

O 33: Oxides and Insulators: Epitaxy and Growth

Time: Tuesday 15:45–17:45

Location: H41

O 33.1 Tue 15:45 H41

Ab-initio study of the epitaxial growth of germanium on SrHfO₃(001) using strontium as surfactant — ●ANDREI REYES HUAMANTINCO and PETER BLÖCHL — Clausthal University of Technology, Institute for Theoretical Physics, Leibnizstr. 10, D-38678 Clausthal-Zellerfeld, Germany

The channel in a MOSFET must consist of layers with smooth morphology and low defect density. When germanium (high mobility channel) is deposited on SrHfO₃ (high-k oxide) it clusters. Nevertheless, we find that depositing a full monolayer of strontium on SrHfO₃(001) and using it as template for germanium overgrowth, inhibits clustering. Formation of the first two epitaxial germanium monolayers occurs via consolidation of so-called germanium zig-zag chains which are pieces of the first and second Ge(001) monolayers, and an structural element of the diamond crystal structure. During consolidation of the zig-zag chains, some atoms from the strontium monolayer diffuse to the surface in order to saturate the germanium dangling bonds. After deposition of two germanium monolayers, the resulting configuration consists of strontium half monolayer at the surface, two epitaxial germanium monolayers, the other half monolayer of strontium that remained at the interface, and SrHfO₃(001). Further deposition of germanium results in a surfactant-mediated epitaxial layer-by-layer growth because half monolayer of strontium stabilizes the germanium surface and strontium is not incorporated into bulk germanium. The interfacial half monolayer of strontium stabilizes the interface, and provides adequate valence and conduction band offsets for transistor applications.

O 33.2 Tue 16:00 H41

Oxidation on the nanoscale - the tungsten-water reaction in high electric fields — ●CARSTEN NOWAK¹, GUIDO SCHMITZ², REINER KIRCHHEIM¹, and CHRISTIAN OBERDORFER² — ¹Institut für Materialphysik, Universität Göttingen, D-37077 Göttingen — ²Institut für Materialphysik, Universität Münster, D-48149 Münster

The oxidation of nanoscale needle-shaped tungsten tips in water vapor at room temperature is strongly depending on the electric field around the nanotip. Above a critical field strength of the order of 10⁹ V/m the natural oxidation process is extended by a field-induced oxidation reaction. Investigation of the oxidation kinetics reveals that the oxidation reaction virtually terminates after some seconds. The morphology of the formed oxide layer shows a distinct pressure dependence in the range of 10⁻⁴ to 10¹ mbar H₂O, with a characteristic size of the formed oxide layer of up to some 100 nm. Using pulsed laser atom probe tomography, the stoichiometry of the formed oxide is determined to be WO₃.

Calculation of the electric field distribution around the tip with the finite element method allows conclusions about the field-influence on oxide growth and the appearance of different morphologies in dependence of the water pressure. Special attention will be paid to the aspect of charge compensation, and it will be discussed to which degree the enhanced oxidation reaction under the influence of the electric field is material independent.

O 33.3 Tue 16:15 H41

Structural and vibrational properties of ultrathin MnO films on Pt(111): An HREELS, STM and LEED study — S. SACHERT¹, B. BOCHMANN¹, CH. HAGENDORF¹, K. KOSTOV², and ●W. WIDDRA¹ — ¹Martin-Luther-Universität Halle-Wittenberg, Institute of Physics, Halle — ²Bulgarian Academy of Science, Sofia, Bulgaria

The atomic structure and the vibrational properties of ultrathin MnO films on Pt(111) have been studied using high-resolution electron energy loss spectroscopy (HREELS), scanning tunneling microscopy (STM), and low-energy electron diffraction (LEED). The formation of several Mn oxide structures during Mn deposition in an O₂ atmosphere has been investigated as a function of film thickness up to 6 ML, substrate temperature and subsequent annealing cycles up to 1200 K. Within the monolayer, three different Mn_xO_y structures with Mn/O ratios between 1 and 2 have characterized by HREELS, STM, LEED, and thermal oxygen desorption: The MnO monolayer grown in an oxygen atmosphere of about 8x10⁻⁸ mbar is characterized by a strong optical phonon at 364 cm⁻¹, a (19x1) superstructure which is stable up to 1100 K. Annealing in pO₂=1x10⁻⁶ mbar converts this phase to a hexagonal structure with a lattice constant of 0.42 nm and MnO₂

stoichiometry. It shows two characteristic vibrations at 580 and 716 cm⁻¹, is stable up to 840 K and identified as single O-Mn-O layer of MnO(111). Reduction of this phase in CO or annealing above 840 K in UHV results in a third oxide structure with two strong phonons at 332 and 391 cm⁻¹. This oxide is stable up to 1000K.

O 33.4 Tue 16:30 H41

Preparation and Investigation of well ordered thick Silica films on Mo(112) — ●MARTIN BARON, DARIO STACCHIOLA, SARP KAYA, SHAMIL SHAIKHUTDINOV, and HAJO FREUND — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Recently our group has demonstrated the preparation of well ordered thin silica films on Mo(112) substrate [1]. The structure of the film has been determined employing various experimental techniques and theoretical calculations [2]. In this work we use a similar approach for growth of thicker silica films which resemble the structure and properties of bulk silica. The experimental results of XPS, IRAS, STM and LEED will be presented.

[1] Schroeder T, Adelt M, Richter B, et al., SURFACE REVIEW AND LETTERS 7 (1-2): 7-14 FEB-APR 2000

[2] Todorova TK, Sierka M, Sauer J, et al., PHYSICAL REVIEW B 73 (16): Art. No. 165414 APR 2006

O 33.5 Tue 16:45 H41

Layer-resolved study of the local electronic structure of ultrathin NiO(001) films on Ag(001): A STS and DFT study — ●S. GROSSER¹, CHR. HAGENDORF¹, M. DÄNE¹, A. ERNST², M. LÜDERS³, Z. SZOTEK³, W. M. TEMMERMAN³, W. HERGERT¹, and W. WIDDRA¹ — ¹Martin-Luther-Universität Halle-Wittenberg, Institute of Physics, Halle — ²MPI for Microstructure Physics, Halle — ³Daresbury Laboratory, Warrington, U.K.

Scanning tunneling microscopy (STM), scanning tunneling spectroscopy (STS), and density functional theory (DFT) have been applied to study the local electronic and atomic structure of thin NiO films on Ag(001). Differential conductance spectra (dI/dV) for precursor phases, oxide bilayer and thin oxide films up to 5 ML exhibit distinct differences in the electronic structure. The region of the unoccupied states up to 4 eV above E_F is dominated by the local density of states within the oxide film. Especially for 2 ML islands and thicker films strong and well-resolved unoccupied Ni 3d-states are found. At energies above 4.5 eV, the experimental spectra exhibit strong field emission resonances which are characteristically modified by the thickness-dependent oxide band structure. The experimental determined electronic structure will be compared with DFT calculations considering also different magnetic ordering within the NiO film. The strong electron correlation effects in the oxide are taken into account via self-interaction corrections. The calculated layer-dependent evolution of the NiO electronic structure and the appearance of a Ni 3d-derived surface state compare well with the experimental results.

O 33.6 Tue 17:00 H41

Electronic structure and quasiparticle calculations of molecules on thin epitaxial films - a DFT and GW study — ●CHRISTOPH FREYSOLDT, PATRICK RINKE, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der MPG, Berlin, Germany

To study insulator surfaces with surface-science techniques that require conducting samples such as photoelectron spectroscopy or STM epitaxial films are often employed. However, the difference in the dielectric properties between the film and the substrate introduces additional polarization effects that modify the electronic states of the film and of molecules adsorbed on it. Here, we present G₀W₀ quasiparticle calculations that incorporate these effects in a natural way, for the electronic structure of molecule/film/substrate system, using NaCl/Ge(001) as a prototypical insulator/semiconductor interface and CO as a model adsorbate. The atomic structure of the NaCl/Ge(001) in interface – so far unknown from experiment – is determined using density-functional theory. We observe that the quasiparticle gap of CO adsorbed on the NaCl film varies as a function of the film thickness. The dielectric response of the substrate also introduces a z-dependence of the quasiparticle corrections within the NaCl film, which then differ by up to 0.6 eV between the Ge-interface and the surface. In experiments ei-

ther metallic substrates are used or the semiconducting substrates are strongly doped to increase their conductivity. We expect that the effects reported here will be even more pronounced for these substrates due to their larger polarizability.

O 33.7 Tue 17:15 H41

Growth of One-dimensional Pd Nanowires on the Reduced SnO₂(101) Surface — ALEXANDER URBAN¹, ●BERND MEYER¹, KHABIBULAKH KATSIEV², MATTHIAS BATZILL², and ULRIKE DIEBOLD² — ¹Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum — ²Department of Physics, Tulane University, New Orleans, USA

The adhesion of metals on insulating surfaces is usually much weaker than the cohesion within the metal itself. Therefore, in vapor deposition experiments metals do not 'wet' most surfaces of insulators, but 3D cluster formation is observed even at very low metal coverage. In a recent STM experiment [1] however, it was observed that Pd, vapor-deposited on the fully reduced SnO₂(101) surface, forms one-dimensional islands with a uniform width of one substrate unit cell and a height of one atomic layer. Neighboring islands do not merge, and the length of the nanowires is only limited by the size of the substrate terraces. DFT calculations have been performed to investigate the atomic processes which lead to this, for metal oxide substrates unusual, overlayer growth [1] It is found that the one-dimensional wires are not the thermodynamically most stable structure, but their formation is dominated by kinetic effects. A pronounced one-dimensional diffusion, combined with a strong interaction 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 one-dimensional islands.

[1] K. Katsiev, M. Batzill, U. Diebold, A. Urban, B. Meyer, submitted to Phys. Rev. Lett.

O 33.8 Tue 17:30 H41

The initial stages of Chromium growth on Titaniumdioxide-Investigations using synchrotron radiation — ●SEBASTIAN MÜLLER and DIETER SCHMEISSER — Brandenburgische Technische Universität Cottbus, Lehrstuhl Angewandte Physik-Sensorik, Postfach 10 13 43, 03013 Cottbus

We investigate the interface of Cr-TiO₂ during the initial stages of Cr deposition. Experiments are carried out at BESSY II (BL U49/2-PGM2). Using XPS, XAS and ResPES we obtain information about electronic structure at the interface. We confirm the results of growth studies by Christian Winde obtained by TEM-EELS. In addition, we find that Cr deposition induces two gap states which appear about 1 eV and 3 eV below E_F . Using ResPES, these states can be identified as being Cr-like and Ti-like respectively. Core-level-XPS and CIS-spectra of the lower gap state indicate the existence of mainly Cr⁴⁺ at low coverage (< 1 ML).

At higher coverage (\approx 2.5 ML) metallic Cr is observed as well as metallic Ti. Oxidized Cr occurs mainly as Cr³⁺. CIS-spectra of higher gap state show metallic behavior with both Cr- and Ti-like character. CIS-spectra of lower gap-state confirm the existence of Cr³⁺.

Reference: Christian Winde, Herstellung und Charakterisierung von Cr Schichten auf TiO₂ (110)Oberflächen, PhD Thesis, University of Stuttgart, 2002