

## O 3: Oxides and insulators I

Time: Monday 11:15–13:00

Location: SCH A01

O 3.1 Mon 11:15 SCH A01  
 $(\sqrt{3}\times\sqrt{3})R30^\circ$  Superstructure in CoO(111) Surfaces —  
 ●WOLFGANG MEYER, KERSTIN BIEDERMANN, MATTHIAS GUBO, LUTZ  
 HAMMER, and KLAUS HEINZ — Lehrstuhl für Festkörperphysik, Uni-  
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CoO(111) films of thicknesses 10–150 Å were prepared by using a  
 Ir(100)-(1×1) surface as a support. At all thicknesses they exhibit  
 a  $(\sqrt{3}\times\sqrt{3})R30^\circ$  superstructure with respect to the hexagonal unit  
 cell of CoO(111). The latter is slightly distorted below the thickness  
 of about 15 Å (due to the films' accommodation to the quadratic unit  
 cell of the Ir substrate) but relaxes to ideal hexagonal symmetry at  
 larger thickness. Thereby, however, the in-plane lattice parameter only  
 gradually approaches that of bulk CoO (3.012 Å) – at a thickness of  
 about 150 Å it is still (but only) 0.6% above that.

Though the  $(\sqrt{3}\times\sqrt{3})R30^\circ$  structure reversibly transforms to a  
 (1×1) phase with temperature increasing beyond 50°C it must be con-  
 sidered as the CoO films' ground state structure. As the thick films ex-  
 hibit a lattice parameter rather close to that of bulk CoO(111) one can  
 assume that the  $(\sqrt{3}\times\sqrt{3})R30^\circ$  termination is intrinsic to CoO(111).  
 This makes the crystallography of the surface even more interesting  
 and, in the light of that, we have investigated it by quantitative LEED  
 and atomically resolved STM. It turns out that the CoO(111) surface  
 is metallic and terminated by a wurtzite-type stacking of layers (as  
 retrieved earlier [1]), whereby the atoms within the unit cell undergo  
 a layer dependent buckling or trimerization.

[1] W. Meyer et al., Phys. Rev. Lett. **101** (2008) 016103

O 3.2 Mon 11:30 SCH A01  
 First-Principles Study of the Growth Kinetics of 1D Pd Is-  
 lands on SnO<sub>2</sub> — ●ALEXANDER URBAN and BERND MEYER — Inter-  
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The vapor deposition of Pd on a reduced SnO<sub>2</sub>(101) surface leads to  
 the formation of one-dimensional (1D) nanowires. Scanning tunneling  
 microscopy reveals the growth of islands with a monoatomic height  
 and a width of 5 Å and a length of up to 350 Å [1]. Nanowires and  
 1D conductors are potential building blocks of nanoscale devices. For  
 the design of nanowires with specific properties it is essential to fully  
 understand the atomistic processes that lead to this for metal oxide  
 substrates unusual overlayer growth. In order to gain insight into the  
 energetics and the kinetics of the growth of Pd islands on SnO<sub>2</sub>(101)  
 surfaces, the system has been studied by first-principles DFT slab cal-  
 culations [1] as well as by kinetic Monte-Carlo (kMC) simulations. It  
 is found that a pronounced 1D diffusion, combined with a strong inter-  
 action of Pd with the surface Sn atoms and the lack of stable binding  
 sites at the sides of the nanowires are responsible for the formation of  
 the 1D islands.

[1] K. Katsiev, M. Batzill, U. Diebold, A. Urban, and B. Meyer,  
 Growth of One-Dimensional Pd Nanowires on the Terraces of a Re-  
 duced SnO<sub>2</sub>(101) Surface *Phys. Rev. Lett.* **98** (2007) 186102

O 3.3 Mon 11:45 SCH A01  
 Interface formation and thin film growth of single crystalline  
 Bi(111) on the NaCl(100) surface — ●THOMAS PAYER, FRANK  
 MEYER ZU HERINGDORF, and MICHAEL HORN-VON HOEGEN — Univer-  
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Starting from the clean and atomically flat NaCl(100) surface [1] we  
 studied the interface formation and the thin film growth of Bi at room  
 temperature using LEED, AFM and TED. The initial few layers of  
 Bi grow layer by layer showing a diffraction pattern identical to the  
 one observed from the clean NaCl surface indicating that the first  
 nanometer of Bi grows in the NaCl lattice. Subsequently an epitaxial,  
 (111)-oriented film grows on top of this wetting layers. Due to the  
 nearly perfect 7:10 epitaxial ratio of lattice constants the film grows  
 in domains up to micrometer size with a very low defect density and  
 a roughness that can be reduced below 1nm rms by a short anneal  
 at 100°C. Subsequent to film growth the free standing Bi membranes  
 could be obtained by dissolving the NaCl substrate in water. Such  
 membranes are mechanically stable down to 20 nm thickness.

[1] Appl. Phys. Lett. **93**, 093102 (2008)

O 3.4 Mon 12:00 SCH A01

Ultrathin titanium oxide films grown on Pt<sub>3</sub>Ti(111): Elec-  
 tronic and structural characterization — ●SÉVERINE LE MOAL,  
 MARCO MOORS, CONRAD BECKER, and KLAUS WANDEL — Institute  
 of Physical and Theoretical Chemistry, University of Bonn, Wegelerstr.  
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As TiO<sub>2</sub>-supported platinum is a well-known catalyst, e.g. for CO hy-  
 drogenation, the formation of titanium oxides on Ti-Pt alloy surfaces  
 raises much interest. In this work the electronic and structural proper-  
 ties of ultrathin titanium oxide films grown on a Pt<sub>3</sub>Ti(111) single crys-  
 tal have been investigated by ultraviolet photoelectron spectroscopy  
 (UPS) and low energy electron diffraction (LEED) as a function of  
 oxygen pressure (10<sup>-8</sup> to 10<sup>-5</sup> mbar), oxygen exposure (up to 9000  
 L) and oxidation temperature (300 to 1000 K). For low oxygen expo-  
 sures (below ~ 200 L) and above 800 K, a quasi-hexagonal structure (a  
 = 3.35 Å, b = 3.25 Å, α = 124°) with two domains rotated by 8° with  
 respect to each other prevails. Upon oxidation at higher exposures and  
 above 900 K a hexagonal structure (a = 3.20 Å) with two domains ro-  
 tated by 8° with respect to each other is predominantly observed. In  
 this case the p(2×2) structure attributed to the Pt<sub>3</sub>Ti(111) substrate  
 is no longer present, indicating a possible segregation of titanium to  
 the subsurface. Despite the variety of ordered structures, which have  
 been found for different oxidation conditions, no significant differences  
 in the shape of the valence band spectra have been observed.

O 3.5 Mon 12:15 SCH A01  
 Investigation of ultra-thin Chromium layers on Titanium  
 Dioxide by resonant photoemission — ●SEBASTIAN MÜLLER and  
 DIETER SCHMEISSER — Brandenburgische Technische Universität Cot-  
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Oxide supported metal films and clusters offer interesting properties  
 with a wide range of possible applications. In this context, Titanium  
 Dioxide is chosen as a model substrate due to its simple electronic  
 structure with a d<sup>0</sup> configuration. We study the interaction of ultrathin  
 Chromium films deposited on TiO<sub>2</sub> film with focus on the modifica-  
 tions of the valence band and band gap region. Normal photoemission  
 in bulk and surface sensitive modes as well as resonant photoemission  
 at the Cr 2p and Ti 2p edges are used to distinguish the different Cr  
 3d and Ti 3d contributions to the valence band. In the initial step we  
 find to gap states of distinct character with a sharp resonance of the  
 Cr 3d related state at the Cr 2p edge. With increasing layer thick-  
 ness we observe that this resonance extends to about 20 eV below the  
 Fermi-Energy. Datasets of valence band spectra measured around the  
 Cr 2p edge show 2 resonant mechanisms in this case i.e. a participator  
 channel for the 3d state accompanied by a spectator channel at fixed  
 kinetic energy.

O 3.6 Mon 12:30 SCH A01  
 Thin iron oxides on corundum - Raman and XRD investi-  
 gations — ●ALEXANDER M. GIGLER<sup>1,2</sup>, MAIKE LÜBBE<sup>1</sup>, ROBERT W.  
 STARK<sup>1,2</sup>, and WOLFGANG MORITZ<sup>1</sup> — <sup>1</sup>Sect. Crystallography, LMU-  
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Iron oxides are a material of great interest as oxidation catalyst [1], for  
 styrene synthesis [2], for corrosion processes [3], as gas sensing material  
 [4]. For its initial growth, a complicated behavior has been supposed  
 including faceting [5], interface expansion [6], or formation of differ-  
 ent iron oxide phases such as an additional metastable FeO like iron  
 oxide phase by LEED measurements [7]. We report on the formation  
 of magnetite (Fe<sub>3</sub>O<sub>4</sub>) and hematite (Fe<sub>2</sub>O<sub>3</sub>) on corundum (Al<sub>2</sub>O<sub>3</sub>) as  
 observed by XRD and Raman spectroscopy. Magnetite appears inde-  
 pendently from the substrate temperature during evaporation and  
 cannot be removed by post-annealing in an oxygen atmosphere. The  
 temperature range for formation of hematite was 400°C to 500°C. For  
 300°C, only magnetite can be observed, since growth of hematite is  
 inhibited by the slow activation kinetics at the surface causing a lack  
 of oxygen. For 600°C, the partial pressure of oxygen is too low for  
 hematite growth and the phase-diagram is in favor of magnetite.

[1] G. Samsonov, The Oxide Handbook (1973). [2] M. Muhler, J. of  
 Catalysis **138**, 413 (1992). [3] S.J. Oh, Hyperfine Int. **112**, 59 (1998).  
 [4] M. Ivanovskaya, Sens. and Act. B **93**, 422 (2003). [5] S.I. Yi, Surf.  
 Sci. **443**, 212 (1999). [6] T. Fujii, Surf. Sci. **366**, 579 (1996). [7] S.  
 Gota, PRB **60**, 14387 (1999).

O 3.7 Mon 12:45 SCH A01

**Oxygen-deficient cobalt oxide monolayer on Ir(100)-(1x1)**

— •CHRISTINA EBENSBERGER, MATTHIAS GUBO, WOLFGANG MEYER, LUTZ HAMMER, and KLAUS HEINZ — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

When cobalt of slightly less than a monolayer deposited on Ir(100)-(1x1) is oxidized under oxygen-deficient conditions a new ultrathin cobalt-oxide is formed. It exhibits a (3x3) superstructure on the substrate which can be transformed reversibly into an oxygen-rich c(10x2) structure as described in ref. [1].

The crystallographic structure of the new oxide was determined by quantitative LEED using an exceptionally large data base of more than 12.000 eV. Excellent agreement between experimental and model inten-

sities was achieved (Pendry R-factor: 0.16). The analysis reveals an extremely oxygen-deficient oxide consisting of eight cobalt and only five oxygen ions per (3x3) unit cell with the oxygen located on top of iridium atoms. Four oxygen ions 3-fold coordinated to cobalt are grouped symmetrically around one oxygen ion which in turn is 4-fold coordinated to cobalt. The cobalt ions are closer to the substrate than the oxygen ions, yet not as much as expected from thin cobalt films on iridium. The iridium atoms with oxygen ions on top are displaced by 0.1 Å into the top Ir layer.

The findings of the LEED analysis are corroborated by STM investigations. Depending on the tunnelling conditions either oxygen or the underlying substrate is imaged.

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