

## O 10: Oxides and insulators II

Time: Monday 15:00–16:45

Location: SCH A01

O 10.1 Mon 15:00 SCH A01

**Ultrathin cobalt oxide-cobalt interface films** — ●MATTHIAS GUBO, CHRISTINA EBENSBERGER, WOLFGANG MEYER, LUTZ HAMMER, and KLAUS HEINZ — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

The deposition of 1.75 monolayers of cobalt on the unreconstructed Ir(100)-(1×1) surface at liquid nitrogen temperature and under oxygen-poor conditions leads – after annealing at about 670 K – to a well ordered c(4×2) superstructure.

The crystallographic structure of this phase was determined by quantitative low-energy electron diffraction (LEED) whereby an excellent agreement between experimental and calculated I(E)-curves was achieved (Pendry R-factor: 0.17). The resulting model reveals that the film is made up by two atomic layers whereby the layer above the substrate consists exclusively of cobalt, i.e. is a metallic layer which however is strained due to epitaxial misfit. All oxygen atoms reside in the second, outermost layer. It is similar to a (compressed) rocksalt-type CoO(100) plane, however with cobalt vacancies in a c(4×2) periodic arrangement equivalent to a Co:O stoichiometry of 3:4. This is consistent with atomically resolved STM images, whereby cobalt ions of the oxide layer are imaged. The same two-dimensional c(4×2) oxide can also be grown on thicker cobalt films on Ir(100) by post-oxidation at 320 K. The interface between the ultrathin cobalt oxide and metallic cobalt is possibly relevant for magnetoelectronic devices.

O 10.2 Mon 15:15 SCH A01

**Growth and atomic structure of epitaxial ultrathin BaTiO<sub>3</sub> films on Pt(100)** — ●STEFAN FÖRSTER, MICHAEL HUTH, ANKE HÖFER, KARL-MICHAEL SCHINDLER, and WOLF WIDDRA — Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

Ultrathin BaTiO<sub>3</sub>(100) films were grown by radio frequency-assisted magnetron sputtering on Pt(100) at room temperature using a Ar/O<sub>2</sub> gas mixture at a pressure of  $2.5 \times 10^{-3}$  mbar. The growth exhibits high reproducibility with respect to film thickness and composition. The Ba/Ti stoichiometry as determined by XPS can be controlled via the gas pressure and the Ar/O<sub>2</sub> ratio during deposition. The long-range order of films with perfect BaTiO<sub>3</sub> stoichiometry can be improved by post annealing in  $1 \times 10^{-4}$  mbar O<sub>2</sub> at 1000 K. These films show sharp BaTiO<sub>3</sub>(100)-(1×1) diffraction spots in LEED which allow a LEED-IV analysis in the range of 20 - 400 eV. STM measurements for a 5 ML film reveal a smooth topography with small islands in the top layer. By annealing in oxygen at temperatures above 1050 K a stoichiometric BaTiO<sub>3</sub>(100)-(4×4) structure is formed.

O 10.3 Mon 15:30 SCH A01

**Long-range ordered manganese oxide bilayer on Pt(111): An in-vivo STM, STS and LEED study at elevated temperatures** — ●BENJAMIN BOCHMANN, STEFFEN SACHERT, CHRISTIAN HAGEDORF, and WOLF WIDDRA — Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

Growth as well as atomic structure of ultrathin epitaxial manganese oxide films on Pt(111) have been studied using STM, STS and LEED. The films have been prepared by reactive Mn deposition in an oxygen atmosphere of  $10^{-8}$  to  $10^{-6}$  mbar. STM measurements performed during growth (in-vivo) at elevated temperatures (400-600 K) reveal three different well-ordered monolayer structures depending on preparation conditions with MnO, Mn<sub>3</sub>O<sub>4</sub> and MnO<sub>2</sub> stoichiometry. Only the MnO monolayer is thermally stable up to 1100 K and long time stable. The others will be reduced slowly by gaseous carbon monoxide. For manganese oxides bilayers, again three different long-range ordered structures are observed depending on the oxygen content similar as in the monolayer. The MnO(001)-like bilayer is less stable than the MnO monolayer. Heating to 780 K in UHV leads to a reorganization of the MnO(001)-like bilayer and the formation of two new uniaxially reconstructed structures with different corrugation heights. All bilayer structures and films up to six layers thickness exhibit characteristic STS spectra in the 1 - 6 eV range.

O 10.4 Mon 15:45 SCH A01

**Preparation and investigation of NdGaO<sub>3</sub>(110) surfaces** — ●RASUOLE DIRSYTE<sup>1</sup>, JUTTA SCHWARZKOPF<sup>1</sup>, JENS LIENEMANN<sup>2</sup>, MARCO BUSCH<sup>2</sup>, HELMUT WINTER<sup>2</sup>, and ROBERTO FORNARI<sup>1,2</sup> —

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Atomically smooth, single terminated surfaces are required for the controlled and epitaxial growth of oxide films. NdGaO<sub>3</sub> is one of the promising substrates for the epitaxial growth of superconducting, ferroelectric, dielectric, and magneto-resistive materials, due to its chemical and structural compatibility. The preparation conditions of NdGaO<sub>3</sub> wafers were optimised by changing the annealing temperature and time in order to obtain surfaces with an atomically smooth step-and-terrace structure. After preparation of a regularly stepped surface the substrates were exposed to different oxygen-argon atmospheres at fixed substrate temperature of 730 °C in order to simulate the thermal conditions met before starting the MO-CVD growth process. The annealing in pure argon atmosphere leads to total degradation of the step-and-terrace structure, while the surface structure could be preserved in argon/oxygen mixture with low oxygen content (2 %). The surface roughness as well as the width of the terraces and the height of the steps was measured by AFM in contact mode. The termination of NdGaO<sub>3</sub>(110) surface was determined by the means of proton- and electron-induced AES.

O 10.5 Mon 16:00 SCH A01

**C-AFM characterization of high-k dielectric films grown by molecular beam deposition** — ●PETER DUDEK, JAREK DABROWSKI, GRZEGORZ KOZLOWSKI, GRZEGORZ LUPINA, GUNTHER LIPPERT, and HANS-JOACHIM MÜSSIG — IHP, Im Technologiepark 25, 15236 Frankfurt (Oder) / Germany

Very thin high-k dielectric films (thickness below 10 nm, dielectric constant k around 100) deposited on metallic electrodes are of particular interest for dynamic random access memories (DRAM). High capacitance density of storage capacitors must be accompanied by extremely low leakage currents: leakage should not exceed about  $10^{-8}$  A/cm<sup>2</sup> at bias around 0.5 V. This study uses conductive atomic force microscopy (C-AFM) to investigate microscopic aspects of electron transport across group-II hafnate and zirconate films deposited by MBE. Typically, most leakage is confined to nano-sized „hot spots”. Analysis of hot spot IV characteristics, including their statistical distribution, provides insight into leakage mechanisms. This analysis is guided by quantum-mechanical simulations for trap-assisted tunnelling and ab initio calculations for the formation energies and electronic structures of point defects. Among the effects discussed in this work is local resistivity switching. We also present the first data obtained for dielectric perovskite films with intentional admixture of TiO, whereby the influence of substrate electrode (TiN, Ru, or Pt) is considered.

O 10.6 Mon 16:15 SCH A01

**Wavefunction-based ab-initio results for the adsorption of N<sub>2</sub>O on CeO<sub>2</sub> surfaces** — CARSTEN MÜLLER<sup>1</sup>, ●BEATE PAULUS<sup>2</sup>, and KERSTI HERMANSSON<sup>1</sup> — <sup>1</sup>Department of Materials Chemistry, The Angstrom Laboratory, Uppsala University, Lägerhyddsvägen 1, 75121 Uppsala, Sweden — <sup>2</sup>Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin

For the ab-initio description of the adsorption process on surfaces it is necessary to model all interactions on the same theoretical footing. The standard density functional methods have their difficulties with describing dispersion forces. But especially for the physisorption, where no covalent bonds are formed between the adsorbant and the surface these interactions are essential. They can only well described with wavefunction based correlation methods like coupled-cluster methods. With the method of increments [1] it is possible to apply these wavefunction based correlation methods to extended systems and absorption processes on surfaces [2]. Here we apply the method to the adsorption of N<sub>2</sub>O on the CeO<sub>2</sub> 111 surface in different adsorption structures. Due to the partitioning of the correlation part of the adsorption energy according to localized orbital groups, it is possible to discuss the individual contributions to the binding. Therefore, the method of increments yields not only highly accurate results for the adsorption energy, but also gain information about the chemical binding on surfaces.

[1] B. Paulus, Phys. Rep. 428, 1 (2006).

[2] C. Müller, B. Herschend, K. Hermansson and B. Paulus, J. Chem.

Phys. 128, 214701 (2008).

O 10.7 Mon 16:30 SCH A01

**Adsorption of CO on TiO<sub>2</sub>(110): A first principles study** —  
•MATTHIAS MEHRING and THORSTEN KLÜNER — Theoretical Chemistry, Carl von Ossietzky University of Oldenburg, 26111 Oldenburg, Germany

Titania plays an important role in materials science. It serves as heterogenous catalyst, photocatalyst, or corrosion protective coating [1]. The wide field of photochemistry, and photodesorption, sparked the interest of theoretical and experimental research. Photodesorption can be described as a prototype of a huge group of non-adiabatic surface reactions [2] like simple rotational and vibrational excitations of small molecules or photodiffusion. These reactions could be a basis for pho-

ton driven molecular switches or molecular rotors [2].

The present study provides an insight into adsorption process of CO from a rutile surface, which is modeled by a finite cluster approach embedded in a field of point charges. The smallest cluster model which describes the system with sufficient accuracy is a Ti<sub>9</sub>O<sub>18</sub> cluster [3], in our case we use a cluster model of the type Ti<sub>15</sub>O<sub>30</sub>. The adsorption of CO on the relaxed rutile surface serves as first step to study the desorption mechanism. Therefore it is necessary to compute potential energy surfaces of the electronic ground state and excited states involved in the desorption process.

In this work, we present first results on CO interacting with TiO<sub>2</sub>(110). The calculated potential energy surfaces will pave the way for a detailed microscopic understanding of surface photochemistry of this important adsorbate-substrate system.