O 91: Epitaxy and growth: Oxides and insulators

Time: Thursday 17:15–19:30 Location: WIL C307

O 91.1 Thu 17:15 WIL C307

DFT study of structure and magnetism of CoO(111) bilayers on Ir(100) — Florian Mittendorfer[1], •Josef Redinger[1], Raimund Podloucky[2], and Michael Weinert[3] — [1]Inst. of Applied Physics, Vienna University of Technology, Vienna, Austria — [2]Inst. of Physical Chemistry, University of Vienna, Vienna, Austria — [3]Dept. of Physics, University of Wisconsin-Milwaukee, Milwaukee, USA

Experimentally, a hexagonal CoO(111) bilayer is formed on square fcc Ir(100) leading to a c(10x2) superstructure (9 CoO/10 Ir) with large lateral displacements and vertical buckling (5 high, 4 low) of the Co atoms [1]. The 4 O atoms above the Co atoms show a (111) NaCl-type arrangement, while the remaining 5 O atoms are found about 1Å lower, almost coplanar with Co, resembling a hexagonal BN-like arrangement. We have performed DFT calculations for the proposed c(10x2) structure and found the structure to be energetically stable and in good agreement with experimental LEED data, provided proper care is taken for the rather complex magnetic arrangement. The 5 high Co atoms couple anti-ferromagnetically (AF), while ferromagnetic (F) coupling is stabilized by the Ir substrate for the 4 low Co atoms. Considering a CoO registry shift on the Ir(100) substrate a new structure with similar energy emerges, but now with 5 high and 4 low Co/O atoms, resembling 9x2 CoO/Pd(100) [2]. The 5 low Co atoms close to Ir favor once more F-coupling, while the remaining 4 high Co couple AF to the former, abandoning an alternating AF-coupling along the high Co rows. [1] C. Ebensperger et al., Phys Rev. B81, 235405 (2010). [2] L. Gragnaniello et al., Surf. Sci. 604, 2002 (2010).

O 91.2 Thu 17:30 WIL C307

STM, LEED, and XPS study of ultrathin $BaTiO_3$ films on Pt(100): switching film orientation by controlling substrate reconstruction — •Hannes Beyer, Klaus Meinel, Stefan Förster, and Wolf Widdra — Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

Ultrathin $BaTiO_3$ films have been prepared on Pt(100) using either reactive rf magnetron sputtering or MBE. For both cases the deposition has been performed at room temperature. The magnetron operates in an Ar/O_2 gas mixture at 3.6×10^{-3} mbar, whereas MBE is performed in an O_2-atmosphere of 1×10^{-6} mbar by reactive co-deposition of Ti and BaO. Long-range ordered films are achieved by post-annealing in O_2 at 950 K using both methods. XPS reveals bulk-like stoichiometry of the $BaTiO_3$ films. With STM smooth films with unit cell islands are observed for film thickness of 4 ML.

By either preserving or quenching of the quasi-hexagonal surface reconstruction of Pt(100), it is possible to control the $BaTiO_3$ orientation. The films grow by MBE epitaxially either in (111) or (100) orientation, respectively. In contrast, the sputter deposition of $BaTiO_3$ films results in an initially amorphous surface. Upon annealing of the $BaTiO_3$ film a brilliant $BaTiO_3$(100)-(1×1) pattern is observed independent of the prior substrate reconstruction for thicknesses above 2 ML.

O 91.3 Thu 17:45 WIL C307

Termination of the hexagonal ice (0001)-surface by admolecule structures — •Anja Michl and Michel Bockstedte — Lehrstuhl Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr 7B2, 91058 Erlangen

Ice grown on metal substrates exhibits a wide range of structures including clusters of varying shape, amorphous and crystalline islands owing to the flexibility of the water bond network and the nature of the water-metal interaction. Focusing on crystalline ice, recent experiments (e.g. [1,2]) have shown that ice (0001)-surface areas are terminated by water admolecule structures rather than by the bi-layer. In particular detailed high-resolution STM-experiments [2] of ice islands grown on Cu(111) analyzed the arrangement of admolecules on top of the bi-layer. Here we address the interaction of admolecules on this surface that eventually leads to the observed admolecule structures theoretically with an *ab initio* method. We find that admolecules coalesce into a nominal (2x1) superstructure forming mutal hydrogen bonds. Furthermore hexagonal rows of admolecules can interact with additional admolecules. The energetics of such structures much depend on the arrangement of dangling OH-groups and the bonding of the row edge to the underneath bi-layer. Undercoordinated edge molecules are found to evolve to the top of the row to enhance their own coordination.

[1] Ph. Parent *et al.*, J. Chem. Phys. **117**, 10842 (2002).

[2] M. Mehlhorn and K. Morgenstern, Phys. Rev. Lett. **99**, 246101 (2007).

O 91.4 Thu 18:00 WIL C307

Strain-induced formation of mixed-oxide films — •Xiang Shao[1], Niklas Nilius[1], Hans-Joachim Freund[1], Livia Giordano[2], and Gianfranco Pacchioni[2] — [1]Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin, Germany — [2]Università di Milano-Bicocca, Via R. Cozzi 53, 20125 Milano, Italy

By means of scanning tunneling microscopy, Auger spectroscopy and density functional theory, we have identified a new mechanism for strain relaxation in ultrathin oxide films grown on metal supports. Due to the considerable lattice mismatch of 8%, only disordered CaO films form on a Mo(001) substrate at low growth temperatures. However, annealing the system above 1000 K induces a phase transition, which becomes manifest in the occurrence of a sharp (2x2) LEED pattern and the formation of an atomically flat oxide surface. In the course of the transition, Mo from the substrate diffuses into the film and replaces 25% of the Ca ions. The resulting rocksalt-type Ca0.75Mo0.25O structure has a negligible lattice mismatch with the Mo(001) and is in perfect registry with the support. Apart from the strain release, the oxidation of Mo atoms provides a strong thermodynamic incentive for the phase transition. A similar behavior is not observed for MgO films grown on Mo(001), where the original lattice mismatch is smaller.

O 91.5 Thu 18:15 WIL C307

LEEM/LEED investigation of Fe3O4 thin film growth on a Pt(111) substrate — •Thomas Schmidt, Alessandro Sala, Helder Marchetto, Shamil Shaikhutdinov, and Hans-Joachim Freund — Fritz-Haber-Institut, Abt. CP, 14195 Berlin

Iron oxide, widely used as a catalyst and as a support for catalytically active systems, has been intensively studied with various techniques [1]. However, controversies in the literature regarding the surface termination and structural inhomogeneities hinder the direct linking of surface electronic and structural properties to chemical properties. Our aim is therefore a comprehensive and consistent characterization of the Fe3O4 film growth on a Pt(111) substrate by using the SMART instrument, specially designed to obtain chemical and structural information with high lateral resolution. In particular, deviating from the optimum preparation conditions [2], the oxide thin film reveals defects like a coexistence of two different stoichiometric phases (Fe3O4 and FeO), a Moiré-like patterned morphology with a mesoscopic periodicity and a predominance of one of two possible rotational domains. In addition, a subsequent annealing at 900K changes significantly the IV-LEED spectra and SPA-LEED profiles, which corresponds to different atomic termination of the magnetite surface. [1] W. Weiss and W. Ranke, Prog. Surf. Sci. 70 (2002) 1-151 [2] Z.-H. Qin, M. Lewandowski, Y.-N. Sun, S. Shaikhutdinov, and H.-J. Freund, J. Phys. Chem. C 112 (2008) 10209-10213

O 91.6 Thu 18:30 WIL C307

Phonon dispersion of ultrathin NiO(100) films on Ag(100) — •Sebastian Polzin, Krassimir L. Kostov, and Wolf Widdra — Martin-Luther-Universität Halle-Wittenberg, Institute of Physics, Halle (Saale), Germany

HREELS is employed to characterize the growth and to measure the phonon dispersion of ultrathin NiO films on an Ag(100) surface. The films have been grown by reactive deposition of Ni in an O_2 atmosphere. The evolution of the spectra observed for different NiO film thickness between 0.5 and 15 ML will be compared to the dielectric response of an oxide film on a metal substrate. For an 15 ML thick NiO(100) film the phonon dispersion along the Γ-X direction has been determined. The data will be compared to NiO(100) single crystal data measured with HREELS [1] and HAS [2]. Due to the improved resolution two additional phonons have been detected which are visible in the entire surface Brillouin zone. In contrast to earlier work the dispersion of the Lucas mode (S_4) and a transverse optical mode (S_2) could be measured from the center to the X point at the zone boundary.

[1] Oshima C., Modern Phys. Lett. 5, (1991)

[2] Toennies J. P., et al., J. Electr. Spectr. Rel. Phen. 64/65, (1993)

O 91.7 Thu 18:45 WIL C307

Epitaxial Polar Europium Oxide on Ir(111) — •Stefan Schumacher, Daniel F. Förster, Carsten Busse, and Thomas Michely — II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, D-50937 Köln

EuO is a ferromagnetic semiconductor with a Curie temperature of 69 K and a band gap of about 1.2 eV. We have grown submonolayer films of EuO by means of reactive molecular beam epitaxy on Ir(111). The initial growth shows atomically flat islands of polar EuO(111) as can be seen from scanning tunneling microscopy (STM) and low energy electron diffraction (LEED). Both in STM images and LEED we see a rotational mismatch of the dense-packed rows of EuO(111) and Ir(111) of up to about 5°.

Using dI/dz spectroscopy and analyzing the Gundlach oscillations in scanning tunneling spectra we find a strong increase of the work function for the first polar bilayer EuO compared to bare iridium. The work function increase also gives rise to a strong reduction of the apparent height of the EuO islands in STM images. We interpret the work function increase to result from the additional surface dipole created by the polar EuO(111) surface.

O 91.8 Thu 19:00 WIL C307

Photo electron spectroscopy study of the stoichiometric composition of ultrathin $La_{0.67}Sr_{0.33}MnO_3$ films — •Åsmund Monsen[1], Fei Song[1], Justin Wells[1], Jos Boschker[2], Zheshen Li[3], Roland Mathieu[4], Matthias Hudl[4], Per Nordblad[4], Thomas Tybell[2], and Erik Wahlström[1] — [1]Dept. of Physics, NTNU, Norway — [2]Dept. of Electronics and Telecommunications, NTNU, Norway — [3]Institute for Storage ring facilities Aarhus, Denmark — [4]Dept. of Engineering Sciences, Uppsala University, Sweden

Ferromagnetic manganites, such as $La_{0.67}Sr_{0.33}MnO_3$ (LSMO), have for a long time been prime candidates for spintronic devices. However, tunneling junctions have yet to display high resistive switching states at room temperature, and reports indicate reduced magnetic properties in ultrathin single films. These observations point towards altered layers at the interfaces.

In order to elucidate the physics of the interface regions we have studied structurally and magnetically well characterized LSMO, grown by pulsed laser deposition, thin films utilizing synchrotron based angle and energy dependent photo electron spectroscopy. We will present an analysis of depth dependent stoichiometry in films ranging from 20 nm down to a few unit cells in thickness. We will especially focus on any changes between surface, film and interface stoichiometry. Changes in valance band electron structure and the effect of the annealing based cleaning procedures will also be assessed.

O 91.9 Thu 19:15 WIL C307

Electronic structure of the c(10x2) cobalt oxide phase on Ir(100): STM and DFT — •C. Tröppner[1], P. Weinhardt[1], M. Reuschl[1], T. Schmitt[1], F. Mittendorfer[2], J. Redinger[2], R. Podloucky[3], M. Weinert[4], L. Hammer[1], and M.A. Schneider[1] — [1]Lst. f. Festkörperphysik, U Erlangen — [2]Inst. of Applied Physics, TU Wien — [3]Inst. of Physical Chemistry, U Wien — [4]Dept. of Physics, University of Wisconsin-Milwaukee, Milwaukee, USA

We studied the electronic properties of the c(10x2) cobalt oxide bilayer on Ir(100) by low-temperature STM and STS in ultra-high vacuum and by DFT. The oxide films representing a bilayer of CoO(111) were produced by oxidation of cobalt deposited onto Ir(100)(1×1) at elevated temperatures. The DFT calculations were performed using the VASP package employing standard PBE as well as PBE+U to assess the importance of on-site correlations. A symmetric repeated 5 layer Ir slab setup separated by ≥ 16Å vacuum with a bilayer CoO on each side was used. The STS signal was calculated in the Tersoff-Hamann approximation. DFT reveals that STM mainly images the oxygen atoms. As a consequence the subtle modulation caused by the local interaction between the cobalt oxide bilayer and the Ir surface becomes obvious in STM. We also performed STS dI/dV mapping of the CoO films and identified signatures, which can be attributed to oxygen and cobalt features by comparison to the theoretical data. However, STS dI/dV spectra of the c(10x2) but also of other thin cobalt oxide phases on Ir(100) show "zero-bias anomalies" tentatively assigned to the Kondo effect that is not captured by the present state of the calculations.