O 77: Oxides and insulators: Epitaxy and growth

Time: Thursday 15:00–18:00 Location: H42

O 77.1 Thu 15:00 H42

Formation of a laterally nanostructured cobalt oxide — •Matthias Gubo, Christina Ebensperger, Wolfgang Meyer, Lutz Hammer, and Klaus Heinz — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

In this study the growth of ultrathin cobalt oxide on a monolayer cobalt and on a monolayer of a Co_4Ir surface alloy - both prepared on a Ir(100) surface - is investigated by means of low energy electron diffraction (LEED) and scanning tunnelling microscopy (STM). The oxide on a monolayer cobalt reveals a c(4x2) periodic LEED pattern. Its structure consists of a compressively strained CoO(100) layer with cobalt vacancies arranged in a c(4x2) periodicity equivalent to a Co_3O_4 stoichiometry of the film. This structure is very different from the oxide on the bare iridium surface [*1*]indicating that the internal structure of this cobalt oxide is strongly coupled to the underlying species of atoms (cobalt or iridium, resp.). Accordingly, by growing the oxide on a well ordered Co_4Ir lateral superlattice - produced via decoration of the reconstructed Ir(5x1)-H phase [*2*] - the cobalt oxide monolayer becomes laterally nanostructured.

So, the oxide's growth appears to be strongly influenced by the local binding conditions to the substrate. In case of a laterally nanostructured substrate the oxide is nanostructured, too.

[*1*] *M. Gubo et al.,* ***J. Phys.: Condens. Matter 21*** *(2009) 474211*

[*2*] *L. Hammer et al.,* ***PRL 91*** *(2003) 156101*

O 77.2 Thu 15:15 H42

Interface Oxides of Eu on Ni(100) — •Jürgen Klinkhammer, Daniel F. Förster, Carsten Busse, and Thomas Michely — II. Physikalisches Institut, 50937 Köln

Eu-oxides of submonolayer to few layer thickness were grown on Ni(100) at 350°C through reactive molecular beam epitaxy with Eu fluxes of $2{,}04{\cdot}10^{14}\,\mathrm{atoms\,m^{-1}s^{-1}}$. The resulting interface oxides are investigated through low energy electron diffraction (LEED) and scanning tunneling microscopy (STM). As a function of the oxygen chemical potential at fixed Eu flux a sequence of interface oxide structures is observed. For the highest oxygen chemical potential polar EuO(111) starts to grow on Ni(100) with the densepacked $[1\bar{1}0]$ EuO direction aligned to the Ni$[(01\bar{1})]$. For medium oxygen chemical potential a phase of small magic clusters coexists with a complex stripe phase. The magic clusters are immobile and decay upon heating. Finally for the lowest oxygen chemical potential applied a 5x5 superstructure forms, which uses as building blocks small, stable square clusters. It turned out that the 5x5 superstructure is well suited as interface oxide for subsequent growth of rather perfect and stoichiometric EuO films. The polar EuO(111) interface oxide decays during subsequent growth through the formation triangular pyramids bounded by {100} facets and the film transforms to the nonpolar (100) orientation.

O 77.3 Thu 15:30 H42

Epitaxial growth of ultra-thin ceria films on Si(111) — •Björn Menkens[1], Jan Ingo Flege[1], Sebastian Gevers[2], Daniel Bruns[2], Joachim Wollschläger[2], and Jens Falta[1] — [1]Institute of Solid State Physics, University of Bremen, 28359 Bremen, Germany — [2]Physics Department, University of Osnabrück, 49069 Osnabrück, Germany

Rare-earth oxides are of major interest in fundamental research due to their intriguing electronic properties, which provide strong potential for multiple applications. Ceria, e.g., is a prominent compound in catalytic converters because of its high oxygen storage capacity, which results from multiple crystallographic phases and their associated oxidation states. In this contribution, we present a growth study of epitaxial ceria films on Si(111) by chemically sensitive x-ray standing waves (XSW) and grazing-incidence x-ray diffraction (GIXRD).

Under ultrahigh-vacuum conditions only Ce_2O_3 can be observed as shown by XPS. Our results show different phases depending on the ceria film thickness. The distinction between a hexagonal phase and the bixbyite (cubic) structure for ultra-thin $Ce_2O_3(111)$ films on Si(111) was achieved by XSW using $Ce3d_{5/2}$ and O1s photoelectrons as secondary signals and subsequent comparison with calculated Fourier components. For film thicknesses exceeding a few nanometers, their crystallinity and surface roughness were investigated by GIXRD and complemented by x-ray relectivity (XRR) measurements. Furthermore, we will discuss the influence of chlorine on ceria growth on Si(111), which acts as a passivating agent for the Si(111) surface.

O 77.4 Thu 15:45 H42

MOS diodes with BaO, SrO and $Ba_{0.7}Sr_{0.3}O$ thin films on Si(001) as a high-k dielectric — •Dirk Müller-Sajak[1], Alexandr Cosceev[2], Herbert Pfnür[1], and Karl R. Hofmann[2] — [1]Leibniz-Universität Hannover, Inst. f. Festkörperphysik — [2]Leibniz-Universität Hannover, Bauelemente der Mikro- und Nanoelektronik

We have grown BaO, SrO and $Ba_{0.7}Sr_{0.3}O$ films on clean Si(001) in order to find a new high-k gate oxide. These films are highly hygroscopic and have to be sealed completely by the metal gate electrode in order to perform ex-situ electrical measurements. We show that complete wetting of a Au layer can be obtained by introducing a thin layer (0.5-1ML) of Al after the oxide growth.

All three oxides have remarkable electrical properties: Dielectric constants near the values for volume material were obtained. Low leakage current densities ($<10^{-6}\,\mathrm{A/cm^2}$ for $Ba_{0.7}Sr_{0.3}O$) have been measured. These results are supported by band offsets measured on the unstructured oxides by XPS and EELS (all above 1eV). Changing the growth conditions at the interface cause a shift in the band offsets induced by states at the interface. Growth of crystalline and lattice matched $Ba_{0.7}Sr_{0.3}O$ turns out to be superior to the amorphous layers of BaO and SrO in terms of defect densities at the interface and of leakage currents. We observed the lowest density of states at the interface of $6.3\cdot10^{10}\mathrm{eV^{-1}cm^{-2}}$ by the Terman method and typically two orders of magnitude lower leakage currents for the crystalline oxide. Structural and chemical reasons will we discussed.

O 77.5 Thu 16:00 H42

Substrate-induced structural modulation of a CoO(111) bilayer on Ir(100) — •Lutz Hammer, Christina Ebensperger, Wolfgang Meyer, Matthias Gubo, and Klaus Heinz — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

Oxidation of a monolayer of cobalt deposited on the unreconstructed Ir(100) surface leads to the formation of a CoO(111) bilayer [1]. Quantitative LEED and STM reveal a cobalt layer next to the substrate covered by an oxygen layer. Both layers' hexagonal atomic arrangements are, however, strongly distorted by the quadratic substrate and form a c(10x2) superstructure. The Co layer's buckling characteristics and atomic bond lengths to Ir atoms are consistent with the hard sphere radius of metallic Co. The binding of the oxide to the substrate appears to be characterized by two types of oxygen ions. One type is close to the expected rocksalt-type stacking with respect to the cobalt layer whilst the other type oxygen ions reside nearly on top of Ir atoms with a very short bond length. They are practically coplanar with the Co layer and so almost form a boron-nitride-type oxide. The bond to Ir can be interpreted as a local pinning of the oxide to the substrate, so modulating the entire oxide bilayer.

[1] C. Giovanardi et al., Phys. Rev. B 74 (2006) 125429

O 77.6 Thu 16:15 H42

Comparing the Structure of Line Defects and Step Edges in the Alumina Film on NiAl(110) – A Dynamic Force and Scanning Tunneling Microscopy Study — •Lars Heinke, Leonid Lichtenstein, Georg Hermann Simon, Thomas König, Markus Heyde, and Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14196 Berlin, Germany

Thin metal oxide films, like aluminum oxide on NiAl(110), are often used as model systems in catalysis. It was found that line defects like step edges and anti phase domain boundaries (APDB) are particularly active sites for catalysis and, therefore, require detailed investigations. In this context, frequency modulated dynamic force microscopy (FM-DFM) and scanning tunneling microscopy (STM) are used to determine the atomic structure of the thin film and its defects in ultra high vacuum at 5 K [1]. The APDBs are orientated along two different directions, i.e. there exist two possible orientations of the film (domain A and B). A detailed analysis reveals that the step edges, which are uniformly distributed on the substrate before the film growth, prefer orientations along these angles. This suggests that the substrate is influenced by the growth of the thin film.

[1] G. H. Simon et al., New J. Phys. 11 (2009), 093009

O 77.7 Thu 16:30 H42

Synchrotron radiation spectroscopy studies of the initial interaction between cobalt and titanium dioxide — •Sebastian Müller and Dieter Schmeisser — BTU Cottbus, Konrad-Wachsmann-Allee 1, 03046 Cottbus

Small metallic particles deposited on oxide surfaces can serve as heterogeneous catalysts, as for example TiO_2 supported cobalt is a known Fischer-Tropsch-Catalyst.

The goal of the presented studies is to investigate the interaction between cobalt and TiO_2 in the initial step of growth by synchrotron radiation based spectroscopy.

PES studies of TiO_2 supported cobalt show a reduction of the oxide support, accompanied by an oxidation of the deposited material. The oxidation is not complete, but metallic cobalt is found already in the very first step of growth. Uniform decrease of both substrate PES lines indicate very weak interaction between overlayer and TiO_2.

An atomic multiplet calculation including charge transfer and crystal field effects is applied to simulate the experimental Co 2p XAS and XPS spectra of the oxidized component. The results allow the identification of the local coordination as well as the identification of the oxidation state of cobalt.

O 77.8 Thu 16:45 H42

From chemisorbed oxygen to ultrathin cobalt-oxides on Ir(100)-(1x1) — •Christina Ebensperger, Matthias Gubo, Wolfgang Meyer, Lutz Hammer, and Klaus Heinz — Institut für Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudstr. 7, 91058 Erlangen

A single monolayer (ML) of cobalt was deposited on Ir(100)-(1x1) and exposed to oxygen at elevated temperatures. As function of oxygen dosage several ordered phases develop, which were studied by means of STM and quantitative LEED.

At low oxygen coverage of 0.25 ML a (2x2) phase develops with hollow site adsorption of chemisorbed oxygen as observed also for other fcc(100) surfaces (R-factor: R = 0.12). With further exposure to oxygen this phase transforms into two different (3x3) phases, $(3x3)_I$ and $(3x3)_{II}$, which can be instantaneously monitored by the LEED intensities. The $(3x3)_I$ structure is a periodic arrangement of isolated suboxide rings with Co_8O_4 stoichiometry (R-factor: R = 0.14), while in the second phase these rings are interconnected by additional oxygen ions (R-factor: R = 0.16). The latter attract the surrounding cobalt ions and reduce their bonding to the substrate. The stoichiometry thereby changes towards Co_8O_5. With even further exposure to oxygen a c(10x2) phase develops which can be regarded as a heavily distorted bilayer of bulk CoO.

O 77.9 Thu 17:00 H42

Mixed interface and charge neutrality in the oxide heterostructure $DyScO_3/SrTiO_3$ — •kourosh rahmanizadeh, gustav bihlmayer, and sbtefan blügel — Institut für Festkörperforschung & Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich

Oxide interfaces have attracted considerable attention in recent years due to the emerging novel behavior, which does not exist in the corresponding parent bulk compounds, e.g. joining two simple band insulators $LaAlO_3$ and $SrTiO_3$ with different polarity can induce new properties ranging from conductivity to magnetism, even to superconductivity. The electrostatic potential diverges due to the polar discontinuity at the interface. But intermixing at the interface, defects, or formation of a polarization in the substrate can help to avoid the divergence of the electrostatic potential.

We carried out density functional theory calculations based on the full-potential linearized augmented planewave (FLAPW) method as implemented in the `FLEUR` code (www.flapw.de) for studying sharp and intermixed $DyScO_3/SrTiO_3$ interfaces. $DyScO_3$ layers induce the same polarity as the lanthanum aluminate. Experimental evidence for intermixing was reported for this system in Ref.[1]. We investigated both scenarios avoiding the polar catastrophe, either by forming a mixed layer at the interface or by formation of a polarization in the $SrTiO_3$ substrate.

[1] M. Luysberg et al., Acta Materialia **57**, 3192 (2009)

O 77.10 Thu 17:15 H42

The surface termination of $Mn_3O_4(001)$ films on Ag(001) — Michael Huth, •Klaus Meinel, Roman Shantyr, Sebastian Polzin, Konrad Gillmeister, Henning Neddermeyer, and Wolf Widdra — Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Germany

Spinel-like Mn_3O_4(001) films can be imagined as an alternating stacking of (2x1)-like Mn_2O_4 and (2x2)-like Mn spinel sublayers (SL). According theory [1], the Mn_2O_4 layer is favored for termination. In our investigations, Mn_3O_4 films have been grown on Ag(001) and analyzed by means of STM and SPA-LEED. The films grow with the lattice vectors of the Mn_3O_4(001) structure aligned along the [110]-like directions of the Ag(001) substrate. This specific film orientation implies an almost vanishing misfit which explains the brilliancy of the LEED spots. In the submonolayer stage, Mn_3O_4 islands are formed displaying either (2x1) or (2x2) surface termination depending on local thickness. For ultrathin continuous films, a (2x1) termination is resolved. However, for film thickness $>$ 12 spinel SL, SPA-LEED yields a (2x2) pattern. STM shows that the films are nevertheless terminated by a Mn_2O_4 layer. But it is now composed not only by (2x1) domains but also by domains where the Mn ions form a c(2x2) pattern. The combination of both structures explains the observed (2x2) LEED pattern. The spreading of this more symmetric structure implies a decrease of density of (2x1) domain boundaries and a corresponding decrease of domain boundary energy.

[1] V. Bayer et al., Phys. Rev. B76 (2007) 165428

O 77.11 Thu 17:30 H42

Epitaxial Europiumoxide on Ni(100) with Single Crystal Quality — •Daniel F. Förster, Jürgen Klinkhammer, Carsten Busse, Zhiwei Hu, L. Hao Tjeng, and Thomas Michely — II. Physikalisches Institut, Univ. zu Köln, Zülpicher Str. 77, 50937 Köln

EuO is one of the rare ferromagnetic semiconductors. Showing a variety of outstanding electronic properties it is e.g. an ideal candidate for spintronic systems. Growth on metal substrates gives rise to additional effects e.g. due to image charge screening or Schottky barriers. Hence the electronic structure is expected to have a different thickness dependence compared to oxide substrates. The initial growth of EuO films on Ni(100) strongly depends on the flux ratio Eu/O and the growth temperature. We use reactive molecular beam epitaxy (MBE) with a flux ratio Eu/O $\approx 3/2$ to grow stoichiometric EuO(100). For two monolayer thick films grown at 450°C in-situ scanning tunneling microscopy (STM) shows films with large monatomic flat terraces and few defects. The EuO grows quasi-pseudomorphically, hence the EuO is in-plane compressed by 3.1%. Low energy electron diffraction (LEED) measurements show the relaxation of the surface lattice constant close to the bulk value within the first 40 monolayers. 100 nm thick films grown at 320°C and annealed at 600°C have a RMS roughness of only 0.5 nm. The step edges are roundly shaped due to the annealing process and the LEED shows spots as sharp as for a single crystal. Ex-situ X-ray adsorption spectroscopy (XAS) was performed after capping with a 4 nm thick Al film. No signs of Eu^{3+} or oxygen vacancies were found, thus the EuO film is stoichiometric.

O 77.12 Thu 17:45 H42

Title: Simulation of deposition and growth of Xe-crystals via the low-temperature atom beam deposition method — •Nicola Toto, Christian Schoen, and Martin Jansen — Max Planck Institute for Solid State Research - Heisenbergstrasse, 1 - 70569 Stuttgart - Germany

We model the deposition of Xe-atoms on a sapphire substrate and the subsequent growth of ordered Xe-phases via the low-temperature atom beam deposition method. This chemical synthesis method (D. Fischer and M. Jansen, J. Am. Chem. Soc. 41, 1755 (2002)) is a successful new way to synthesize metastable solid compounds. The modeling procedure consists of several steps, where we use empirical potentials to model the interactions within the substrate, the Xe-Xe-interactions in the gas phase and the solid, and the interactions between the Xe-atoms and the substrate. In a first step, we established that under the experimental conditions, no Xe-clusters form in the gas phase, and thus the deposition could be described by the adsorption of single Xe-atoms on the substrate at low temperatures. Next, we simulate the Xe deposition process and we study the growth mode depending on various synthesis parameters such as the deposition rate and the temperature of the substrate. Finally, the deposited Xe-layers are annealed, and the structure of the resulting compound is analyzed. We studied the establishment of locally ordered regions as a function of time, both during the deposition and the annealing. We observed that the final configuration is always crystalline, although defects such as stacking faults and dislocations are likely to form.