# DS 7: Thin Film Properties: Structure, Morphology and Composition (XRD, TEM, XPS, SIMS, RBS, AFM, ...): Session I

Time: Monday 15:00–17:45 Location: H 2032

DS 7.1 Mon 15:00 H 2032

**Stoichiometry determination of chalcogenide superlattices by means of X-ray diffraction and its limits** — Felix R. L. Lange[1,2], Henning Hollermann[1], Stefan Jakobs[1], •Peter Kerres[1], and Matthias Wuttig[1,2] — [1]I. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen Germany — [2]JARA-FIT Institute Green-IT, RWTH Aachen University and Forschungszentrum Jülich, 52056 Aachen, Germany

In this study we explore the potential of stoichiometry determination of $GeTe/Sb_2Te_3$ superlattices (CSLs) by means of X-ray diffraction (XRD). For this purpose a series of sputter-deposited CSLs with varying ratios of the GeTe and $Sb_2Te_3$ layer thicknesses is analyzed. Kinematical scattering theory is applied to link the change in average chemical composition with the specific CSL diffraction features. It is found that the lattice parameters of the reference unit cell of the superlattice follow Vegards law, which allows for a straight-forward model for stoichiometry determination.

DS 7.2 Mon 15:15 H 2032

**Revealing the Interfaces of MgO/Co/GaAs(001): A Structural and Chemical Investigation with XPS and XPD** — •Karim Shamout[1,2], Philipp Espeter[1,2], Peter Roese[1,2], Richard Hönig[1,2], Ulf Berges[1,2] und Carsten Westphal[1,2] — [1]Experimentelle Physik 1 - Technische Universität Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund, Germany — [2]DELTA - Technische Universit
ät Dortmund, Maria-Goeppert-Mayer-Str. 2, 44221 Dortmund, Germany

We report a synchrotron radiation based x-ray photoelectron spectroscopy (XPS) and x-ray photoelectron diffraction (XPD) study on the system MgO/Co(bcc)/GaAs(001)-$c(8 \times 2)$ and its interfaces. Co substitutes As at the Co/GaAs interface and forms a $Co_3Ga$ alloy in $D0_3$-structure with Ga due to interdiffusion. The GaAs surface reconstruction is lifted in favor of the newly formed alloy that serves as a template for the metastable Co(bcc) structure. No indication for Co oxidation was found at the MgO/Co interface. The MgO film grows amorphously up to a thickness of $\leq 4$ ML. After 5 ML of MgO deposition, the amorphous phase crystallizes into a distorted unit cell.
Keywords: Topological insulator, MTJ, TMR, PED, XPD, XPS

DS 7.3 Mon 15:30 H 2032

**Ti valence mapping in LAO/STO with Resonant Soft X-ray Reflectometry** — •Martin Zwiebler[1], Emiliano Di Gennaro[2], Jorge Enrique Hamann-Borrero[4], Fabio Miletto Granozio[2], Enrico Schierle[3], Eugen Weschke[3], Bernd Büchner[4], George Sawatzky[5], Robert Green[5], and Jochen Geck[1] — [1]Institut fuer Festkörper- und Materialphysik Technische Universität Dresden, 01062 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]IFW Dresden, Helmholtzstraße 20, 01069 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. We performed X-ray reflectivity measurements at the Ti L2,3 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 and interacts strongly with the lattice degrees of freedom. From the polarization dependence of the reflectivity we gain new results on the anisotropy of orbital energies and valence orbital occupation.

DS 7.4 Mon 15:45 H 2032

**Investigation of wake-up and local polarization switching behavior in La doped HfO2 structures** — •Pratyush Buragohain[1], Tony Schenk[2], Uwe Schroeder[2], and Alexei Gruverman[1] — [1]Dept. of Physics and Astronomy, University of Nebraska-Lincoln, Lincoln, NE 68588, USA — [2]NaMLab gGmbH, Noethnitzer Str. 64, 01187 Dresden

The discovery of ferroelectricity in hafnium oxide (HfO2) based thin films is a promising step towards the realization of ferroelectric based memory devices due to their inherent advantages over conventional perovskite materials, especially their compatibility with existing CMOS technology. Although several studies have reported the integral behavior of the capacitors, an in-depth investigation of the local ferroelectric characteristics has not yet been performed. Here, we will discuss the wake-up behavior and the polarization switching dynamics in ultrathin La-doped HfO2 capacitors investigated by means of Piezoresponse Force Microscopy (PFM). Evolution of the domain structure as a function of the applied voltage confirmed that de-pinning of domains is responsible for the increase in polarization upon field cycling. Step-by-step switching of the polarization coupled with PFM imaging revealed that the domains grow from grain boundaries or pinned domains, if present, following the nucleation limited switching (NLS) model.

DS 7.5 Mon 16:00 H 2032

**Revealing the actual structure of the oxygen-rich surface of $\alpha$-$Fe_2O_3$(0001)** — •Jesús Redondo[1], Petr Lazar[2], Benjamín Mallada[1], Aleš Cahlik[1], Pavel Procházka[3], Martin Vondráček[1], Jan Čechal[3], Pavel Jelínek[1], and Martin Švec[1] — [1]Institute of Physics, Czech Academy of Sciences, Praha, Czech Republic — [2]Regional Center for Advanced Materials and Technologies, Olomouc, Czech Republic — [3]Central European Institute of Technology, Brno, Czech Republic

The surface of metal oxides reconstructs in many ways depending on the crystallographic planes and preparation procedures. In the case of iron oxides, the surface reconstruction of $\alpha$-$Fe_2O_3$(0001) is still controversial. Under oxidizing conditions, it partially reconstructs in the so-called "biphase" structure, which traditionally has been explained by the coexistence of small islands of FeO and $Fe_2O_3$(0001). Furthermore, other phases are present, and there is no recipe to obtain large domains of single phases on the surface, which hinders an unambiguous interpretation of spectroscopic and microscopy data.

In this work, we present a procedure to obtain micrometer-sized domains of single stoichiometry under reducing and oxidative conditions. This has allowed us to thoroughly characterize the two main phases of the $\alpha$-$Fe_2O_3$(0001) by means of STM, AFM, LEEM, $\mu$LEED, XPS, and NEXAFS. Moreover, we have solid evidence that that the "biphase" structure may, in fact, be a novel 2D material rather than a truncated bulk. Complementary DFT calculations support the model of an O-Fe-O trilayer ($FeO_2$) on the surface.

**15 min. break.**

DS 7.6 Mon 16:30 H 2032

**Effect of stress on structural properties of Fe/Cr multilayers.** — •Magnifouet Tchinda Gladice Claire, Dacosta Manu, Meny Christian, and Pierron-Bohnes Véronique — 23 rue du Loess, 67200 Strasbourg

Cr/Fe/Cr tri-layers were deposited by sputtering with an average total thickness of 100nm on MgO(100) and STO(100) substrates. In order to have good epitaxy, the first chromium was deposited at high temperature (400°C), iron at 400°C, 300°C, 200°C and room temperature and; the capping chromium at room temperature. X-ray diffraction is used to study the structure of Cr/Fe/Cr tri-layer. Both the specular scan and pole figure mapping showed good epitaxy of the films along the [100] direction when the temperature of the deposited iron is low (200°C and room temperature). Presence of the residual strain was quantified by *sinus2 * method*. This method revealed that the values of the free lattice stress parameter determined on the tri-layers are sometimes low or high compare to the massive one as I will show it during the presentation.

DS 7.7 Mon 16:45 H 2032

**Effect of alkali post-deposition treatments on the formation of the CdS buffer layer / Cu(In,Ga)Se2 thin-**

**film solar cell absorber interface** — •Jakob Bombsch[1], Enrico Avancini[2], Romain Carron[2], Thomas Kunze[1], Evelyn Handick[1], Roberto Félix[1], Raul Garcia-Diez[1], Yuefeng Zhang[1,4], Stephan Buecheler[2], Regan Wilks[1,3], and Marcus Bär[1,3] — [1]Renewable Energy, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH (HZB), Berlin, Germany — [2]Laboratory of Thin Films and Photovoltaics, Empa-Swiss Federal Laboratories for Materials and Science and Technology, Dübendorf, Switzerland — [3]Energy Materials In-Situ Laboratory Berlin (EMIL), HZB, Berlin, Germany — [4]Department of Physics, Xiamen University, Xiamen, China

Cu(In,Ga)Se2 (CIGSe) - based devices are considered to be high-efficient alternatives to silicon-wafer based solar cells. The performance of chalcopyrite-based thin-film solar cells has recently been improved by performing alkali post-deposition treatments (PDT), where the highest efficiency so far has been reached using an RbF PDT. We used soft and hard x-ray photoelectron spectroscopy to study the impact of NaF/RbF PDT on the chemical and electronic properties of low temperature processed CIGSe absorbers as a function of alkali content. Evidence for the presence of Cu(II) - scaling with RbF - is found at the absorber (surface). Further, the (wet chemically) deposited CdS buffer layers contain a significant fraction of a sulfate. Finally, in our contribution, we will present and discuss the impact of the PDT on the electronic structure of the CdS/CIGSe interface.

DS 7.8 Mon 17:00 H 2032

**Defects investigation in black anatase** — •Dmitry Zyabkin[1], Juliana Schell[3], Ulrich Vetter[1], Haraldur Pall Gunnlaugsson[3], Hilary Masenda[2], Peter Schaaf[1], and the ISOLDE Collaboration[2] — [1]Chair materials for Electronics, Institute of Materials Engineering and Institute of Micro- and Nanotechnologies MacroNano®, Gustav-Kirchhoff-Str. 5, 98693 Ilmenau, Germany — [2]School of Physics, University of the Witwatersrand, Johannesburg 2050, South Africa — [3]European Organization for Nuclear Research (CERN), CH-1211 Geneva, Switzerland

Black anatase has been considered as the promising material for dye-sensitized solar cells and efficient water splitting under light exposure [1]. While defects play the essential role in the enhanced photocatalytic activity it has received plenty of attention to expand studies of their roles as well as further advancing of light absorption [2]. Thin films were obtained by means of reactive sputtering and treated at room and 573K temperatures. The current Mössbauer study was done on black anatase thin films at the ISOLDE mass separator at CERN. Implantation of $^{57}$Mn ($T_{1/2}$ = 1.5 min) was accomplished at ion energies of 50 keV, with the measurements performed online within an interval from 301 to 735K. Hyperfine parameters are given relative to the centre of the spectrum of $\alpha$-Fe at RT.

[1] S.Zhang *et al.* Energy Environ. Sci., 2013,6, 1443-1464

[2] F.Amano *et al.* J. Phys. Chem. C, 2016, 120 (12), pp 6467-6474

DS 7.9 Mon 17:15 H 2032

**Friction behavior of graphene on polished steel surfaces** — •Dogus Ozkan[1], Cem Kincal[2], Egemen Sulukan[3], Yaman Erarslan[4], Baris Yağci[5], and Oğuzhan Gurlu[6] — [1]National Defense University, Naval Academy, Istanbul-Turkey. — [2]Istanbul Technical University, Istanbul-Turkey — [3]National Defense University, Naval Academy, Istanbul-Turkey — [4]Yildiz Technical University, Istanbul-Turkey — [5]Koç University, KUYTAM, Istanbul, Turkey — [6]Istanbul Technical University, Istanbul-Turkey

Application of graphene in tribological problems is gaining importance. In this work, single/multi-layer graphene was growth on copper foils by CVD and transferred on to different polished steels samples, which had different surface roughness (Figure). Lateral force microscopy (LFM) was used to investigate the influence of graphene on the friction behaviour of polished steel surfaces. Effects of surface roughness on the adhesion of single/multi layer graphene was also looked upon. Elastic properties of single/multilayer graphene on steel surface were characterized by AFM in force modulation mode (FMM). Results showed that graphene reduced friction coefficient of steel surface when compared to bare steel surface under different load conditions.

DS 7.10 Mon 17:30 H 2032

**Supramolecular Heterostructures - expanding molecular self-assembly beyond 2D** — •Vladimir Korolkov[1], Kenji Watanabe[3], Takashi Taniguchi[3], Matteo Baldoni[2], Elena Besley[2], Nicholas Besley[2], and Peter Beton[1] — [1]School of Physics and Astronomy, The University of Nottingham, UK — [2]University Park — [3]University of Nottingham, University Park

For a long time the molecular self-assembly has been limited to engineering 2D molecular structures on surfaces. Here we demonstrate a successful approach that extends self-assembly into 3D by creating supramolecular heterostructures - layered organic materials stabilized by hydrogen bonds in plane and by van der Waals interactions between layers. SHs are formed by growing sequential layers of bi- and mono-component two-dimensional supramolecular arrays. The heterostructures are formed on hexagonal boron nitride by depositing of cyanuric acid/melamine, 5,10,15,20-tetrakis(4-carboxylphenyl) porphyrin, trimesic acid and terephthalyc acid. We analyzed this heterostructures with ambient Atomic Force Microscopy that routinely achieve 0.1 nm resolution. AFM has confirmed that there is a clear epitaxial arrangement between these layers. We demonstrate that heterostructure formation may be used to control the functional properties of supramolecular layers through a shift of the fluorescence peak position.

1 - Korolkov et al. Nature Chemistry, 2017