

DS 11: Thin Film Properties: Structure, Morphology and Composition (XRD, TEM, XPS, SIMS, RBS, AFM, ...): Session II

Time: Tuesday 9:30–13:15

Location: H 0111

DS 11.1 Tue 9:30 H 0111

Ni:SrTiO₃ thin films — ●FATIMA ALARAB^{1,2}, ROSTISLAV MEDLIN², LUCIE PRUSAKOVA², PAVOL SUTTA², LAURENT NICOLAI², CHRISTINE RICHTER¹, KAROL HRICOVINI¹, and JAN MINAR² — ¹University of Cergy-Pontoise, Paris, France — ²University of West-Bohemia, New technologies research centre, Plzen, Czech Republic

Strontium titanate (SrTiO₃, STO) is a bulk insulator with a band gap of 3.2 eV in its cubic phase at room temperature. Specific properties of pure STO like very large dielectric constant and high resistivity make it an interesting material for different applications in microelectronics, optics and in advanced ceramics. By doping with transition metals or oxygen vacancies, STO becomes electrically conductive and the band gap width is modified. Here we report the fabrication, structure and electronic properties of Nickel doped STO (Ni:STO) thin films. The films with different Ni concentrations were prepared by reactive co-sputtering in reactive magnetron units using pure STO and Ni targets. X-ray diffraction, TEM, EELS and XPS techniques were used to characterize the effect of Ni concentration in STO on crystallinity and electronic properties as compared to pure STO. We performed as well calculation of the band structure using SPR-KKR package.

DS 11.2 Tue 9:45 H 0111

Experimental and computational analysis of grain growth in ultrafine-grained thin films — ●AHU ÖNCÜ¹, THORSTEN HALLE², and DANA ZÖLLNER³ — ¹Institute of Experimental Physics, Otto-von-Guericke University Magdeburg, Germany — ²Institute of Materials and Joining Technology, Otto-von-Guericke University Magdeburg, Germany — ³B CUBE Center for Molecular Bioengineering, Technische Universität Dresden, Germany

Grain microstructures of polycrystalline solids have an immense impact on materials properties. While investigations of bulk materials it is generally assumed that surfaces or interfaces are negligible. For thin films, surface effects are very important. If during grain growth in such films the average grain size reaches the order of the layer thickness, grain growth slows down or even comes to a halt. Analytic theories of nano- and microcrystalline grain growth of thin films are often in good agreement with numerical results using computer simulations, analytic size distributions or topological correlations between grains rarely capture the experimental features. One reason for this disagreement can be found in the simple fact that the experimental samples are of 3D nature, but are commonly measured in 2D and compared to 2D simulations. In the present work, we analyze the grain microstructures of ultrafine-grained thin metallic films experimentally and compare the results to 3D computer simulations.

DS 11.3 Tue 10:00 H 0111

Structural and magnetic properties of FePt-Tb alloy thin films — ●NATALIJA SAFONOVA and MANFRED ALBRECHT — Experimental physics IV, Institute of Physics, University of Augsburg, D-86159, Augsburg

Magnetic materials designed for ultrafast all-optical switching of magnetization are of high interest from a fundamental as well as technological point of view [1, 2]. In this study, two series of (FePt)(1-x)Tb(x) ternary alloy thin films with a thickness of about 10 nm were sputter deposited on MgO(100) substrates at 530°C (series I) and 700-770°C (series II). The Tb content x was varied in the range 5 - 28 at.%. Series I reveal limited L10 chemical ordering with an in-plane easy axis at room temperature. By addition of Tb higher than 11 at.%, a loss in crystallinity was observed. It is suggested that Tb is located as an interstitial atom to the FePt lattice, adding elastic stress to the lattice, eventually leading to amorphization of the local Tb environment. At low temperatures a spin reorientation transition (SRT), indicated by the appearance of strong perpendicular magnetic anisotropy (PMA), was observed. The SRT temperature increases linearly with addition of Tb. Higher deposition temperatures of 700-770 °C (series II) promote L10 chemical ordering with (001) orientation and strong PMA of 1.2 MJ/m³ at 300 K. However, with addition of Tb up to 6 at.%, PMA as well as coercivity get strongly reduced.

[1] A. Kirilyuk et al., Rev. Mod. Phys. 82, 2731 (2010).

[2] A. Hassdenteufel et al., Phys. Rev. B 91, 104431 (2015).

DS 11.4 Tue 10:15 H 0111

Structural analysis of epitaxial Ba₂SiO₄ thin films grown on Si(100) — ●JULIAN KOCH and HERBERT PFNÜR — Leibniz Universität Hannover, Inst. für Festkörperphysik, Appelstr. 2, 30167 Hannover

Ba₂SiO₄ is a very promising candidate as a high-k dielectric. Epitaxial films grown in a previous study [1] have shown a dielectric constant of 22.8 ± 0.2 , band offsets to p-Si(100) of over 2 eV, a high temperature stability up to desorption at around 750 °C and an acceptable leakage current of 3 mA/cm² at -1 V. Unfortunately, these films still feature a high density of interface traps. The primary cause of this is most likely the growth mode of the silicate films, which were produced by heating the Si(100) substrate during the growth of a BaO film, so that a diffusion of Si from the substrate to the film occurred turning the BaO into Ba₂SiO₄. This process resulted in an atomically rough interface in a geometric and possibly also in a chemical sense. Moreover, only the first 5 nm close to the interface turned out to be crystalline.

This study aims to improve the structural quality of the Ba₂SiO₄ films by employing a co-deposition growth method, in which Ba and Si are evaporated simultaneously in an oxygen atmosphere. This eliminates the need for the Si diffusion. The chemical composition and the crystallinity of the films are investigated using XPS and SPA-LEED, respectively. To further investigate the crystalline growth, crystal orientation and thickness HRTEM is used.

DS 11.5 Tue 10:30 H 0111

Ionic and Ferroelectric Behavior of SbSI Films — ●SARA SAND, KA KAN WONG, SUSANNE T. BIRKHOFF, EUGEN ZIMMERMAN, and LUKAS SCHMIDT-MENDE — University Konstanz, Konstanz, Germany

Thin film solar cells display many benefits due to their solution-based processing, allowing for inexpensive manufacturing and the possibility of devices on flexible substrates. Recently, perovskite solar cells have dominated this area of research due to their rapidly increasing efficiency, but this material still has many drawbacks due to its toxicity and lack of durability. Antimony sulfide (SbSI) has been identified as a promising material for these applications, because it is much more stable and is similarly defect tolerant. It also has ferroelectric behavior with phase transition around room-temperature and its ionic characteristics. These two properties have been largely discussed in reference to perovskites, but, as of yet, their role in solar cell function is not well understood. The aim of this study is to investigate the ferroelectric and ionic characteristics of SbSI and their impact on solar cell devices. However, SbSI solar cells have not yet been reported in literature, as typical SbSI films possess very uneven surface structures composed of large crystallites. Here we present a novel approach to control the film formation of SbSI. By performing the two-step conversion process of SbSI under elevated pressure within a hot press, even and dense films of SbSI are achieved. Application of these films into devices will allow us to compare ferroelectric and ionic properties of perovskite and SbSI solar cells.

DS 11.6 Tue 10:45 H 0111

Orientation-dependent chemistry and band-bending of Ti thin layers on polar ZnO surfaces — ●PATRIZIA BORGHETTI¹, YOUNES MOUCHAAL^{1,2}, ZONGBEI DAI¹, GREGORY CABAILH¹, RÉMI LAZZARI¹, and JACQUES JUPILLE¹ — ¹Sorbonne Universités, Institut des NanoSciences de Paris, F-75005, Paris, France. — ²Laboratoire de Physique des Couches Minces et Matériaux pour l'Electronique (LPCMME), Université d'Oran 1 31000, Oran, Algeria

Next to its use to create ohmic contacts, the deposition of titanium on ZnO is known to promote adhesion for noble metals in optical coatings for glazings, to enhance the gas sensor properties of ZnO and to set up resistive random access memories. However the detailed mechanism of interface reactivity and the role of the surface orientation of ZnO in terms of species profile and chemical state are not yet resolved. In the present work, orientation-dependent reactivity and band-bending are evidenced by X-ray photoemission spectroscopy upon Ti deposition (1-10 Å) on the polar ZnO(0001)-Zn and ZnO(000-1)-O surfaces [1]. On Zn-ZnO, Ti reduces ZnO to form a Ti oxide, while on O-ZnO, the deposition of Ti gives rise to the formation of a (Ti, Zn, O) compound. A similar chemistry is observed upon annealing the Ti adlayers, although

with very different activation temperatures, 500 K on O-ZnO and 700 K on Zn-ZnO. Those orientation-dependent behaviours are expected to strongly affect applications relying either on thin Ti/ZnO films and partly explain why Ti/ZnO electrical contact properties are quite scattered and depend on annealing treatments and crystal orientation.

[1] P. Borghetti et al., Phys. Chem. Chem. Phys., 2017, 19, 10350.

DS 11.7 Tue 11:00 H 0111

Vertically aligned metal-ceramic nanocomposites: Self-assembly of ultrathin metallic nanowires embedded in oxide matrices — ●MARCEL HENNES¹, XIAORONG WENG¹, DOMINIQUE DEMAILLE¹, SARAH HIDKI¹, EMILIANO FONDA², YUNLIN ZHENG¹, and FRANCK VIDAL¹ — ¹INSP, UPMC Sorbonne Universités, CNRS UMR 7588, 4 place Jussieu, 75005 Paris, France — ²Synchrotron SOLEIL, 91192 Gif-sur-Yvette, France

Vertically aligned metal-ceramic thin films constitute a novel class of hybrid materials characterized by the presence of metallic nanopillars embedded in a planar oxide matrix. For the development of these nanocomposites, pulsed laser deposition (PLD) synthesis relying on self-organized growth has recently emerged as a novel technique, complementing conventional template-assisted methods. On the one hand, self-assembly based procedures avoid cumbersome intermediate steps and permit to create arrays of ultrathin nanowires ($d < 5$ nm) with extremely high densities ($\rho > 10^{11}/\text{cm}^2$). On the other hand, the metallic and oxide phases exhibit vertical epitaxial coupling, which paves the way for strain engineering and synthesis of artificial multiferroics. In the present contribution, we present results on magnetic nanocomposites and put special emphasis on the possibility to grow alloy wires ($\text{Co}_x\text{Ni}_{1-x}$ and $\text{Co}_x\text{Pt}_{1-x}$), a simple and efficient strategy to control the magnetic anisotropy of the system. We also address remaining hurdles that have to be overcome to achieve full control of the final thin film nanoarchitecture.

15 min. break.

DS 11.8 Tue 11:30 H 0111

Growth of organic thin films on modified TiO₂(110) surfaces — ●KONRAD SZAJNA¹, MARKUS KRATZER², DOMINIK WRANA¹, WOJCIECH BELZA¹, BENEDYKT JANY¹, JACOB GENSER², FRANCISZEK KROK¹, and CHRISTIAN TEICHERT² — ¹Marian Smoluchowski Institute of Physics, Jagiellonian University, Krakow 30-348, Poland — ²Institute of Physics, Montanuniversität Leoben, Franz Josef Straße 18, 8700 Leoben, Austria

The detailed growth morphology of vapor deposited para-hexaphenyl (6P) as model system of small organic molecules on modified TiO₂(110) surfaces has been investigated by means of scanning probe microscopy. As substrates, atomically flat, air passivated and rippled ion beam modified TiO₂(110) surfaces have been used. On pristine TiO₂(110) crystalline needles consisting of flat lying 6P molecules are formed which extend along the [1-10] substrate direction. In contrast, on air exposed and ion beam modified surfaces island growth with an upright standing molecular configuration is favored. [1,2,3] The mechanisms that trigger the transition from flat lying to upright standing structures are discussed. Further the change in the stability of the 6P structures due to ion beam induced substrate rippling was tested by atomic force microscopy and is discussed.[3]

[1] M. Kratzer et al. PCCP 16, 26112 (2014)

[2] D. Wrana et al. JPCC 119, 17004 (2015)

[3] K. Szajna et al. JCP 145, 144703 (2016)

DS 11.9 Tue 11:45 H 0111

Hafnium oxide interface formation during ALD oxide growth on pure Hf films for resistive switches — ●STEPHAN AUSSSEN, ALEXANDER HARDTDEGEN, THOMAS HEISIG, CHRISTOPH BÄUMER, REGINA DITTMANN, and SUSANNE HOFFMANN-EIFERT — Peter Grünberg Institut and JARA-FIT, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

Oxygen exchange and drift/diffusion processes play a major role in redox-based resistive switching random access memories. Therefore, understanding oxidation/reduction reactions taking place already during the growth process is of utmost importance. In this study we investigate the oxidation behavior of pure Hf during atomic layer deposition (ALD) of stoichiometric oxide films (M'O) as Al₂O₃, TiO₂ and HfO₂ and the switching behavior of the resulting stacks. 25 nm thick sputtered Hf films with a low surface roughness < 0.2 nm were transferred under ultra-high vacuum conditions into an ALD system. Oxide lay-

ers were deposited at temperatures between 160 °C and 280 °C from amino-based precursor and O₂-plasma. The resulting stacks were investigated by angle resolved X-ray photoelectron spectroscopy to determine the thickness of the formed interfacial HfO_x layer as well as the valence states of the involved metal cations. The effect of the different ALD processes, e.g. Al₂O₃ as passivation layer, and influence of the temperature on Hf oxidation are discussed. In addition, complementary resistive switching experiments performed on equivalent stacks, i.e. Pt/M'O/HfO_x/Hf, revealed influence of the HfO_x interface formation on the switching behavior.

DS 11.10 Tue 12:00 H 0111

Epitaxial Ag thin films grown on biaxially textured IBAD-MgO template layers — ●SEBNEM YAZICI¹ and MATTHIAS WUTTIG² — ¹I. Physikalisches Institute, RWTH Aachen, Germany — ²I. Physikalisches Institute, RWTH Aachen, Germany

The heteroepitaxial growth of thin metal films on ceramic substrates is of great scientific and industrial interest, due to their applications in electronic interconnects as well as catalysis and optical coating applications. Therefore, it is very important to examine the growth mechanism of the metal layer including wetting behavior to control crystalline properties and to determine the grain orientations as well as strain relaxations and electron transport mechanisms.

Biaxially ordered films produced by ion beam assisted deposition (IBAD) provides good templates for the heteroepitaxial growth of the functional layers. MgO is a very promising template layer for epitaxial Ag thin film growth since MgO can be deposited with rapid biaxial texture formation via IBAD technique. Besides, very similar in-plane lattice constants of Ag(100) and MgO(100), results in 4-fold symmetric cube-on-cube epitaxy. In this work, Ag thin films were deposited via magnetron sputtering on IBAD-MgO layers in order to study epitaxial relationship and electron transport mechanism of very thin Ag films. Biaxial texture formation in MgO layer depending on MgO layer thickness was investigated. Additionally, effects of post deposition annealing on Ag films grown on IBAD MgO films were analysed regarding crystallinity-texture improvement, stress relaxation and surface roughness via high resolution X-ray diffraction and AFM, respectively.

DS 11.11 Tue 12:15 H 0111

Influences of growth kinetics on interface structure and magnetism in La_{1/3}Sr_{2/3}FeO₃/La_{2/3}Sr_{1/3}MnO₃ heterostructures — ●MARKUS WASCHK¹, JÖRG VOIGT¹, PAUL ZAKALEK¹, JURI BARTHEL², and THOMAS BRÜCKEL¹ — ¹Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS-2) and Peter Grünberg Institut (PGI-4), JARA-FIT, 52425 Jülich, Germany — ²Forschungszentrum Jülich GmbH, Ernst Ruska-Centre for Microscopy with Electrons (ER-C-2), 52425 Jülich, Germany

Transition metal oxide heterostructures like La_{1/3}Sr_{2/3}FeO₃/La_{2/3}Sr_{1/3}MnO₃ (LSFO/LSMO) has been chosen as a model system to study the interfacial coupling between an antiferromagnet (LSFO) and a ferromagnet with regard to different growth kinetics. Two epitaxial heterostructures (LSFO/LSMO and LSMO/LSFO) were grown with a combination of oxide molecular beam epitaxy and high oxygen sputtering on (001)-oriented SrTiO₃ substrates. Subsequent structural analysis with e.g. scanning transmission electron microscopy and energy dispersive X-ray spectroscopy revealed that the interface morphology depends crucially on the growth order. The interface in LSMO/LSFO is dominated by iron interdiffusion from the LSFO into the LSMO layer in at least nine monolayers, where Fe occupies the Mn sites. This leads to significant changes of the magnetic properties within the interface region. In contrast, LSFO/LSMO exhibits a sharp interface. Polarized neutron reflectometry was used to investigate the magnetization profile of both samples and revealed a highly reduced magnetization at the interface for the case of interdiffusion.

DS 11.12 Tue 12:30 H 0111

Room temperature atomic layer deposition for perovskite solar cells — ●MALGORZATA KOT¹, LUKAS KEGELMANN², PETER KUS³, NATALIYA TSUD³, IVA MATOLINOVA³, STEVE ALBRECHT², VLADIMIR MATOLIN³, and DIETER SCHMEISSER¹ — ¹BTU Cottbus-Senftenberg, Konrad-Wachsmann-Allee 17, 03046 Cottbus — ²Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium-Photovoltaik, Kekuléstraße 5, 12489 Berlin, Germany — ³Department of Surface and Plasma Science, Charles University, Prague, 18000, Czech Republic

After few years of efficiency driven research on perovskite solar cells, the focus now is shifting to understand the underlying processes gov-

erning the high efficiency and also to obtain long-term stable devices. Among various deposition methods, atomic layer deposition (ALD) may represent one of the best options, being possible to coat substrates in a very efficient way and at very low temperatures. In our previous work [1] we reported that the efficiency of the solar cell containing aged perovskite film can be enhanced twice while covering the perovskite with a thin ALD alumina film at room temperature. In this work, the chemical, electronic and morphological properties of the fresh perovskite film treated by ALD pulses of the trimethylaluminium and water at room temperature investigated using X-ray Photoelectron Spectroscopy and Field Emission Scanning Electron Microscopy will be discussed and correlated with the solar cells performance and stability.

[1] M. Kot et al., ChemSusChem 2016, 9, 3401.

DS 11.13 Tue 12:45 H 0111

Fabrication and structural characterization of diamond coated tungsten tips — •ALEXANDER TAFEL¹, MINGJIAN WU², ERDMANN SPIEKER², PETER HOMMELHOFF¹, and JÜRGEN RISTEIN¹ — ¹Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen — ²Department Material Science, Institute of Micro- and Nanostructure Research Center for Nanoanalysis and Electron Microscopy (CENEM), Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen

Coating metal nanotips with a negative electron affinity material like hydrogen terminated diamond promises a high brightness photocathode. Dip seeding in detonation diamond suspensions in combination with nitrogen flow towards the tip apex and subsequent plasma enhanced chemical vapor deposition results in thin and dense diamond films along the tip from shaft to apex. The seeding density can even be controlled locally by the nitrogen flow, which counteracts forces occurring during solvent evaporation. With this technique a homogeneous coating of a complete tip with a dense and 100 nm thin diamond film as well as a selective coating of the tip apex only with 20 nm thin di-

amond were achieved. (HR)TEM and electron diffraction reveal that columnar nanocrystalline diamond with $\langle 110 \rangle$ texture and graphitic tissue between the grains was grown on the tungsten tip. An average of 17 % sp^2 -bonded carbon is estimated from the fine structure of the C(1s) electron energy loss spectrum.

DS 11.14 Tue 13:00 H 0111

Formation and thermal stability of co-evaporated lead halide perovskite thin films (ABX_3 , A=MA,Cs; B=Pb; X=I,Br,Cl) analysed by in situ XRD — •PAUL PISTOR, THOMAS BURWIG, CARLO BRZUSKA, RENE CSUK, WOLFGANG FRÄNZEL, and ROLAND SCHEER — Martin-Luther-Universität Halle-Wittenberg, Halle(Saale), Deutschland

Methyl ammonium (MA) lead halide perovskites (e.g. MAPbI₃) are widely used to prepare efficient solar cells. In our group we have built a co-evaporation chamber equipped with a dedicated X-ray diffractometer, which allows us to study the formation and evolution of the different phases during thin film growth and under thermal stress. In this contribution, we show our investigation of the formation of single halide MAPbI₃, MAPbBr₃ and MAPbCl₃ thin films and their thermal decomposition into lead halides at temperatures between 150°C -250°C. Furthermore, the miscibility of MAPbI₃ and MAPbBr₃ is analyzed in detail. We find a preference for phase segregation if the formation is induced with PbBr₂ precursors, in contrast to the case where PbI₂ is used.

Then, MAPbX₃ is compared to its inorganic CsPbX₃ counterparts, where e.g. a stable cubic perovskite structure is easily obtained for CsPbBr₃, while for CsPbI₃ two polymorphs with cubic and orthorhombic crystal structure are observed at room temperature. Finally, we find that the inorganic CsPbX₃ thin films are thermally more stable and decompose at much higher temperatures (>300°C) through the evaporation of the PbX₂, leaving behind the corresponding cesium halide.