrial polymers polyethylene (PE) and polyoxymethylene (POM) serve as model substrates in the present work. In order to examine the effect of the carbonaceous layers on PE and POM thin diamond-like carbon films were realized via PECVD. The topography of the different coatings was detected by AFM and SEM uncovering the different influence of the substrate material, e. g. interlayer formation for PE. The composition of the surface structures were analyzed in more detail by NEXAFS, showing the hybridization of carbon atoms in chemical different surroundings from the pure polymer to the carbon coating. The comparison of carbon coated PE- and POM-composites enables valuable insights into the interaction between soft substrates and hard coatings. For the chosen settings in PECVD, POM showed incomplete coating, while on PE a very stable and robust composite has formed.

DS 43.21 Thu 16:00 P1

**Sputter yield amplification of carbon by serial magnetron co-sputtering** — ●PATRICK RIES<sup>1</sup>, RÜDIGER SCHMIDT<sup>1</sup>, ANDREAS PFLUG<sup>2</sup>, TOMAS KUBART<sup>3</sup>, and MATTHIAS WUTTIG<sup>1,4</sup> — <sup>1</sup>I. Physikalisches Institut (IA), RWTH Aachen, Germany — <sup>2</sup>Fraunhofer IST, Braunschweig, Germany — <sup>3</sup>Solid State Electronics, Uppsala University, Sweden — <sup>4</sup>JARA - Fundamentals of Future Information Technology

Carbon has been doped by serial co-sputtering with two different elements, namely Tungsten and Niobium. Both elements provide a significant rate increase for the doping concentrations analyzed. A dopant concentration of 3 at.% Nb increases the deposition rate of carbon by 130%, whereas W increases it by 280%. Due to its higher mass, W is significantly more effective than Nb. TRIDYN simulations have been performed which reproduce the experimental data and show that saturation occurs at higher dopant concentrations, which have not been reached in the experiments. Additionally our experiments indicate very long residual times of the dopant in the target as a result of recoil implantation.

DS 43.22 Thu 16:00 P1

**Al-doped zinc stannate thin films as amorphous transpar-**

**ent conductive oxides prepared by reactive DC magnetron sputtering** — ●ROLAND SITTNER, RÜDIGER MATTI SCHMIDT, and MATTHIAS WUTTIG — I. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen, Germany

Transparent conductive oxides (TCOs) combine the contrary material properties of low electrical resistivity and high optical transparency. Indium tin oxide and aluminum doped zinc oxide are widely used in optoelectronic devices such as photovoltaic modules and flat panel displays. Amorphous TCOs, like indium gallium zinc oxide and zinc stannate, are utilized as channel material in transparent thin film transistors. The most common stoichiometries of the  $Zn_xSn_yO_z$  system are  $ZnSnO_3$  and  $Zn_2SnO_4$ , with the latter possessing a lower electrical conductivity in the amorphous state.

In this work, we deposited aluminum doped  $Zn_xSn_yO_z$  thin films with a high Zn to Sn ratio via reactive DC magnetron sputtering. Doping occurred in a serial co-deposition process in order to obtain films with improved electrical properties compared to undoped zinc tin oxide films. The process parameters and dopant concentrations were varied to deposit films with optimized properties. The electrical, optical and structural properties were determined via van der Pauw method, UV/Vis spectroscopy and X-ray diffraction.

DS 43.23 Thu 16:00 P1

**Influence of film thickness on structural properties of TiO<sub>2</sub> films coated with RF and DC magnetron sputtering** — ●SEBASTIAN SCHIPPOREIT<sup>1</sup>, SANAT KUMAR MUKHERJEE<sup>1</sup>, ABDELKADER NEBATTI<sup>2</sup>, FARHAD MOHTASCHAM<sup>1</sup>, CHRISTIAN NOTTHOFF<sup>2</sup>, and DIETER MERGEL<sup>1</sup> — <sup>1</sup>Faculty of Physics, University Duisburg-Essen — <sup>2</sup>Faculty of Engineering, University Duisburg-Essen

TiO<sub>2</sub> thin films were deposited by reactive sputtering of a Ti target on unheated substrates and post-heated at 300 °C and 500 °C. The dc-sputtered films are amorphous after deposition and crystallize to pure anatase only at 500 °C. The rf-deposited films are crystalline (purely anatase) already after deposition without post-heating. Above a thickness of 100 nm, the crystallite size is constant at 35 nm and decreases to zero when the thickness decreases to 25 nm. Below 25 nm the films are x-ray amorphous. Height and half-width of the XRD peaks of rf-sputtered films do not change upon post-heating at 300 or 500 °C, contrary to the intensity of Raman lines [1]. A larger lattice parameter ratio  $c/a$  is observed compared to the bulk value that decreases with increasing film thickness and is about 1 % larger for a film thickness larger than 100 nm.

[1] Sanat Kumar Mukherjee, Dieter Mergel, *J. Appl. Phys.* 114, 013501 (2013).

DS 43.24 Thu 16:00 P1

**Pulsed Laser Deposition of thin Metal-Oxide Multilayers for thermal barrier coatings** — ●ANNA MAJOR<sup>1</sup>, FLORIAN DÖRING<sup>1</sup>, CHRISTIAN EBERL<sup>1</sup>, SARAH HOFFMANN<sup>2</sup>, FELIX SCHLENKRICH<sup>1</sup>, and HANS-ULRICH KREBS<sup>1</sup> — <sup>1</sup>Institute for Materials Physics, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — <sup>2</sup>Institute for X-Ray Physics, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Multilayers consisting of metals and oxides are highly interesting for modern high-quality coatings especially with regard to their unique thermal conducting properties which could be used for thermal barrier coatings in different applications like gas turbine coatings, cryogenic applications or modern power plants.

Therefore, we have studied pulsed laser deposited (PLD at 248 nm) multilayers consisting of various metals (e.g. W, Ti, Cu) and oxides (e.g. ZrO<sub>2</sub> or MgO) with different layer thicknesses. Their structure, interface roughness and thermal stability were characterized by X-Ray-Reflectivity, Scanning-Electron-Microscopy and cross-sectional Transmission-Electron-Microscopy. Especially we focus on the material combination of W and ZrO<sub>2</sub>, which is highly useful for high temperature applications due to its high thermal stability. For effective multilayer insulation it is necessary to produce very thin individual layers with a high interface density and therefore many scattering and reflection centers for heat transporting phonons.

In this contribution, we show our results in producing these multilayers with high quality and thin individual layer thicknesses.

DS 43.25 Thu 16:00 P1

**High quality TiN as bottom electrode for zinc ferrite based magnetic tunnel junctions grown by pulsed laser deposition** — ●MICHAEL BONHOLZER, MICHAEL LORENZ, and MARIUS GRUNDMANN — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr.

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A highly conductive interlayer is required for a successful device implementation of spinel oxides in magnetic tunnel junctions (MTJs) [1]. We use zinc ferrite ( $\text{ZnFe}_2\text{O}_4$ ) as ferromagnetic electrodes. To reduce the series resistance of these devices we add a highly conductive titanium nitride (TiN) layer between the magnesium oxide (MgO) substrate and the  $\text{ZnFe}_2\text{O}_4$  layer. We have achieved to grow atomically smooth hetero-epitaxial TiN thin films on (001) MgO single crystals by pulsed laser deposition (PLD).

In order to generate perfect conditions for two-dimensional growth of TiN on MgO, the substrates are annealed at  $950^\circ\text{C}$  for 2h in vacuum using a  $\text{CO}_2$  laser heater. The annealed substrates show smooth and uniformly stepped surfaces. The terrace height is half a unit cell of MgO; a value of 0.21 nm was measured by atomic force microscopy (AFM). On these substrates we grew TiN thin films by pulsed laser deposition (PLD). In situ RHEED oscillations indicate two dimensional growth mode up to a film thickness of about 50 nm. This is confirmed by AFM measurements; the TiN films show smooth, stepped surfaces with a uniform terrace height of about 0.21 nm. The existence of intensity fringes in the X-ray pattern indicates a high film quality, as well.

[1] M.Opel *et al.*, Phys. Status Solidi A **208**, 232 (2011)

DS 43.26 Thu 16:00 P1

**Structural and magnetic properties of ultrathin epitaxial magnetite films grown on  $\text{SrTiO}_3$  (001)** — ●OLGA SCHUCKMANN<sup>1</sup>, NICO PATHE<sup>1</sup>, TOBIAS SCHEMME<sup>1</sup>, FREDERIC TIMMER<sup>1</sup>, TIMO KUSCHEL<sup>2</sup>, FLORIAN BERTRAM<sup>3</sup>, KARSTEN KÜPPER<sup>1</sup>, and JOACHIM WOLLSCHLÄGER<sup>1</sup> — <sup>1</sup>Osnabrück University, Germany — <sup>2</sup>Bielefeld University, Germany — <sup>3</sup>Lund University, Sweden

In this study, structural and magnetic properties of ultrathin magnetite ( $\text{Fe}_3\text{O}_4$ ) films grown on  $\text{SrTiO}_3$  (STO) have been investigated. The films of thicknesses between 10 - 120 nm, as determined by x-ray reflectivity (XRR), were deposited on single crystalline niobium doped STO(100) substrates by reactive molecular beam epitaxy (RMBE, Fe evaporation in  $\text{O}_2$  atmosphere).

The stoichiometry of the oxide films was controlled by x-ray photoelectron spectroscopy (XPS). The film structure was characterized by high-energy surface x-ray diffraction (HESXRD) using 85 keV photons as well as lab based conventional XRD. The in-plane and out-of-plane lattice parameters show that compressive strain (-7.5 % lattice mismatch) is reduced with increasing film thickness. In addition, the magnetic properties were studied by magnetooptic Kerr effect (MOKE) showing that the thickness and epitaxial strain affect the magnetic anisotropy of the films.

DS 43.27 Thu 16:00 P1

**Thickness dependency of the magnetic anisotropy of iron oxide on  $\text{MgO}$ (001)** — ●TOBIAS SCHEMME<sup>1</sup>, NICO PATHE<sup>1</sup>, TIMO KUSCHEL<sup>2</sup>, and JOACHIM WOLLSCHLÄGER<sup>1</sup> — <sup>1</sup>Barbarastr. 7, 49076 Osnabrück — <sup>2</sup>Universitätsstr. 25, 33615 Bielefeld

Iron oxide films with different thicknesses were prepared on  $\text{MgO}$ (001). The  $\text{MgO}$  substrates were cleaned by annealing at  $400^\circ\text{C}$  in a  $10^{-4}$  mbar oxygen atmosphere. Afterwards, the surface quality and cleanness was checked in-situ by low energy electron diffraction (LEED) and x-ray photoelectron spectroscopy (XPS), respectively. Iron oxide films with different thicknesses were grown using reactive molecular beam epitaxy (MBE) at  $250^\circ\text{C}$  depositing Fe in a  $10^{-4}$  mbar oxygen atmosphere. Film thickness and the lattice constants were analyzed by x-ray reflectometry (XRR) and x-ray diffraction (XRD), respectively. These experiments reveal the singlecrystalline and epitaxial state of the films. XPS spectra and LEED patterns indicate the stoichiometry and the surface structure of magnetite. Ex-situ magneto optic Kerr measurements were performed to investigate the magnetic properties. While the thinnest film shows a magnetic isotropic behavior, the thicker films exhibit a fourfold magnetic in-plane anisotropy. However, the anisotropy gets weaker with increasing film thickness.

DS 43.28 Thu 16:00 P1

**Pseudo-rotational Epitaxy of Octadecyltrichlorosilane Monolayers on Sapphire (001)** — ●HANS-GEORG STEINRÜCK<sup>1</sup>, ANDREAS MAGERL<sup>1</sup>, MOSHE DEUTSCH<sup>2</sup>, and BEN OCKO<sup>3</sup> — <sup>1</sup>Lehrstuhl für Kristallographie und Strukturphysik, Universität Erlangen Nürnberg, Germany — <sup>2</sup>Bar-Ilan University, Ramat-Gan, Israel — <sup>3</sup>Brookhaven National Laboratory, Upton NY, USA

Octadecyltrichlorosilane (OTS) self-assembled monolayers (SAMs) on the (001) sapphire surface are vertically aligned, well-packed and have hexagonal ordering like the underlying sapphire as shown by X-ray grazing incidence diffraction. The SAM lattice planes are preferentially aligned along the sapphire in-plane structure albeit with an angular rotational distribution, which is well described by a Lorentzian profile with a FWHM of 10 degrees. The hexagonal SAM lattice constant is incommensurate with the sapphire by 1.2% at room temperature, and the degree of incommensuration increases at higher temperatures. The radial correlation length of  $232 \text{ \AA}$  is three times larger than for the same monolayers on a native silicon oxide surface and scales with the orientation  $\phi$  of domains via  $\xi \sim 1/\sin \cdot \phi$ . Our results suggest that a commensurate epitaxial arrangement is distorted by steric hindrances caused by both the packing density of the alkyl chains and the dimension and the cross-linking of the head groups. This results in a size-dependent strain within the OTS domains. We call these novel structural properties of a SAM pseudo-rotational epitaxy.

DS 43.29 Thu 16:00 P1

**High-resolution TEM investigation of an epitaxially strained  $\text{LaNiO}_3/\text{LaGaO}_3$  superlattice** — ●HAOYUAN QI<sup>1</sup>, MICHAEL KINYANJUI<sup>1</sup>, EVA BENCKISER<sup>2</sup>, HANNS-ULRICH HABERMEIER<sup>2</sup>, BERNHARD KEIMER<sup>2</sup>, and UTE KAISER<sup>1</sup> — <sup>1</sup>University of Ulm, Central Facility of Electron Microscopy, Electron Microscopy Group of Materials Science, Albert Einstein Allee 11, D-89069 Ulm, Germany — <sup>2</sup>Max Planck Institute for Solid State Research, Heisenbergstrasse 1, D-70579 Stuttgart, Germany

An epitaxially strained  $\text{LaNiO}_3/\text{LaGaO}_3$  (LNO/LGO) superlattice grown on (001)  $\text{SrTiO}_3$  (STO) has been investigated. Due to the lattice mismatch, the superlattice is subject to tensile strain. The strain-induced distortions and deformations of the octahedral network may drastically influence the magnetic, electrical and structural functionalities of the heterostructures. We have studied the structural change, particularly the tilt system, of the octahedral network by means of aberration-corrected high-resolution transmission electron microscopy (AC-HRTEM). Each atomic column can be resolved clearly by applying negative Cs conditions. The two different octahedral tilt angles viewed in [110] projection indicate non-identical tilt systems in LNO and LGO layers. The atomic structure of the superlattice has been resolved, including in-plane and out-of-plane lattice parameters, distortions and rotation of the oxygen octahedral.

DS 43.30 Thu 16:00 P1

**Soft X-ray emission spectroscopy used for the characterization of a-C and  $\text{CN}_x$  thin films** — SERGEJ NEPIJKO<sup>1</sup>, ALISA CHERNENKAYA<sup>1</sup>, KATERINA MEDJANIK<sup>1</sup>, ●SERGEY CHERNOV<sup>1</sup>, MICHAEL KLIMENKOV<sup>2</sup>, OLEKSANDR VLASENKO<sup>3</sup>, SVETLANA PETROVSKAYA<sup>4</sup>, LARISA ODNODVORETS<sup>3</sup>, YAROSLAV ZAULICHNYY<sup>5</sup>, and GERD SCHÖNHENSE<sup>1</sup> — <sup>1</sup>Institute of Physics, University of Mainz, Germany — <sup>2</sup>Institute for Applied Materials, Karlsruhe Institute of Technology, Germany — <sup>3</sup>Sumy State University, Sumy, Ukraine — <sup>4</sup>Frantsevich Institute for Problems of Materials Science, National Academy of Sciences of Ukraine, Kiev, Ukraine — <sup>5</sup>National Technical University of Ukraine (KPI), Kiev, Ukraine

We have studied a-C and  $\text{CN}_x$  films characterized by an outstanding mechanical properties (hardness, elasticity, low friction coefficient) and chemical inertness thus being a good protection against corrosion and mechanical damage for underlying layers. We present the results of a soft X-ray emission spectroscopy study of a-C and  $\text{CN}_x$  films on Si(100) and glass substrates. Also for the characterization of the homogeneity in depth electron energy loss spectroscopy measurements with localization better than 4 nm were carried out. In case of  $\text{CN}_x$  films the highest diamond-like modification occurs in the region close to Si(100) substrate. Film density decreases with increasing distance from the substrate and becomes almost constant in range of thicknesses more than 2 nm. By means of X-ray absorption and photoelectron spectroscopies it was shown that a  $\text{CN}_x$  film (a-C film also) as thin as 1.5 to 2 nm thickness effectively prevents oxidation of the underlying Co film.

DS 43.31 Thu 16:00 P1

**Measurement of lattice parameters of ultrathin films with an improved Guinier diffractometer** — ●MARKUS MEYL and ARNO EHRESMANN — Institute of Physics and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Straße 40, D-34132 Kassel

Lattice parameters of ultrathin films are quantified with the X-ray Guinier thin film diffractometer Huber G 653. One advantage of

this Guinier diffractometer includes the use of a focussing monochromator between the X-ray tube and the sample for achieving strictly monochromatic X-rays. Another benefit lies in the very small angle of incidence ( $< 10^\circ$ ) between the incident X-rays and the surface of the sample to attain a large distance in the ultrathin films and thereby higher diffraction intensities. Furthermore the sample surface is aligned with height accuracy by utilizing a home built adjustment stage. The measurement setup behind the monochromator is the one of a Seemann-Bohlin camera. In this camera the focal line of the

monochromator, the surface of the sample and the detector entrance slit are situated on a constant focussing cylinder. Before a measurement the angle of incidence is appointed and reflected X-rays are measured when Bragg's law is fulfilled. As a consequence the Guinier thin film diffractometer is especially suitable for analysing thin polycrystalline films on a crystalline or amorphous substrate. From the diffraction spectrum e.g. lattice parameters can be calculated. Exemplary results of Si / Cu / Ir<sub>17</sub>Mn<sub>83</sub> / Ti samples deposited by radio frequency sputtering will be presented.