O 44: Poster: Oxide and Insulator surfaces: Structure, Epitaxy, Growth and Adsorption

Time: Tuesday 18:15–20:30 Location: Poster A

O 44.1 Tue 18:15 Poster A

Formation of cobalt ferrite on $SrTiO_3(001)$ by Interdiffusion of Fe_3O_4/CoO bilayers — •Jannis Thien, Jari Rodewald, Martin Hoppe, Karsten Küpper, and Joachim Wollschläger — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany

Ultrathin epitaxial cobalt ferrite ($CoFe_2O_4$) films are in the focus of both spintronics and spin caloritronics since they combine semiconducting properties with ferrimagnetic properties and high Curie temperature. Therefore, cobalt ferrite films can be used as spin filters [1] or as supports for Pt films which are used to obtain deeper insight into the Spin Seebeck effect (SSE) [2].

One approach to prepare ultrathin $CoFe_2O_4$ films is reactive solid phase epitaxy where the interdiffusion of Fe_3O_4/CoO bilayers is used. Therefore, Fe_3O_4/CoO bilayers were consecutively grown by reactive molecular beam epitaxy on $SrTiO_3(001)$. Afterwards, the samples were post-annealed at different temperatures. The effects of interdiffusion were examined after each annealing step by means of x-ray reflectivity (XRR), soft x-ray photoelectron spectroscopy (Soft XPS), hard x-ray photoelectron spectroscopy (HAXPES) and x-ray diffraction (XRD) using synchrotron radiation.

XRR, Soft-XPS as well as HAXPES revealed interdiffusion of Fe_3O_4 and CoO layers after an annealing temperature of 673K and probable formation of $Co_xFe_{3-x}O_4$ layers with $0.4 \leq x \leq 1$.

[1] J.-B. Moussy, J. Phys. D: Appl. Phys. 46, 143001 (2013)
[2] K. Uchida et al., Nature (London) 455, 778-781 (2008)

O 44.2 Tue 18:15 Poster A

Temperature dependent spin polarization in EuO thin films investigated by high resolution ARPES — •Tristan Heider[1,2], Timm Gerber[1], Patrick Lömker[1], Claus Michael Schneider[1,2], Lukasz Plucinski[1,2], and Martina Müller[1,3] — [1]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich GmbH, 52428 Jülich, Germany — [2]Fakultät für Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany — [3]Experimentelle Physik I, TU Dortmund, 44227 Dortmund, Germany

The ferromagnetic insulator EuO is predicted to show 100% spin polarization at the valence band maximum, which makes this material a prototype candidate for research in the field of spintronics. Our goal is to interface it with a topological insulator to introduce time-reversal symmetry breaking without an external magnetic field.

As a first approach we studied MBE growth of EuO on Cu(001), because Cu is a very good electrical conductor, thus, ideally suited as an aid for charging problems in band mapping from an insulating thin film. After we could narrow down the EuO synthesis to a very small parameter window, in which single-crystalline growth is mastered, we performed temperature dependent high resolution spin-ARPES measurements. A non-vanishing spin polarization of the O 2p band as well as up to 52% in the Eu 4f band could be obtained. Furthermore the temperature dependence of the Eu 4f polarization can be described by the Brillouin function and confirm the literature value of $T_C = 69$ K.

O 44.3 Tue 18:15 Poster A

Ni on Fe_3O_4: Post deposition annealing treatments and Ni diffusion into Fe_3O_4 — •Andreas Alexander, Martin Hoppe, Joachim Wollschläger, and Karsten Küpper — Fachbereich Physik, Universität, Barbarastr. 7, 49076 Osnabrück, Germany

One approach of preparing the magnetic insulating ferrite $NiFe_2O_4$ is the interdiffusion of Fe_3O_4/NiO bilayers [1]. Very recently, it has been demonstrated that the surface properties of spinel ferrites can be precisely controlled by diffusion of metallic Co into Fe_3O_4 [2]. Here we study the diffusion of metallic Ni into Fe_3O_4. We have grown Ni/Fe_3O_4 by reactive molecular beam epitaxy (RMBE) on $SrTiO_3(001)$. Then the samples were post-deposition annealed (PDA) at three different temperatures, i.e. 400°C, 500°C, and 700°C, in UHV and 10^{-4} mbar O_2 to tackle the diffusion process. The structural surface characterization was performed by low energy electron diffraction (LEED) after each PDA step, whereas x-ray photoelectron spectroscopy (XPS) was employed to investigate the surface chemical composition. In order to gain information about the Ni incorporation into the bulk of the magnetite layer, we employed hard x-ray photoelectron spectroscopy (HAXPES) due to its enhanced electron escape depth. HAXPES was performed at the beamline I09 of DLS.

[1] O. Kuschel et al., Phys. Rev. B 94, 094423 (2016).
[2] R. Gargallo-Caballero et al., J. Chem. Phys. 144, 094704 (2016.)

O 44.4 Tue 18:15 Poster A

Corundum surface energies from DFT and MD simulations — •Lilit Amirkhanyan, Hemanth Nagaraj, and Jens Kortus — TU Freiberg, Institute for Theoretical Physics, Germany

The surface energy is a very important property for a broader understanding of materials features. The knowledge of oxide surfaces like e.g. Al_2O_3 is essential to understand crystal growth, corrosion or sintering phenomena.

We examined the surface energy of the stable α - Al_2O_3 using first principles density functional theory (DFT) and molecular dynamics (MD) simulation.

This is a study of α - Al_2O_3 relaxed surfaces, surface energies. Our results indicate possible growth planes and interfaces which may have implication for morphology or catalytic behaviour.

O 44.5 Tue 18:15 Poster A

The Growth and Fluorescence of Phthalocyanine Monolayers and Thin Films on Hexagonal Boron Nitride — •Manal Alkhamisi, Vladimir Korolkov, and Peter Beton — School of Physics & Astronomy, University of Nottingham, Nottingham NG7 2RD, U.K.

We have investigated the adsorption of metal-free phthalocyanine (Pc) thin films on hexagonal boron nitride (hBN) using high resolution atomic force microscopy under ambient conditions. The Pc molecules are sublimed onto hBN under vacuum conditions. A set of samples were grown at room temperature with wide range of film thickness (0.2nm-32nm) and the effect of temperature variation of the substrate was also investigated. At low coverage, metal-free phthalocyanine form needle-like islands in which the molecules are coplanar with the substrate. With increasing thickness in the range 4nm to 32nm the morphology of the islands changed to form dendritic-like disordered islands which are attributed to cofacial stacking of molecules. At growth temperatures close ˜100 oC we observe the formation of large monolayer islands and we are able to obtain AFM images with molecular resolution from which we can identify the packing and ordering of the molecules. The photoluminescence of the Pc films was measured with a fluorescence microscope and we find a very intense red-shifted zero-phonon peak for the monolayers with additional peaks for multilayer samples which appear at lower energy and are close to those observed for Pc powder. We discuss these red shifts in relation to substrate and intermolecular interactions.

O 44.6 Tue 18:15 Poster A

Surface terminations of oxidized Nb(110), from Nb_2O_5 to $NbO_{1\approx x}$ — •Kuanysh Zhussupbekov[1], Brian Walls[1], Killian Walshe[1], Emma Norton[1], Sergey I. Bozhko[2], Karsten Fleischer[1], Andrey M. Ionov[2], Valery N. Semenov[2], and Igor V. Shvets[1] — [1]School of Physics and Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College, University of Dublin, Dublin 2, Ireland — [2]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Russia

The oxidation of single crystalline Nb(110) is investigated by low-energy electron diffraction (LEED), X-ray photoelectron spectroscopy (XPS), scanning tunneling microscopy (STM) and spectroscopy (STS). Oxidizing at low temperature and/or high oxygen partial pressure results in the formation of Nb_2O_5. STM measurements reveal an amorphous surface which is found to be insulating by STS measurements. Annealing in ultra-high vacuum (UHV) above 700^oC removes this native oxide and sees the formation of $NbO_{x\approx 1}$ surface [1]. This surface is characterized by stick-shaped $NbO_{x\approx 1}$ nanocrystals. The terrace step width is defined by the nanocrystal stick length and one-dimensional terrace states are observed by STS measurements. Ion bombardment of this surface and subsequent annealing forms a $NbO_{x\approx 1}$ surface with a different terrace structure. Finally, the oxidation of the $NbO_{x\approx 1}$ nanocrystal surface is investigated; room temperature oxidization and subsequent UHV annealing results the extra oxygen sitting in between the $NbO_{x\approx 1}$ nanocrystals.

[1]. I. Arfaoui et al., Physical Review B 65, 115413 (2002).

O 44.7 Tue 18:15 Poster A

Acetone on the TiO_2 rutile surfaces: Adsorption, reaction and IR spectra — Tim Würger[1], Wolfgang Heckel[1], •Kai Sellschopp[1], Heshmat Noei[2], Yuemin Wang[3], Andreas Stierle[2,4], Stefan Müller[1], and Gregor Feldbauer[1] — [1]Institute of Advanced Ceramics, Hamburg University of Technology — [2]DESY NanoLab, Deutsches Elektronensynchrotron, Hamburg — [3]Institute of Functional Interfaces, Karlsruhe Institute of Technology — [4]Physics Department, Hamburg University

Acetone is often present in chemical reactions during the formation of hybrid interfaces, and thus is a potential competitor to coupling agents like carboxylic acids. Moreover, acetone can be oxidized via photo-catalysis at TiO_2 surfaces. Here, we studied the adsorption geometry, energetics and vibrational modes of acetone molecules on the TiO_2 rutile (110) surface with density functional theory (DFT) and IR spectroscopy. Studying a large number of possible adsorption geometries in DFT calculations, we found that even at high coverage the adsorbed acetone is able to change its configuration by thermal activation. IR spectra were recorded while dosing acetone on rutile powder particles at low temperature and agree very well with the calculated IR spectra. Increasing the temperature resulted in a reaction of the adsorbed acetone. The nature of this reaction is examined using DFT.

O 44.8 Tue 18:15 Poster A

LEED I(V) analysis of the physisorption system C_2H_2 $(3\sqrt{2}\times\sqrt{2})\mathrm{R}45^\circ/\mathrm{NaCl}(100)$ — •Jochen Vogt — Chemisches Institut der Uni Magdeburg, Magdeburg, Germany

The first layer acetylene adsorbed on the NaCl(100) surface is known to form long-range ordered structures with $(3\sqrt{2}\times\sqrt{2})\mathrm{R}45^\circ$ and $(7\sqrt{2}\times\sqrt{2})\mathrm{R}45^\circ$ translational symmetry, respectively [1,2]. The comparatively large unit cells in this system are assumed to be induced by a moderate lattice mismatch with the substrate. In both cases, however, the adsorbate structure is not known in full detail. The poster presents first results of an I(V) structure analysis for the $(3\sqrt{2}\times\sqrt{2})\mathrm{R}45^\circ$ phase. Calculated full dynamical LEED intensities are fitted to experimental data of seven diffraction spot orders. An unusual feature of the in-house search algorithm for R-factor minima is the use of rigid molecule structure parameters instead of individual atomic site coordinates, with the advantage of a reduced number of free parameters. According to LEED (Pendry R-factor=0.27), the substrate exhibits a small site specific surface rumpling. The acetylene molecules are placed in average 2.71 Å above the Na^+ ions in a nearly parallel orientation with respect to the surface plane. Lattice mismatch induced strain appears to be released by small lateral shifts of the molecules from the exact on-top positions over Na^+.

[1] A. Glebov, R. Miller, J. P. Toennies, J. Chem. Phys. **106** (1997) 6499. [2] A. G. Cabello-Cartagena, J. Vogt, H. Weiss, J. Chem. Phys. **132** (2010), 74706.