O 48 Oxide und Isolatoren II

Zeit: Dienstag 15:45–18:30 Raum: TU EB107

O 48.1 Di 15:45 TU EB107

Ordered alumina film on NiAl(110): Structure and nucleation centers — •E. Napetschnig[1], G. Kresse[2], L. Köhler[2], M. Schmid[1], and P. Varga[1] — [1]Institut f. Allgemeine Physik, Vienna University of Technology, Austria — [2]Institut fuer Materialphysik, University of Vienna, Austria

Transition metal clusters on alumina support are one of the most frequently used model systems for investigations of heterogenous catalysis. Oxidation of the (110) surface of NiAl at elevated temperatures leads to the formation of an alumina film of uniform thickness and structure [1]. In spite of many attempts of structural analysis, the atomic structure of the unit cell was unknown until now. Unexpectedly our atomically resolved STM images of the topmost oxygen layer show squares with oxygen atoms at the edges in addition to areas with hexagonal structure. The unit cell has a p2g symmetry. This is an atomic arrangement not found in the known bulk structures of alumina. Based on these STM images the complete determination of the oxide film structure was possible by ab-initio calculations [2]. This was the starting point to determine the nucleation centers of platinum clusters on the alumina film.

[1] M. Bäumer et al., Prog. Surf. Sci. 61 (1999) 127

[2] G. Kresse et al, to be published

O 48.2 Di 16:00 TU EB107

Growth of vanadium oxides on Cu$_3$Au(111) — •Michael Hafemeister, Jürgen Middeke, Ralf-Peter Blum, and Horst Niehus — Humboldt-Universität zu Berlin, Institut für Physik/ASP, Newtonstraße 15, D-12489 Berlin

Systematic studies of the deposition of transition metals on different oxidic substrates illustrate the trend of increased wetting and enhanced growth depending on the oxygen affinity of the deposit. According to the concept of an oxygen-containing substrate we found that different transition metal oxide films (VO$_x$, NbO$_x$, MoO$_x$) of high quality can be obtained on Cu$_3$Au(100). In order to analyze the influence of structural factors of the substrate, the growth of VO$_x$ on Cu$_3$Au(111) has been investigated. STM studies show the 2D growth of a single-phase VO$_x$ film with a honeycomb structure (2.7nm), that can be recognized as a Moiré pattern created by a hexagonal superlattice with a lattice parameter of 0.3nm. This structure could be confirmed by LEED images. The evaluation of AES data suggests a VO stoichiometry. From low energy ion scattering we conclude that the top layer is composed of oxygen. Finally the formation of a VO(111) layer is proposed, exposing a lattice of 0.3nm which is just slightly lager than 0.28nm known from the bulk vanadium monoxide.

O 48.3 Di 16:15 TU EB107

Oxidation and reduction of thin molybdenum oxide layers on Cu$_3$Au(100) — •Jürgen Middeke, Ralf-Peter Blum, and Horst Niehus — Humboldt-Universität zu Berlin, Institut für Physik, ASP, Newtonstr. 15, 12489 Berlin

Recently it has been shown that well defined two dimensional vanadium oxide layers can be created on a Cu$_3$Au(100) surface [1]. The most important step of the preparation technique seems to be oxygen implantation and subsequent annealing of the alloy substrate prior to the transition metal evaporation. Meanwhile the technique was also successfully applied to niobium oxide and molybdenum oxide formation. In this presentation we will focus on oxidation and reduction processes observable at different phases of MoO$_x$ that exhibit either rectangular or hexagonal symmetry. The oxidation and reduction has been followed in situ on an atomic scale by scanning tunneling microscopy.

[1] H. Niehus R.-P. Blum and D. Ahlbehrendt, phys. stat. sol. (a) **187** (2001) 151

O 48.4 Di 16:30 TU EB107

Structural Studies of thin VO_x films grown on TiO_2 using NIXSW — •Emily Kröger[1], Francesco Allegretti[2], Martin Polcik[1], Matthew Knight[2], Vin Dhanak[3], and Phil Woodruff[1,2] — [1]Fritz-Haber-Institut, Faradayweg 4-6, 14195, Berlin — [2]Department of Physics, University of Warwick, Coventry CV4 7AL, UK — [3]Daresbury Laboratory, UK

The aim of this project is to use quantitative structural techniques to obtain information on transition metal oxide surfaces. The Normal Incidence X-Ray Standing Waves (NIXSW) technique is used to investigate the growth of sub-nanometre vanadia films on the rutile titanium dioxide (110) surface. The bulk NIXSW structural parameters for TiO_2 have been successfully fitted. Three different Bragg reflections were used to triangulate the V atom positions and epitaxial film growth for vanadia films grown by post-oxidation has been confirmed. The measurements allowed the decrease in film quality with film thickness to be monitored. In addition, a series of experiments on as-deposited sub-monolayer films were completed. Two components in the X-ray photoelectron spectrum of the V 2p suggest two different V species on the surface and this NIXSW study shows that they take different surface positions.

O 48.5 Di 16:45 TU EB107

Tieftemperatur-STM-Untersuchungen der Morphologie und Defektstruktur von dünnen MgO-Filmen — •Martin Sterrer, Markus Heyde, Niklas Nilius, Hans-Peter Rust und Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Abteilung Chemische Physik, Faradayweg 4-6, 14195 Berlin

Die genaue Kenntnis der Struktur und elektronischen Eigenschaften von Defekten ist unumgänglich für die Aufklärung des Zusammenhangs zwischen Struktur und Reaktivität von Oberflächenzentren. Mittels Raster-Tunnel-Mikroskopie bei 4K wurde die Morphologie eines 4 Monolagen dünnen MgO-Films auf Ag(100) untersucht. Mindestens 4 atomare Lagen des Films sind exponiert, wobei die Terrassen nahezu perfekt georndet sind, Stufen jedoch eine hohe Anzahl von Defekten wie Kinken und Ecken aufweisen. Es wird gezeigt, dass mittels Landungsinjektion von der STM-Spitze elektronische Defekte auf der Oberfläche erzeugt werden können, deren Energieniveaus innerhalb der Bandlücke von MgO liegen. Durch geeignete Wahl der Polarität der Probenspannung ist es möglich, den Ladungszustand der Defekte gezielt zu verändern. Der Vergleich mit theoretischen Berechnungen legt den Schluss nahe, dass es sich bei den Defekten um Farbzentren handelt.

O 48.6 Di 17:00 TU EB107

ESR-spektroskopische Untersuchung zur Bildung und Reaktivität von Oberflächen-Farbzentren auf dünnen MgO-Filmen — •Esther Fischbach, Martin Sterrer, Thomas Risse und Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Abteilung Chemische Physik, Faradayweg 4-6, 14195 Berlin

Die chemischen und physikalischen Eigenschaften von Oxid-Oberflächen werden entscheidend von der Anwesenheit von Defekten beeinflusst. Die Aufklärung der Reaktivität der Oberfläche erfordert daher eine genaue Untersuchung der Natur und elektronischen Eigenschaften von Defektstrukturen. Farbzentren, i.e. neutrale oder einfach positiv geladene Anionenfehlstellen auf MgO, sind in diesem Zusammenhang von herausragender Bedeutung, da sie einerseits durch die Möglichkeit eines Elektronentransfers auf molekulare Adsorbate zur chemischen Reaktivität der Oberfläche beitragen, andererseits die elektronischen Eigenschaften von adsorbierten Metallclustern verändern.

In der vorliegenden Arbeit wurden dünne MgO-Filme (20ML) auf einkristallinen Substraten hergestellt und mittels Elektronen-Spin-Resonanz-Spektroskopie untersucht. Während auf den frisch gewachsenen MgO-Filmen keine Farbzentren detektiert werden konnten, bewirkt Elektronenbeschuss eine deutliche Veränderung der Oberflächen-Morphologie und führt zu einem den Farbzentren zuzuordnenden ESR-Signal. Die Reaktivität der Oberflächen-Farbzentren gegenüber einfachen molekularen Adsorbaten wie O$_2$, CO, N$_2$O und NO wurde untersucht.

O 48.7 Di 17:15 TU EB107

On the electronic structure of LiCoO2 and related compounds used as battery cathodes — •Thissen Andreas[1], David Ensling[1], Qi-Hui Wu[2], Francisco Javier Fernandez Madrigal[1], Stefan Laubach[1], Peter C. Schmidt[1], and Wolfram Jaegermann[1] — [1]FB Material- und Geowissenschaften, Fachgebiet Oberflächenforschung, TU Darmstadt, Petersenstr. 23, D-64287 Darmstadt — [2]Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum, Universitätsstr. 150, D-44780 Bochum

Electronic structure of transition metal oxides is often discussed in terms of ionic bonding in a rigid band model. In this approach the introduction of electrons by alkaliation leads to filling of metal 3d states. In most cases those two approximations are too simple, because of polarcovalent bonding, electron correlation, localization, polaron formation and structural influences, like Madelung-potentials, ligand-field effects and Jahn-Teller-distortion. Stoichiometric, polycrystalline LiCoO2 thin films in the high temperature modification have been prepared by RF magnetron sputtering. From XPS data it has been shown, that the Co-ions are in the formal 3+ low-spin oxidation state. The interpretation of the ResPES data is complicated, because of ligand-hole screening effects. At the Co3p-3d threshold an anti-resonance occurs, from that the O2p and Co3d PVBDOS have been derived, showing good agreement with DFT calculations. Via the preparation of an all solid state micro-battery a route to in-situ measurements of the electronic structure as a function of the lithium content in parallel to electrochemical measurements is presented. This work is funded by DFG (SFB595) and BMBF.

O 48.8 Di 17:30 TU EB107

Surface x-ray analysis of Co grown on NiO(100) — •Christian Tusche[1], Holger Meyerheim[1], Jürgen Kirschner[1], Ulrich Hillebrecht[2], and Carlos Quiros[3] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle — [2]Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich — [3]ESRF, 6 rue Jules Horowitz, F-38043 Grenoble

Ultra-thin ferromagnetic films grown on antiferromagnetic oxides are of interest for fundamental studies of exchange biased systems. Still the role of the microscopic structure of the metal/oxide interface is subject to discussion. Of particular interest is the well known antiferromagnet NiO with thin overlayers of the ferromagnetic elements Fe, Co, Ni.

We have carried out a surface x-ray structure analysis of the Co/NiO(100) interface. About one monolayer of Co was deposited at room temperature on the nonpolar NiO(100) surface. The formation of two layer high CoO islands covering about 25% of the surface area is observed. The interfacial region consists of about one monolayer of a substoichiometric mixed oxide [NiCo]O$_x$ with $x \approx 0.5$. Comparing with bulk NiO the interlayer spacing is expanded by 9%.

The oxygen deficiency in the interface region gives strong evidence for the presence of metal-like Ni and Co in the interface. By formation of uncompensated interfacial spins, this is generally considered to play a major role in exchange bias effects.

O 48.9 Di 17:45 TU EB107

Field emission resonances investigated by scanning tunneling spectroscopy on Ag(001) surfaces and CoO islands on Ag(001) at low temperatures — •Stephan Grosser, Christian Hagendorf, and Wolf Widdra — Martin-Luther-Universität Halle-Wittenberg, FB Physik, Hoher Weg 8, D-06120 Halle(Saale)

Scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) have been applied to study the clean Ag(001) surface and CoO islands on Ag(001). CoO has been grown by reactive deposition of Co in an O$_2$ atmosphere. dI/dV and z(V) spectra in the range from 0 to 19 eV are used to investigate field emission resonances. In constant current mode the STS spectra on Ag(001) show up to 44 resonances.
The influence of the surface band structure, the tip radius and the tip structure on the field emission resonances have been examined. Qualitativ different spectra for the metallic Ag(001) surface and different structural phases of CoO islands have been obtained and will be discussed with respect to the different electronic band structures and work functions.

O 48.10 Di 18:00 TU EB107

A Tensor LEED Structure Determination of a CoO Ultrathin Film on Ag(100) — •Karl-Michael Schindler, Jian Wang, Wolf Widdra, and Henning Neddermeyer — Martin-Luther-Universität Halle-Wittenberg, FB Physik, D-06099 Halle, Germany

A four monolayer thick CoO film has successfully be grown in nearly layer by layer mode on a Ag(100) substrate by evaporating Co in 10^{-6} mbar oxygen with the substrate heated to 470 K. Previous LEED and STM investigations have shown that such films grow pseudomorphic i.e. the CoO accepts the lattice of the substrate, Furthermore, they exhibit maximal long range order and minimal variation in thickness. This makes them the most suitable systems for a structure determination by the analysis of LEED I(V) curves. The one of this study is based on the measurement of 5 inequivalent beams in the range from 30 to 400 eV, with a total energy range of 1025 eV. The calculation of the I(V) curves was performed using the Barbierie-van Hove Symmetrized Automated Tensor LEED(SATLEED) package. As an initial structure bulk values were assumed for the Ag substrate and the CoO film. Regarding the lattice relations at the interface, all three possibilities of high symmetry were tried as initial model structures. In addition films with a thickness of 2, 3, 4, and 5 layers were tried. In the optimization the z positions of the atoms in the two topmost layers, the distance between the CoO film and the Ag substrate, the inner potential and the Debey temperatures were optimized. The structural results of the best-fit model (r-factor: 0.20) will be discussed in comparison to related systems.

O 48.11 Di 18:15 TU EB107

Submonolayer growth of KCl on pristine and oxygen covered Cu(110) — •Michael Vogelgesang, Lars Diekhöner, Vitali Lucia, M. Alexander Schneider, and Klaus Kern — Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart

By forming insulating ultrathin films on metal surfaces one can decrease the interaction of adsorbates with the metal electron system. In the monolayer regime these films are transparent enough to allow electron tunneling. As an example of such a system potassium chloride on Cu(110) has been investigated by low temperature scanning tunneling microscopy. For submonolayer growth at room temperature we find that KCl (100) forms large islands on Cu terraces and grows with its [010] direction along the [$2\bar{2}1$] direction of the Cu(110) substrate. On a Cu(110) O(2x1) substrate the nucleation can be steered as KCl nucleates preferentially on the oxygen covered regions. First results of spectroscopic measurements will also be presented.