DS 28: Poster: Thin Film Properties: Structure, Morphology and Composition

Time: Wednesday 15:00-18:00

DS 28.1 Wed 15:00 P1A

Long-time stability of swift-heavy ion irradiated LiNbO₃ — •VERONICA LOPEZ MARCOS¹, ELKE WENDLER¹, LIANG-LING WANG^{1,2}, ALMA DAULETBEKOVA³, MAXIM ZDOROVETS³, and CARSTEN RONNING¹ — ¹Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Germany — ²School of Physics and Technology, University of Jinan, P. R. China — ³L. N. Gumilyov Eurasian National University, Nur-Sultan, Kazakhstan

Lithium niobate (LiNbO₃) has been a material of interest in optics for many years. For the production of photonic devices, ion-beam induced amorphisation can be applied, which is connected with a reduced refractive index. In order to satisfy optical application requirements, thick layers of amorphous material may be needed, which can be achieved by implantation of swift heavy ions. However, the longterm stability of the amorphous structure must be guaranteed, which is investigated in this presentation. LiNbO₃ samples were irradiated with 66 MeV Xe-ions at ion fluences from 5×10^{10} to 3×10^{13} cm⁻². Later the samples were analyzed with Rutherford backscattering spectrometry in channeling mode using 1.4 MeV He-ions. It was found that the fluence-dependent increase of damage is well represented by the direct impact model. The obtained radius of the amorphous tracks produced by individual ions is in agreement with previous results which were measured right after ion irradiation. This indicates that no annealing of amorphous tracks in a crystalline surrounding occurred. In order to understand the damage structure obtained when the tracks overlap forming a complete amorphous layer, further studies are in progress.

DS 28.2 Wed 15:00 P1A

Characterization of photochromic diarylethene films produced via spin-coating — •VIKTOR UDACHIN¹, SVEN NAGORNY², SEBASTIAN DAHLE¹, JÖRG ADAMS³, ANDREAS SCHMIDT², and WOLFGANG MAUS-FRIEDRICHS¹ — ¹TU Clausthal, Institut für Energieforschung und Physikalische Technologien, Deutschland — ²TU Clausthal, Institut für Organische Chemie — ³TU Clausthal, Institut für Physikalische Chemie

Thin photochromic films that can reversibly change physico-chemical properties under suitable electromagnetic radiation have received considerable attention. Such functional coatings are crucial in development of novel optical imaging and lithography applications using photochromism [1, 2]. A promising photochromic substance is 4,4"-(perfluorocyclopent-1-ene-1,2-diyl)bis(5,5'-dimethyl-2,2'bithiophene) (BTE-1) due to its comparatively high thermal- and photo-stability [2]. However, specifications of a spin-coating procedure to obtain homogeneous BTE-1 films with different optical properties are not well defined. In this study, we investigated the behaviour of BTE-1 during spin-coating and determined a set of parameters for the production of defect-free BTE1/PMMA coatings with different thicknesses. The films were produced on quartz substrates by changing spin-coating conditions and properties of solutions. The optical parameters, morphology and thickness of the films as well as the structure of the dye were studied via spectroscopic and microscopic techniques. [1] Kowarsch R. et al. Optics express 26.5 (2018): 5327-5341. [2] Andrew T. L., Tsai H. Y., Menon R. Science 324.5929 (2009): 917-921.

DS 28.3 Wed 15:00 P1A

Shaping silver nanoparticles using low energy ion irradiation — •SHIVA CHOUPANIAN¹, ALESSANDRO NAGEL², CLAUDIA PACHOLSKI², and CARSTEN RONNING¹ — ¹Institute for Solid State Physics, Friedrich Schiller University Jena, Germany — ²Institute of Chemistry, University of Potsdam, Germany

Ion irradiation of surfaces always comes up with other effects such as sputtering or/and ion beam mixing. When nanoparticles are irradiated with ions having an ion range comparable to the size of the object, strong deviation from the behavior of surfaces occurs. In this work, the morphology changes of silver nanoparticles on top of silicon substrates irradiated with Ga^+ ions with energies ranging from 1 to 30 keV were investigated. For higher energies, the morphology change of the nanoparticles occurs dominantly due to enhanced sputtering. However, by decreasing the energy to 8 and 5 keV, a combination of sputtering, ion beam mixing and Ostwald ripening results in the reforming of new particles on top of the surface. Location: P1A

DS 28.4 Wed 15:00 P1A

XPS characterization of ZnO thin films prepared by TALD — •CHRISTOPH JANOWITZ¹, ALI MAHMOODINEZHAD¹, FRANZISKA NAUMANN², PAUL PLATE², HASSAN GARGOURI², KARSTEN HENKEL¹, and JAN INGO FLEGE¹ — ¹Brandenburg University of Technology Cottbus-Senftenberg, K.-Zuse-Str. 1, 03046 Cottbus, Germany — ²SENTECH Instruments GmbH, Schwarzschildstraße 2, 12489 Berlin, Germany

Among the transparent conducting oxides (TCO's) like SnO_2 and In_2O_3 respectively In_2O_3 :Sn (ITO), zinc oxide (ZnO) with comparable electronic and optical properties has attracted interest as an alternative due to its low cost, non-toxicity and high durability. Advances in the production of high quality films of ZnO, foster the realization of TCO based devices in optoelectronics and photovoltaics. Several approaches have been pursued for the deposition of ZnO films in which thermal atomic layer deposition (TALD) facilitates low temperature layer by layer growth for high-quality thin films. Zinc oxide films were deposited on Si (100) substrates using diethyl zinc (DEZn) as a zinc precursor and H_2O as an oxidizing co-reactant within a temperature window of 80 °C to 200 °C. The chemical composition and bonding states of the films were quantitatively determined using X-ray photoelectron spectroscopy (XPS) by decomposition of Zn2p and O1s corelevel spectra. The films exhibited only a slight deviation from ideal stoichiometry with a small excess of oxygen. Also the carbon contamination dependence on the growth temperature was studied. The lowest carbon concentration was found for the sample grown at 150 $^{\circ}\mathrm{C}.$

DS 28.5 Wed 15:00 P1A

2D Extended crystalline films for organic electronics applications — •FABIAN STRELLER, TIM HAWLY, and RAINER FINK — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg

Excelling in applications where large area coverage, low cost and flexibility are limiting factors of device fabrication, organic semiconductors are of high interest as alternative functional layers in modern electronic devices. While well-established preparation methods for organic thin films such as physical vapor deposition (PVD) offer good process control via parameters, such as deposition rate, they suffer from intrinsic limitations, namely the formation of polycrystalline layers, leading to charge trapping at grain boundaries and hence, reduced charge carrier mobilities. Herein, we report on the formation of highly oriented, long range-ordered thin films created in a novel approach via surfactant assisted self-assembly at the liquid-liquid interface.[1] Thin films with thicknesses of only few monolayers crystallized out of solution, utilizing a surfactant-modified water surface as a substrate. Thus prepared film were characterized by microscopic (AFM, SAED) and spectroscopic (NEXAFS, STXM) methods. To further investigate their suitability in organic electronics (OFETs, OLEDs), charge transfer characteristics were measured, exceeding those of reference devices by at least an order of magnitude.

[1] Q. Wang, F. Yang, Y. Zhang, M. Chen, X. Zhang, S. Lei, R. Li, W. Hu J Am Chem Soc. 2018, 140, 5339-5342

DS 28.6 Wed 15:00 P1A

Light element analysis using an external proton beam — •FELIX JUNGE¹, MASAHIRO SAITO^{1,3}, KIM HOLM^{1,2}, FELIPE LIPP BREGOLIN¹, and HANS HOFSÄSS¹ — ¹II. Institute of Physics, Georg-August-Universität Göttingen, 37077 Göttingen, Germany — ²Institut für Physik, 06120 Halle, Germany — ³Toray Research Center Inc., 3-3-7, Sonoyama, Otsu, Shiga 520-0842, Japan

In this work, we describe the new setup for light element depth profiling using a 2.7 MeV external proton beam and helium gas atmospheric pressure conditions. This setup is used to simultaneously perform backscattering spectrometry (BS) and H-H coincidence elastic recoil detection analysis (C-ERDA) in transmission. The beam is extracted through a 170 nm diamond membrane of 1 mm² size. Polyamide and Mylar foils were used as reference samples. In addition, thin titanium layers were deposited on 100 nm to 500 nm thick Si_3N_4 membranes by magnetron sputtering and loaded with hydrogen using an inductively coupled plasma. H concentration profiles were investigated as a function of film preparation and plasma loading conditions. Furthermore, thin amorphous carbon layers with hydrogen content were produced by magnetron sputter deposition and examined with simultaneous BS and C-ERDA measurements. In order to investigate the possibility of detecting all light elements, samples of lithium manganese oxide were examined and the lithium was measured by NRA. The aim of our research is the development of an efficient method for the quantitative analysis and depth profiling of all light elements of a sample.

DS 28.7 Wed 15:00 P1A

GTSAXS measurements on resistively switching strontium titanate thin film structures — •RICHARD VALENTA, KILIAN WILDEN, CHRISTOPH BOEHNKE, and UWE KLEMRADT — 2. Physikalisches Institut, RWTH Aachen, Deutschland

We present an application of a novel variant of small angle x-ray scattering (Granzing incidence transmission small angle x-ray scattering (GTSAXS)) for structural analysis of resistively switching thin oxide films. Resistive Random Access Memory is a promising candidate for novel data storage techniques. Our samples consist of a thin strontium titanate layer sandwiched between a bottom electrode and a structured top electrode. By means of voltage pulses the devices can be switched reversely between different resistive states distinguished by creation and rupture of conductive filaments. Using GTSAXS we were able to detect a strong signal sensitive to the different resistive states which can be related to the shape of the filaments.

DS 28.8 Wed 15:00 P1A

The new Neutron Depth Profiling Instrument N4DP at the FRM2 — •LUKAS WERNER¹, MARKUS TRUNK¹, ROMAN GERNHÄUSER¹, RALPH GILLES², BASTIAN MÄRKISCH¹, and ZSOLT REVAY² — ¹Technische Universität München — ²Heinz Maier-Leibnitz Zentrum

Neutron Depth Profiling (NDP) is a non-destructive nuclear analytical technique. It uses charged particles produced in neutron capture reactions (for example the neutron capture on $^{6}\mathrm{Li}$) to map isotope depth distributions in thin film samples. At the Forschungsneutronenquelle München 2 (FRM2) the new Neutron Depth Profiling instrument N4DP has been set up. The high neutron flux available at the experimental site allows for ex-situ as well as for operando studies of thin film samples (e.g. battery anodes during cycling). We will present the capabilities of the instrument alongside several application examples.

$\mathrm{DS}~28.9 \quad \mathrm{Wed}~15{:}00 \quad \mathrm{P1A}$

Electron beam induced defect formation and evolution in single-layer WSe₂ — •ROBERT LEITER, YUELIANG LI, and UTE KAISER — Electron Microscopy Group of Materials Science, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany

Lattice defects in two-dimensional TMD monolayers, such as tungsten diselenide (WSe₂) can alter the electronic properties of the material [1]. Artificially creating such defects by means of an electron beam may be used to tailor the structure and properties of these monolayers for use in future devices [2].

Here, we use the C_c/C_s - corrected SALVE (Sub Ångström Low Voltage Electron microscopy) instrument to observe the dynamics of the formation and evolution of defects in WSe₂ atom by atom [3]. Single point defects are highly mobile and accumulate fast to more extended defects. With continued electron beam irradiation, inversion domains form, which contain several types of mirror twin boundaries (MTBs), previously reported to possess interesting electrical and magnetic properties. We also observe MTBs that were previously unreported for tungsten diselenide as well as a completely new type of boundary, not reported in any TMD so far. We show that with further increased electron dose, highly defective W-rich regions within the WSe₂ matrix form, paving interesting ways towards device engineering.

[1] Y.-C. Lin et al., Nat. Commun. 6, 6736 (2015)

[2] H.-P. Komsa and A. V. Krasheninnikov, Adv. Electron. Mater. 3, 1600468 (2017)

[3] M. Linck et al., Phys. Rev. Lett. 117, 076101 (2016)

DS 28.10 Wed 15:00 P1A

Electron-beam-stimulated structure evolution of single-layer MoTe₂: From point to extended defects — •JANIS KÖSTER¹, TIBOR LEHNERT¹, MAHDI GHORBANI-ASL², ZHONGBO LEE¹, ARKADY KRASHENINNIKOV², and UTE KAISER¹ — ¹Electron Microscopy Group of Materials Science, University of Ulm, Ulm 89081, Germany — ²Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden 01328, Germany The SALVE instrument is equipped with a Cc/Cs-corrector and operates between 20-80kV at atomic resolution. It enables the investigation of electron-beam-stimulated structural transformations in 2D materials on an atomic level. Here, we report the electron-beam-induced atomby-atom evolution of single Te vacancies and Te divacancies in singlelayer 2H-MoTe₂. At 40kV electron accelerating voltage, defect creation due to elastic interaction can be excluded because of the high mass of Te and Mo, and the observed defects originate from more complex interactions as a combination of inelastic and elastic events. We found different types of tetravacancies and trefoil-like defect structures as well as line defects in zigzag direction. Additionally, electron-beam-driven dynamics of defects were observed and their kinetic pathways were proven with DFT calculations. Our results may allow one-dimensional magnetic quantum systems in single-layer 2H-MoTe₂, by creating locally metallic quantum dots consisting of T' phase.

DS 28.11 Wed 15:00 P1A

Benefits of Ion-beam-assisted Sputtering on Chalcogenides — •KAI SCHEUVENS¹, PETER KERRES¹, and MATTHIAS WUTTIG^{1,2} — ¹I. Physikalisches Institut (IA), RWTH Aachen University — ²JARA-FIT, RWTH Aachen University

Chalcogenide phase change materials (PCM) have been of great interest for research as well as application in fast switching data storages. Our sputter chamber, which is part of an UHV cluster, allows producing high quality textured thin films with a broad range of deposition parameters while keeping the oxygen contamination at a minimum. However, due to the chamber design, the fabrication of dense amorphous layers has been proven difficult. XRR Measurements on amorphous thin films show roughly 10% less density compared to other sputtered films of the same material, hinting at voids in the thin film. The formation of voids can be suppressed by applying additional energy to the film during deposition in the form of an ion beam. The influence of this ion beam assisted deposition (IBAD), specifically in terms of film density and stoichiometry, will be investigated in this study. Samples with varying ion fluxes will be produced and characterized via XRD, XRR, XPS and AFM.

DS 28.12 Wed 15:00 P1A Interface effects in the electronic structure of chalcogenide heterostructures — •PETER KERRES¹, MATTHIAS DÜCK¹, KAI SCHEUVENS¹, and MATTHIAS WUTTIG^{1,2} — ¹1st Institute of Physics "new Materials", RWTH Aachen University, 52066 Aachen, Germany — ²JARA-FIT, RWTH Aachen University, Germany

While thin film devices containing homogenous films of GeSbTe based phase change materials (PCM) have already found their way into applications, heterostructure applications of phase change materials, i.e. chalcogenide superlattices are still topic of ongoing research. In the heterostructures, the focus of study lies in the interface region between the two constituents. In this study, we focus on the GeTe/Sb₂Te₃ Interface and employ X-ray photoelectron spectroscopy (XPS) to find differences in the electronic structure of the heterostructure compared to single films of GeTe, $\mathrm{Sb}_2\mathrm{Te}_3$ and an alloyed GeSbTe compound. Several thin film stacks of textured crystalline films were prepared with heated sputter deposition in an UHV cluster and afterwards transferred to the analysis chamber for in-situ XPS measurements. Angle dependent core level spectroscopy (ARXPS) is employed to extract depth dependent data and attribute parts of the spectra to interface effects. The structure of the thin films is additionally verified with X-ray diffraction (XRD) and reflectometry (XRR) measurements.

DS 28.13 Wed 15:00 P1A

Investigation of in-plane texture of GeTe thin films — MARC POHLMANN¹, MARVIN KAMINSKI¹, ●MARIA HÄSER¹, and MATTHIAS WUTTIG^{1,2} — ¹I. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen Germany — ²JARAFIT Institute Green-IT, RWTH Aachen University and Forschungszentrum Jülich, 52056 Aachen, Germany

Chalcogenide-based Phase Change Materials (PCM) are a prominent candidate for energy efficient memory devices. This material class shows a strong difference in its electrical and optical properties between the amorphous and crystalline state. To understand the crystalline state in thin film devices the preparation of highly textured films for structural characterization is crucial. In this study, Molecular beam epitaxy is employed to grow GeTe thin films on two different Si(111) surfaces: A 7x7 Reconstruction and a R30°- $\sqrt{3} \times \sqrt{3}$ -Sb-termination. Using X-Ray Diffraction methods (Θ -2 Θ -Scans, Reciprocal space maps and Φ -Scans) two very different in-plane textures for the two surfaces

were investigated. Additionally, a simulation of the mismatch between the 7x7 reconstructed Si(111) surface and thin film was performed and compared to the XRD results.

DS 28.14 Wed 15:00 P1A Ultrathin (SrO)₂ buffer layer actuates strain relaxation in La_{0.7}Sr_{0.3}MnO₃/SrTiO₃(100) — •VITALY BRUCHMANN-BAMBERG¹, ALEXANDR BELENCHUK², YURY KHAYDUKOV^{3,4}, VLADIMIR RODDATIS⁵, and VASILY MOSHNYAGA¹ — ¹I. Physik. Inst., G.-A.-Universität Göttingen, Germany — ²IIEN, Academy of Sciences of Moldova, Kishinev, Republic of Moldova — ³Max Planck Institute for Solid State Research, Stuttgart, Germany — ⁴Max Planck Society Outstation at the Heinz Maier-Leibnitz Zentrum, Garching, Germany — ⁵GFZ German Research Centre for Geosciences, Potsdam, Germany

Strain and oxygen octahedral distortions imposed by the substrate play a crucial role in epitaxially grown perovskites, e.g. they strongly affect electrical transport and magnetic properties of the double exchange manganite La_{0.7}Sr_{0.3}MnO₃ (LSMO) films. Instead of changing the substrate, a buffer layer can also be used to structurally decouple the film from the substrate. We report on the in-plane strain relaxation of an LSMO film grown on a (SrO)₂ buffered SrTiO₃(100). The buffer layer manifests itself as the Ruddlesden-Popper defect at the interface which disrupts the integrity of the octahedral network imposed by the epitaxy. Strain relaxation as well as the structural decoupling of perovskites through a rock-salt interface, directly visualized by TEM, significantly improves electric and magnetic properties of LSMO (e.g. the Curie and metal-insulator transition temperatures were increased by 30 K). The financial support from DFG via the SFB 1073 (TP A02) and the FRM II at the MLZ Garching are acknowledged.

DS 28.15 Wed 15:00 P1A Investigation and Deposition of Methylammonium Lead Iodide Thin Films for Perovskite Solar Cell — •Young Un JIN¹, NIELS BENSON², and DORU C. LUPASCU¹ — ¹Institut für Materialwissenschaft, Universität Duisburg-Essen und Center for Nanointegration Duisburg-Essen (CENIDE) — ²Institut für Nanostrukturtechnik, Universität Duisburg-Essen und Center for Nanointegration Duisburg-Essen (CENIDE)

The organic-inorganic lead halide perovskites have been getting the limelight due to their excellent performance in photovoltaic devices which contain charge transport and hole transfer materials. Recently, methylammonium lead iodide (CH3NH3PbI3, MAPI) light harvester has contributed to be recorded in the highest power conversion efficiency, over 23% of perovskite solar cell by NREL. A thin film of MAPI is demonstrated that it has broad light absorption, high carrier mobility and leads to be therefore appropriate to engineering of direct bandgap structure of interlayers in a photovoltaic device expected.

In this study, we focus on a progressive method to deposit a clean MAPI thin film for the surface quality and its material properties to figure out the key how these properties affect charge transport and the relationship with its defect density. On the overall proeprties to understand the fundamental physical properties and their influence we characterize the morphology of the surface and local defect densities in MAPI and investigate how morphological problems are associated with charge mobility and what defects can impact on the electrical and optical features.

DS 28.16 Wed 15:00 P1A

Comparison of surface preparation techniques for topological materials — AI HAMODI¹, T HÖKELEK¹, YASER HAMODI², O. ABDULKAREEM³, •NAMI NAKAMORI⁴, OMAR ISAM², N.BASHEER MAHMOOD⁵, KARAM NAJI⁶, WARD SHEIKO⁷, and ALI JIHAD⁸ — ¹1Hacettepe University, Ankara, Turkey — ²2Minstry of higher education and scientific research, Baghdad, Iraq — ³3 Central Piedmont Community College, Texas, USA — ⁴4Shanghai Institute of Ceramics, China — ⁵5Ministry of education, Baghdad, Iraq — ⁶6Lafargeholcim Company, France — ⁷7Siemens Company, Oman — ⁸8Thermoplastics company GmbH, Germany

The surface state of this type of material are heavily oxide at atmosphere pressure, to avoid the oxidation, grown of capping layer (Te or Se) is necessary directly after fowh of the films in ultra-high vacuum. Surface treatment can be classified in to i) Sputtering and annealing method which is really powerful technique for all type of materials ii) Top boost method, which is work only on some of these Topological material. Here we shows x-ray photoemission (XPS), low energy electron diffraction (LEED) and Angle-resolved photoemission spectroscopy (ARPES) results in detailed that prove our samples getting fresh surface after treatment. Additionally, we did overview surface treatment measurements for non-capped materials.

DS 28.17 Wed 15:00 P1A **Functionalization of Metal Oxid Surfaces with Porphyrins** — •KLAUS GÖTZ^{1,2}, ANNEMARIE PRIHODA^{1,2}, and TOBIAS UNRUH^{1,2} — ¹Lehrstuhl für Kristallographie und Strukturphysik, Universität Erlangen-Nürnberg, Staudtstr. 3, 91058 Erlangen — ²Interdisziplinäres Zentrum für Nanostrukturierte Filme, Universität Erlangen-Nürnberg, Cauerstr. 3, 91058 Erlangen

Porphyrins are widely studied for their use as catalysts and in dye sensitized solar cells. In these systems the porphyrins are bound to metal oxide surfaces as a functionalizing layer.

We study the binding mechanism in the porphyrin - metal oxide interface on TiO_2 and Co_3O_4 . Special emphasis of our work is focused on the exchange process of organic stabilizing molecules with porphyrins.

One method is the combination of small angle x-ray and neutron scattering (SAXS and SANS) experiments. These are well suited to study core/shell systems. X-rays interact mainly with electrons and therefore SAXS yields information about the inorganic core of the nanoparticles. Neutrons on the other hand are very sensitive to hydrogen and therefore SANS is well suited to get information about the organic stabilizer shell.

Additionally, X-ray reflectivity (XRR) measurements can be used to study layered systems on flat substrates. This offers the possibility to study the exchange of oleic acid with porphyrins on TiO_2 Wafers as a test system.

The poster will show the complementary methods, focusing on the XRR measurements.

DS 28.18 Wed 15:00 P1A

 $\begin{array}{l} \label{eq:Miniaturization of patterns formed in graded thin elastic film \\ -- \bullet SUNITA SINGH^1 and JAYATI SARKAR^2 -- ^1 Indian Institute of technology, Delhi, India -- ^2 Indian Institute of technology,$

We study the instability and morphology of a thin incompressible, inhomogeneous elastic soft film, whose shear modulus is exponential function or arbitrary function of film thickness. An LSA (linear stability analysis) has been done to obtain the minimum stress or force required to perturb the top surface of the film. In our study, we obtained the smaller length scale features can be formed at the interface in these anisotropic (non-homogeneous) materials where the anisotropy exists only in the normal direction. The present work constituted the range of length scale of instability is $0.3h < \lambda < 2.96$, lower critical stiffness from LSA and total energy minimization, to look out the evolved morphology with high aspect ratio at the interface of film and contactor. The similar length scale of instability can be obtained using different techniques like patterned substrates and bilayers where it was possible to decrease the length scale by about an order of magnitude than those formed in simple elastic thin films because of antagonistic energies (elastic and interaction) present. These techniques are also cost-effective than the existing techniques of lithography suitable for hard materials. The LSA gives a 4th order ordinary differential equation, which cannot be solved analytically, so we discretized it using finite difference method with 2nd order accuracy throughout the process. The studies involved numerical techniques for energy minimization, and also finite element schemes to tackle non-linearities.