DS 3: Thin Film Characterisation: Structure Analysis and Composition I

Time: Monday 9:30–13:00 Location: CHE 91

DS 3.1 Mon 9:30 CHE 91

Ti valence mapping in LAO/STO with resonant soft X-ray reflectometry — •Martin Zwiebler[1], Emiliano Di Gennaro[2], Jorge Enrique Hamann-Borrero[1], Fabio Miletto Granozio[2], Enrico Schierle[3], Eugen Weschke[3], Bernd Büchner[3], George Sawatzky[4], Robert Green[4], and Jochen Geck[5] — [1]IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — [2]CNR-SPIN and Dipartimento di Finica, Complesso Universitario di Monte S. Angelo, Via Cintia, 80126 Naples, Italy — [3]Helmholtz-Zentrum Berlin, BESSY, Albert-Einstein-Str. 15, 12489 Berlin, Germany — [4]University of British Columbia 6224 Agricultural Road Vancouver, B.C. V6T 1Z1 Canada — [5]Institut fuer Strukturphysik Technische Universität Dresden, 01062 Dresden, Germany

The two dimensional electron gas (2DEG) at the LaAlO3/SrTiO3 heterointerface exhibits intriguing features, which are currently not well understood. When at least four UCs of LAO are deposited on a STO substrate, mobile electrons accumulate at interfacial Ti sites. In order to establish the underlying physics, it is essential to know the charge density distribution of the 2DEG around the interface. Exactly this point, however, remained highly controversial so far. In order to clarify this issue, we performed X-ray reflectivity measurements at the Ti $L_{2,3}$ edge to determine the Ti stoichiometry and the depth-dependent electron content at the interface with resolution at the atomic scale. We demonstrate that the electron distribution is strongly T-dependent. From the polarization dependence of the reflectivity we gain new results on the anisotropy of orbital energies and electron density.

DS 3.2 Mon 9:45 CHE 91

XPD experiments and simulation of GaAs(001)-c(8x2) — •Karim Shamout[1,2], Philipp Espeter[1,2], Peter Roese[1,2], Ulf Berges[1,2], and Carsten Westphal[1,2] — [1]Experimentelle Physik I - Technische Universität Dortmund, Otto-Hahn-Str. 4a, D-44221 Dortmund — [2]DELTA - Technische Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D-44221 Dortmund

The III-V compound semiconductor gallium arsenide is an applicable substrate for spin-tronic multilayer systems due to its electronical and magnetic properties. GaAs(001) is found in various reconstructions determined by the Ga-As ratio in the top atom surface layer. In this work, we analyse of the GaAs surface reconstructions, and here especially the GaAs(001)-c(8x2) structure where huge uncertainties arise. Photoelectron diffraction (XPD) provides detailed information of the surface and interface of the sample. Thereby Ga or As dimers located 5 Å beneath the surface can be resolved. In literature, 8 different possible structures of the GaAs-c(8x2) surface have been shown. These structures differ by the number of Ga dimers, the sub-dimers or the arrangement of Ga-As rings. Here we present the experimental data of the GaAs-c(8x2) surface measured with XPD at the U55 beamline 11 at DELTA. For each possible structure an XPD pattern has been simulated and compared to the experimental data. As a result, the structure suggested by Kumpf et al. fits best to the data. Further, the precise location of the Ga-dimers is found. Moreover, we analyse the interface of Co/GaAs(001)-c(8x2) and investigate on the stability of the GaAs reconstruction beneath Co.

DS 3.3 Mon 10:00 CHE 91

ARXPS study of the growth behaviour of ultrathin ionic liquid layers on metal surfaces — •Matthias Lexow, Benjamin May, Florian Maier, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

Ionic liquids (IL) are ionic compounds with a relatively low melting point, often even below room temperature. In addition to numerous applications as a solvent or electrolyte, the extremely low vapour pressure of ILs also led to the development of completely new concepts for catalytically active systems. Thin layers of ILs on solid materials are applied e.g. in SCILL (Solid Catalyst with Ionic Liquid Layer) catalysis.

In this context, the structure and composition of the IL/solid interface is studied by our group with angle-resolved X-ray photoelectron spectroscopy (ARXPS). Recently it was shown that by deposition of sub-monolayer amounts of Pd on single-crystalline Au(111) the growth mode of ILs can be switched from three-dimensional to two-dimensional growth, i.e. from non-wetting to wetting behaviour.

Aiming to understand the behaviour of applied catalyst systems containing Ag and Pd, the ARXPS studies are extended to the Ag(111) surface. The results offer possible explanations for the beneficial influence of the IL layer on heterogeneous metal alloy catalysts.

M.L., B.M and H.P.S. thank the European Research Council (ERC) for financial support of this research in the context of an Advanced Investigator Grant to H.P.S.!

DS 3.4 Mon 10:15 CHE 91

Multiparamter Characterization of Subnanometre Cr/Sc Multilayers Based on Complementart Measurements — •Anton Haase[1], Saša Bajt[2], Philipp Hönicke[1], Victor Soltwisch[1], and Frank Scholze[1] — [1]Physikalisch-Technische Bundesanstalt (PTB), Abbestr. 2-12, 10587 Berlin, Germany — [2]Photon Science, DESY, Notkestr, 85, 22607 Hamburg, Germany

Cr/Sc multilayer systems can be used as near-normal incidence mirrors for the water window spectral range. It is shown that a detailed characterization of these multilayer systems with 400 bilayers of Cr and Sc, each with individual layer thicknesses below < 1 nm, is attainable by the combination of several analytical techniques. We used EUV and X-ray reflectance measurements, resonant EUV reflectance across the Sc L edge, as well as X-ray standing wave fluorescence measurements. The parameters of our multilayer model were determined based on a particle swarm optimizer and validated using a Markov-chain Monte Carlo maximum likelihood approach. For the determination of the interface roughness, diffuse scattering measurements were conducted.

DS 3.5 Mon 10:30 CHE 91

3D-Analysis of fine-grained metallic thin films. — •Ahu Öncü[1], Thomas Hempel[1], Bodo Kalkofen[2], Thorsten Halle[3], and Dana Zöllner[1] — [1]Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg — [2]Institute of Micro and Sensor Systems, Otto-von-Guericke-University Magdeburg — [3]Institute of Materials and Joining Technology, Otto-von-Guericke-University Magdeburg

Fine-grained thin films play an important role in many technical applications. It is also known that grain microstructures of polycrystalline metals and alloys have an immense impact on materials properties. That is why it is important to understand the processes of grain growth not just as surface effects, but also as mechanisms in the entire layer like in bulk materials.

Commonly, thin layers are measured in 2D and compared with 2D simulations and analytic theories. However, two-demensional analytic size distributions or topological correlations between grains rarely capture the experimental features. One reason of this disagreement can be found in the simple fact that the experimental samples are of 3D nature. In the present work, we analyze the grain microstructures of thin aluminum films experimentally and compare the results to 3D computer simulations.

DS 3.6 Mon 10:45 CHE 91

Synchrotron radiation damage on Copper Naphthalocyanine layers — •Peter Roese[1,2], Philipp Espeter[1,2], Karim Shamout[1,2], Ulf Berges[1,2], and Carsten Westphal[1,2] — [1]Experimentelle Physik I - Technische Universität Dortmund, Otto-Hahn-Str. 4a, D-44221 Dortmund — [2]DELTA - Technische Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D-44221 Dortmund

The organic semiconductor naphthalocyanine includes a delocalized π-electronic system. The fascinating properties of naphthalocyanine are based on the delocalized π-electronic system. For applications the molecule is being studied as a perspective candidate for organic solar cells, organic LED's and molecular switches. Furthermore, using naphthalocyanines as a photosensibilisator in cancer treatment utilizes the strong absorption properties in the visible spectrum. Here, we present the investigation of synchrotron radiation damage on copper- and free-base naphthalocyanine layers (CoNc, H2Nc) on an Ag(110) surface using x-ray photoelectron spectroscopy (XPS) at the U55 beamline 11 at DELTA. In this study we report on synchrotron radiation damage induced changes at the nitrogen bonds while no changes at the C 1s signals occur. Furthermore, the reduction of the photon density by moving the experimental chamber out of focus reduced radiation

damage significantly. Now, it was possible to perform photoelectron diffraction (XPD) measurements with these systems.

DS 3.7 Mon 11:00 CHE 91

Real time investigation of optical properties and morphology during the co-sputter deposition of Au/Ag nanoparticles — •Deniza Chekrygina[1], Matthias Schwartzkopf[2], André Rothkirch[2], Ivan Baev[1], Pallavi Pandit[2], Marc Gensch[1], Calvin Brett[1,2], Wiebke Ohm[2], Bjoern Beyersdorff[2], Jan Rubeck[2], Stephan Roth[2,3], Wilfried Wurth[1], and Michael Martins[1] — [1]UHH, Luruper Chaussee 149, D-22761 Hamburg — [2]DESY, Notkestr. 85, D-22607 Hamburg — [3]KTH, Teknikringen 56-58, SE-100 44 Stockholm

Binary alloys and multicomponent metallic thin films containing one or more noble metals are of great interest now due to their possible applications as catalysts, sensors and photonic devices. We concentrated in our work on investigation of the binary alloy system of Au/Ag, which is considered to be very promising in the field of nonlinear optical materials [1]. In this work, we present the results of in situ Grazing Incidence Small-Angle X-ray scattering (GISAXS) and UV/Vis spectroscopy for the simultaneous radio-frequence (r.f) co-sputtering process from two metallic targets with different ratio and geometry of deposition. Post-sputtering growth characterization for the set of samples was made using Atomic Force Microscopy (AFM), GISAXS, Grazing Incidence Wide-Angle X-ray scattering (GIWAXS) and X-ray emission spectroscopy (XES). We will present comparison of the physical and structural properties depending on the ratio of the metal in bialloys and the geometry of the deposition. [1] Faupel et al., Adv. Eng. Mater. 12, 1177 (2010).

15 min. break.

DS 3.8 Mon 11:30 CHE 91

Reactive ion beam sputter deposition of TiO2: Influence of deposition parameters on thin film properties — •Thomas Lautenschläger, Daniel Spemann, Annemarie Finzel, Erik Thelander, Micheal Mensing, Frank Frost, and Carsten Bundesmann — Leibniz-Institut für Oberflächenmodifizierung, Permoserstraße 15, 04318 Leipzig, Germany

In physical vapor deposition (PVD), the properties of film forming particles strongly influence the growth process. Ion beam sputter deposition (IBSD) is a versatile PVD technique, as it offers several possibilities to alter the properties of the film forming particles. Reactive IBSD was used to deposit TiO2 thin films. The influence of sputtering geometry, ion energy, and ion species on thin film characteristics was investigated. The growth rate shows an over-cosine angular distribution, tilted in forward direction, and was found to increase with increasing ion energy and incidence angle. This behavior is in good agreement with the well-known dependence of the sputtering yield. The deposited films were amorphous, stoichiometric, and contained a considerable amount of primary particles. The concentration of inert gas was found to depend mainly on sputtering geometry and ion species. Surface roughness was well below 1 nm and depends mainly on sputtering geometry. Similarly, the refractive index changes systematically with the scattering geometry. These changes are strongly correlated with systematic variations in the mass density. The observations are assigned to variations of the angular and energy distribution of the sputtered target particles and the backscattered primary particles.

DS 3.9 Mon 11:45 CHE 91

Properties of SiO2 films grown by ion beam sputter deposition — •Maria Mateev, Thomas Lautenschläger, Daniel Spemann, Annemarie Finzel, Michael Mensing, Frank Frost, and Carsten Bundesmann — Leibniz-Institut für Oberflächenmodifizierung, Permoserstraße 15, 04318 Leipzig, GER

Ion beam sputter deposition (IBSD) is an established physical vapor deposition technique that provides several possibilities to study the influence of certain process parameters on the film properties. Sputtering of a Si target in a reactive oxygen atmosphere using Ar and Xe as primary ions was used to grow SiO_2 films on silicon substrates. The sputtering geometry, ion energy and ion species were varied systematically and their influence on the sputtering yield and film properties was investigated. Thickness, index of refraction, composition, mass density, and surface roughness were determined with the help of ellipsometry, Rutherford backscattering spectrometry, X-ray reflectometry and atomic force microscopy, respectively. The SiO_2 growth rate increases with increasing ion energy and incidence angle between ion beam and target normal. Furthermore, thickness, index of refraction, stoichiometry, mass density and surface roughness show a strong correlation with the sputtering geometry. The ion species also has an impact on the film properties, the influence of the ion energy is rather small. A considerable amount of primary inert gas particles is found in the deposited films.

DS 3.10 Mon 12:00 CHE 91

Magneto-optical polarization spectroscopy on graphene-metal interfaces in the soft-x-ray regime — •Christine Jansing[1], Hans-Christoph Mertins[1], Markus Gilbert[1], Maxim Krivenkov[2], Andrei Varykhalov[2], Oliver Rader[2], Andreas Gaupp[2], Andrey Sokolov[2], Hud Wahab[3], Heiko Timmers[3], Dominik Legut[4], and Peter M. Oppeneer[5] — [1]Münster University of Applied Sciences, Stegerwaldstr. 39, D-48565 Steinfurt — [2]HZB, Albert Einstein Str. 15, D-12489 Berlin — [3]Uni. of New South Wales, Canberra, ACT 2600, Australia — [4]IT4Innovations Center, VSB-Technical University of Ostrava, CZ-708 33 Ostrava, Czech Republic — [5]Dept. of Physics and Astronomy, Uppsala University, Sweden

We present magneto-optical polarization and x-ray natural linear dichroism measurements [1] at the C 1s edge of graphene on metallic substrates. Graphene-metal interfaces show a strong hybridization between graphene π-states and 3d-states of the metallic substrate. Intercalation of gold in the graphene/Ni system leads to a change in the orientation and strength of this bonding which is deduced quantitatively. Additionally we observe a shift of the conduction bands (CB) at the Dirac point while the CB at the M-point is not affected. Furthermore the XMCD as well as T-MOKE of graphene/Ni is presented, which allows for the determination of the spin split density of states of the CB and the determination of the magnetic moment of magnetized graphene showing that magnetism in graphene is carried by the π-orbitals. [1] C. Jansing, H.-Ch. Mertins et al., Phys. Rev. B 94, 045422 (2016)

DS 3.11 Mon 12:15 CHE 91

Insights into epitaxial growth of thin film samples of the ferromagnetic shape memory alloy Fe_7Pd_3 — •Alina J. Bischoff[1], Kenneth Hua[1], and Stefan G. Mayr[1,2] — [1]Leibniz-Institut für Oberflächenmodifizierung, Leipzig — [2]Abteilung Oberflächenphysik, Fakultät für Physik und Geowissenschaften, Universität Leipzig

Single crystalline-like thin film Fe_7Pd_3 samples allow to study the physics of this promising ferromagnetic shape memory alloy. We demonstrate how to prepare such samples using electron beam evaporation and investigate the impact of variable deposition parameters such as growth temperature and deposition interruptions. We are able to epitaxially grow 500 nm thin Fe_7Pd_3 samples in austenitic and martensitic phases and the latter with visible surface twinning structures. Ideal growth conditions are given around 700 °C because deposition at temperatures below 690 °C results in demixing of samples while film quality is reduced at higher temperatures due to lattice misfit effects. Our investigations enabled us to identify a deposition procedure, which is realizable without much effort, to grow samples of increased and satisfyingly good quality so that subsequent processing of samples is rendered unnecessary.

DS 3.12 Mon 12:30 CHE 91

Interphase Formation and Band Bending in Organic and Inorganic Semiconductor Films Examined with Hard X-ray Photoelectron Spectroscopy — •Martin Schmid, Benedikt P. Klein, Claudio K. Krug, Stefan R. Kachel, Malte Sachs, Min Chen, and J. Michael Gottfried — Fachbereich Chemie, Philipps-Universität Marburg

Hard X-ray photoelectron spectroscopy (HAXPES) allows to extend the information depth of photoelectron spectroscopy up to several tens of nanometers into a bulk material. This is achieved by using high energy photons ($h\nu = 2 - 10$ keV) to generate photoelectrons with high kinetic energies and accordingly larger mean free paths within solid materials. In a HAXPES experiment one integrates the signal contributions from many layers within the material, however the extraction of quantitative local information with regard to individual layers from the integral signal is in general not trivial. We will demonstrate how genetic optimization routines can be used to accomplish this task with two examples. In a first example we use this approach to characterize the reaction zone between 2H-tetraphenylporphyrin (2HTPP)

films and metallic cobalt and iron layers. We find that the width of the reaction zone crucially depends on the sample temperature during preparation. In a second example we examine the depth dependent, local electrostatic potential (band bending) at a GaP/Si(001) heterojunction. Funding by DFG through SFB 1083 and by Verband der Chemischen Industrie e.V. is gratefully acknowledged.

DS 3.13 Mon 12:45 CHE 91

The effect of substrate miscut in epitaxial PMN-PT thin films — •Paul Chekhonin[1,3], Michael Mietschke[1,2], Darius Pohl[1], Frank Schmidt[1,2], Sebastian Fähler[1], Werner Skrotzki[3], Kornelius Nielsch[1,2], and Ruben Hühne[1] — [1]Institute for Metallic Materials, IFW Dresden — [2]Institut für Werkstoffwissenschaft, Technische Universität Dresden — [3]Institut für Strukturphysik, Technische Universität Dresden

The perovskite (1-x)Pb(Mg1/3Nb2/3)O3-xPbTiO3 (or (1-x)PMN-xPT) exhibits excellent ferroelectric and electrocaloric properties. The use of epitaxial films of PMN-PT facilitates the analysis of predetermined crystal orientations and the application of strain. Therefore, PMN-PT thin films were grown on SrTiO3 (STO) substrates using pulsed laser deposition. In comparison to standard (001) oriented substrates, such with a certain miscut allow the growth in a much broader parameter range. To advance the understanding of the substrate miscut, the microstructure of 0.68PMN-0.32PT thin films grown on La0.7Sr0.3CoO3 buffered STO substrates, with and without miscut, is compared in detail applying X-ray diffraction and high resolution transmission electron microscopy. The PMN-PT layers in both cases exhibit strain relaxation. While in the film without miscut perfect misfit dislocations are observed, in the film with miscut partial dislocations and stacking faults dominate the microstructure. These results may be useful to comprehend the stabilisation of the perovskite PMN-PT phase on miscut substrates.