O 56: Metal substrates: Epitaxy, growth and adsorbates

Time: Thursday 15:00–19:15

O 56.1 Thu 15:00 SCH A316

The Cu(110) surface state anisotropy as a probe for the initial stages of homoepitaxial growth — •MICHAEL HOHAGE, LIDONG SUN, ALEXANDER DORNINGER, and PETER ZEPPENFELD — Institut für Experimentalphysik, Johannes Kepler Universität Linz, A-4040 Linz, Austria

Reflectance Difference Spectroscopy (RDS) revealed that the Cu(110)surface state anisotropy is an extremely sensitive probe to study adsorption and growth. The high sensitivity originates from the quenching of surface state contribution to the optical anisotropy at 2.1 eV, due to surface state scattering at adsorbates or point defects. Here, we apply this phenomenon to the investigation of the homoepitaxial growth of Cu on Cu(110). The transition from a step-flow growth at high temperatures to a 3D-island growth and finally to a re-entrant layer-by-layer growth at low temperatures can be easily observed. In addition, we were able to study the morphological changes occurring upon annealing after depositing 0.04 ML Cu at 10 K, by monitoring the partial recovery of the surface state anisotropy. The recovery proceeds mainly in two steps: (i) the onset of the adatom diffusion and nucleation of tiny clusters (90 K to 120 K) and (ii) the onset of adatom detachment and ripening of the clusters (> 190 K). Detailed analysis of the data with the help of a kinetic-Monte-Carlo code allows simulating the experimental results quantitatively and permits to quantify the effective cross-section of small ad-clusters for depolarization of the surface state.

O 56.2 Thu 15:15 SCH A316

Evidence for Cu dimer mobility on $Cu(001) - \bullet$ ANJA MICHL, ANDREAS DOBLER, and THOMAS FAUSTER — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

We investigated the homoepitaxial submonolayer growth of Cu on Cu(001) at 300 K. The density of stable Cu islands n_x was measured by scanning tunneling microscopy after thermal deposition at pressures below 5×10^{-11} mbar.

Variation of coverage θ and particle flux F lead to a characteristic behavior of $n_x \propto \theta^{0.20\pm0.05}$ for $\theta \leq 0.11$ ML and $n_x \propto F^{0.40\pm0.02}$ at saturation for $F = 10^{-5}$ to 10^{-2} ML/s. This result is not compatible with standard models of nucleation which predict an exponent i/(i+2)for the flux dependence with the atom number i of the largest unstable islands.

A recent theoretical study [1] concludes that dimer mobility is dominant at 300 K in the experimentally available range of flux. The predicted behavior $n_x \propto \theta^{1/5}$ and $n_x \propto F^{2/5}$ is in excellent agreement with our experimental results.

[1] P. A. Mulheran and M. Basham, Phys. Rev. B 77 (2008) 075427

O 56.3 Thu 15:30 SCH A316

Non adiabatic processes during homoepitaxy of silver and gold films — \bullet Domocos Kovacs¹, Eckart Hasselbrink², and Detlef Diesing² — ¹Institut für Experimentalphysik, Universität Duisburg Essen — ²Institut für Physikalische Chemie, Universität Duisburg Essen

Thin film metal-insulator-metal (MIM) tunnel junctions have been employed in the last years in the investigation of electronic excitations induced by particles at metal surfaces. Such type of junctions act simultaneously as target and detector: While the electronic excitation is produced by the irradiation of the top metal layer, the excited charge carriers (electrons and holes) are detected in the bottom metal layer as an internal emission current. A major advantage offered by the present method in comparison with the methods measuring the external emission is the possibility of detecting excited charge carriers of very low energy (< 5 eV). We show that a MIM junction is suitable for the investigation of the electronic effects accompanying the adsorption of metal atoms from the gas phase onto the surface of a metal film consisting of the same atomic species. Thus, we show that the adsorption of Au(Ag) Atoms at the surface of the top Au(Ag) film of a Au(Ag)-TaO_x-Ta tunnel junction generates hot charge carriers which are finally detected in the bottom Ta film. The relatively large emission yield, of the order of 10^{-4} electrons per incident atom, measured for 15-20 nm Au(Ag) films, indicates that the binding energy of 3-4 eV/atom, released during adsorption, is primarily transferred into the electronic system.

Location: SCH A316

The temperature dependence of film stress in epitaxial Co monolayers on Pt(111) — •SAFIA OUAZI^{1,2}, ZHEN TIAN², ANITA DHAKA², DIRK SANDER², HARALD BRUNE¹, and JÜRGEN KIRSCHNER² ⁻¹Institut de Physique des Nanostructures, EPFL, Station 3, CH-1015 Lausanne, Switzerland — ²Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

We perform combined stress and low energy electron diffraction (LEED) studies to investigate the correlation between film strain and stress during the deposition of several monolayer thin Co films on Pt(111) in the temperature range 250 to 400 K. The quantitative analysis of our cantilever stress measurements indicates a tensile stress of +4.3 GPa in the thickness range between 3 to 7 ML for the investigated growth temperature range. LEED indicates a Moiré-like diffraction pattern, where our quantitative analysis of the in-plane lattice spacing gives a film strain of +1.2% from 1 to 7 ML. We apply continuum elasticity and calculate +5 GPa for the strain-induced film stress, in close agreement with the experimental value. In thinner films, the measured film stress is found to depend sensitively on the growth temperature. We ascribe this strong temperature dependence of the initial stress to the thermally activated Co incorporation into Pt, which relieves surface stress. We discuss our results in view of STM [1], LEED [2], and SXRD[3] studies, and indicate the implication of Pt-Co intermixing for the magnetic anisotropy of this system.

[1] Varga et al., phys. Stat. sol. 187 (2001) 97 [2] Tsay et al., Surf. Sci. 96 (1998) 313 [3] Ferrer et al., Phys. Rev. B 56 (1997) 9848

O 56.5 Thu 16:00 SCH A316 Growth of ultra-thin Ag films on $Ni(111) - \bullet AXEL MEYER^1$, JAN INGO FLEGE¹, SANJAYA SENANAYAKE², FAISAL ALAMGIR³, and JENS FALTA¹ — ¹Institute of Solid State Physics, University of Bremen, 28359 Bremen, Germany — ²Chemistry Department, Brookhaven National Laboratory, Upton, NY 11973-5000, USA — ³Georgia Institute of Technology, Atlanta, GA 30332-0245, USA

The physical and chemical properties of ultra-thin metal films on metallic substrates strongly depend on their morphology and the structure of the buried interface. Hence, detailed knowledge of the growth mechanisms is essential for the creation of new functional materials with novel characteristics. In this contribution, we present a comprehensive structural study of the growth and properties of epitaxial Ag films on Ni(111) by in-situ low energy electron microscopy (LEEM).

For lower temperatures, the growth of the Ag film proceeds in a Stranski-Krastanov mode after completion of the wetting layer, while for higher temperatures layer-by-layer growth is observed. Quantitative information about the film structure were obtained by analyzing the intensity-voltage (I-V) dependence of the local electron reflectivity (IV-LEEM). The corresponding I(V) spectra showed intensity oscillations depending on local thickness of the Ag film due to the quantum size effect (QSE). Modeling of the I(V) spectra was performed both within the framework of a one-dimensional Kronig-Penney model and multiple scattering IV-LEED calculations. The results of both approaches concerning the variation of the layer spacings and interface characteristics for different temperatures and film thicknesses will be discussed.

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Floating of PtRu and PdRu surface alloys on Ru(0001) studied by STM and AES — • ANDREAS BERGBREITER, HARRY E. HOSTER, and R. JÜRGEN BEHM — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm

According to previous studies by scanning tunnelling microscopy (STM) with chemical contrast and Auger electron spectroscopy (AES), deposition of submonolayer Pt (Pd) on Ru(0001) and subsequent annealing to T = 1300 K (1150 K) results in atomically smooth and laterally equilibrated PtRu (PdRu) surface alloys on Ru(0001) confined to the outermost layer [1]. To verify whether or not these surface alloys reflect local equilibrium, the prepared alloys were deliberately buried by > 1 ML of vapor deposited Ru. After surface analysis by STM and AES, these samples were again annealed to the respective surface alloy formation temperature. Both STM and AES confirm that the initially formed surface alloy is recovered by this final annealing step, i.e., both types of surface alloys exhibit a surfactant-like floating

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behavior. We discuss, in how far this behaviour depends on the transport mechanism involved in the surface alloy formation process, and for which types of surface alloys a similar inherent stability is to be expected.

[1] H.E. Hoster et al., Phys.Chem.Chem.Phys. 10 (2008) 3812.

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Atom distribution and interactions in Ag_xPt_{1-x} and Au_xPt_{1-x} surface alloys on $Pt(111) - \bullet RALF$ T. RÖTTER, ANDREAS BERGBREITER, HARRY E. HOSTER, and R. JÜRGEN BEHM — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm

The atom distributions in $Ag_xPt_{1-x}/Pt(111)$ and $Au_xPt_{1-x}/Pt(111)$ surface alloys were studied by high resolution UHV-STM. These surfaces were prepared by submonolayer Ag (Au) metal deposition on Pt(111), followed by annealing at 900 K or 1000 K, respectively, which in both cases results in surface confined 2D alloys, with equilibrated distribution of the components. Both systems show a tendency towards two-dimensional clustering, which fits well to their known bulk immiscibility. Effective cluster interactions (ECIs) will be derived by a quantitative evaluation of the 2D atom distributions in the surface alloys [1]. By comparing the ECIs for PtAg and PtAu on Pt(111), and considering that Ag and Au have almost similar lattice constants, the results allow conclusion on the physical origin of the tendency for clustering.

[1] A. Bergbreiter et al., Phys.Chem.Chem.Phys. 9 (2007) 5127.

O 56.8 Thu 16:45 SCH A316

Growth on nanopatterned gold surfaces — •YASMINE NAHAS^{1,2}, VINCENT REPAIN¹, and SYLVIE ROUSSET¹ — ¹Laboratory Material and Quantum Phenomena, University Paris 7, UMR 7162, 10 rue Alice Domon et Léonie Duquet, 75205 Paris, France — ²Physikalisches Institut, Universität Karlsruhe (TH), Wolfgang-Gaede-Str., D-76131, Karlsruhe, Germany

The magnetic properties of nanometer size objects cause a large interest in technological applications as well as in the fundamental point of view. Ordered growth allows to obtain controlled size and density structures, as shown by the Co/Au(788) system and others [1]. Although basic mechanisms for this ordered growth have been found out, the complexity of atomistic processes on surfaces (and especially on nanopatterned ones) makes the behaviour of such system generally very surprising. I will show variable temperature experiments of the growth of various elements (Fe, Pt, Co, Au) on different naturally patterned surfaces (Au(111) and Au(788)). I will extract some common features to these systems but I will also explain how the thermodynamic properties of each element (crystallographic phase, lattice parameter, binary phase diagram ...) have a strong influence on some characteristics of the nucleation and growth process. Finally, results on the ordered growth of codeposited iron and platinum atoms will be shown. Different experiments varying the relative concentration of iron and the substrate temperature will be discussed in the framework of the nucleation and growth kinetic theory.

[1] V. Repain et al., J. Phys.: Condens. Matter. 18 (2006) S17-S28

O 56.9 Thu 17:00 SCH A316

Novel mechanism of growth of atomic wires on (110) surfaces driven by intermixing — OLEG V. STEPANYUK¹, •NIKOLAY N. NEGULYAEV², PAVEL A. IGNATIEV³, MAREK PRZYBYLSKI³, WOLFRAM HERGERT², ALEXANDER M. SALETSKY¹, and JÜRGEN KIRSCHNER³ — ¹Faculty of Physics, Moscow State University, 119899 Moscow, Russia — ²Fachbereich Physik, Martin-Luther-Universität, D06099 Halle, Germany — ³Max-Planck-Institut für Mikrostrukturphysik, D06120 Halle, Germany

We reveal a novel mechanism of nanowire growth on fcc (110) metal surfaces, which is promoted by interface intermixing of deposited and substrate atoms. We present a theoretical investigation of the selfassembly of 1D nanostructures during room temperature thermal deposition of Fe and Co atoms on Pd(110) in the sub-monolayer regime. Calculations performed by means of density functional theory demonstrate that incorporation of the deposited Fe (Co) atoms into the topmost substrate layer is energetically and kinetically feasible at room temperature. Kinetic Monte Carlo simulations based on ab initio calculated diffusion barriers of relevant atomic processes indicate that the surface diffusion of expelled substrate atoms is responsible for the growth of atomic wires consisting mainly of Pd atoms. We suggest that scanning tunneling spectroscopy could allow to distinguish between Fe (Co) and Pd atomic chains on Pd(110) to confirm our predictions.

O 56.10 Thu 17:15 SCH A316 Kinetic Monte Carlo Simulations of Temperature Programmed Desorption — •THOMAS FRANZ — Faculty of Physics, University of Vienna

We present a simulation of Temperature Programmed Desorption (TPD) experiments using single- and multi-site models on the basis of Density Functional Theory (DFT) calculations. The system under consideration was O/Rh(111), for which adsorption in both fcc and hcp hollow sites was taken into account. The lateral interactions of the adsorbed oxygen atoms were determined by fitting to a set of DFT energies. The calculations of these energies were performed using the Vienna ab-initio simulation package (VASP). Applying Cross Validation, we maximized the predictive power of our parametrization. The calculated desorption spectra were compared with experimental data. We found that for the investigated system the application of a multi-site model is necessary to obtain good agreement with experiment.

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First-principles initial sticking coefficient for O₂ **at Pd(100)** — •JÖRG MEYER and KARSTEN REUTER — Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin (Germany)

Although the first steps in the oxidation of metal surfaces are of fundamental importance e.g. in heterogeneous catalysis, first-principles investigations of the sticking behavior of oxygen molecules are still scarce and center on simple metals like Al(111) [1]. To address catalytically much more interesting transition metals, we apply a divide and conquer approach [2] to study sticking of oxygen on Pd(100): First, an analytical six dimensional potential energy surface (PES) is generated using a neural network to interpolate between several thousand energy data points obtained from density-functional theory in the generalized gradient approximation. After that, the initial sticking S_0 as a function of initial kinetic energy E_0 of the impinging oxygen molecules is calculated by evaluating a sufficiently large number of classical molecular dynamics trajectories on the previously constructed PES. We detail on technical aspects of the employed interpolation strategy, focusing on how symmetry of the (100) surface is exploited to reduce the necessary amount of input data and optimize the interpolation quality. In light of the good agreement of the obtained sticking curve $S_0(E_0)$ with the sparse experimental data, we critically discuss the employed frozen-surface approximation and the importance of electronically nonadiabatic effects for this system.

[1] J. Behler et al., Phys. Rev. Lett. 94 (2005) 036104.

[2] A. Gross, Surf. Sci. Rep. 32 (1998) 291.

O 56.12 Thu 17:45 SCH A316 Adsorption induced surface stress change of O and H on Pt(111) — •ZHEN TIAN, DIRK SANDER, and JÜRGEN KIRSCHNER — Max-Plank Institute of Microsctructure Physics, 06120, Halle, Germany

Surface stress changes induced by adsorption of oxygen and hydrogen on clean Pt(111) surface are measured in a UHV system with an optical beam bending method. Combined low energy electron diffraction (LEED) and stress measurements identify a compressive surface stress change of -2.2 N/m upon formation of a p(2×2)-O structure for an exposure of 120 L oxygen at 5×10^{-7} mbar at room temperature. The exposure of clean Pt(111) to H₂ at $P_{\rm H_2} = 5 \times 10^{-7}$ mbar leads to a compressive surface stress change of -0.5 N/m, which saturates after 5 L. We found that the magnitude of the H-induced surface stress change depends on the H₂ partial pressure. Exposure at higher partial pressure induces larger compressive stress change, e.g. partial pressure of $P_{\rm H_2} = 5 \times 10^{-6}$ mbar induces a compressive stress change of -0.73 N/m. These results are discussed in view of other experimental studies on surface stress[1] and calculations[2] on adsorbate-induced surface stress of Pt(111).

A. Grossmann, W. Erley, and H. Ibach, Surf. Rev. Lett. 2 (1995)
543. [2] P. J. Feibelman, Phys. Rev. B, 56 (1997) 2175.

O~56.13 Thu 18:00 SCH A316 Influence of C-adsorption on the segregation profile of $Pt_{25}Rh_{75}(100)$

 WOLFGANG LANDGRAF, TOBIAS KERSCHER, and STEFAN MÜLLER
Universität Erlangen-Nürnberg, Lehrstuhl für Theoretische Physik 2, Staudtstr. 7, D-91058 Erlangen

As found earlier by experiment [1] and theory [2], the (100) and (111)surfaces of the alloy system Pt₂₅Rh₇₅ show a strong Pt enrichment in the top atomic layer and a Pt depletion in the layer underneath. However, from experiment [1], it appears that for the (100) orientation even a small amount of carbon impurity leads to a considerable decrease in the Pt top layer concentration. We applied density functional theory to analyze quantitatively the influence of C-adsorption on the segregation profile of $Pt_{25}Rh_{75}(100)$. Indeed, we find that the segregation profile tremendously change as function of the C-coverage: Already at $\Theta = 0.5$ the configuration being lowest in energy consists of carbon atoms in hollow sites and pure Rh-layers in the near surface regime. The correlations between structural and energetic properties will be discussed. The corresponding energetics can be used for the construction of a cluster expansion Hamiltonian in order to predict the alloy's most stable segregation profile for arbitrary carbon coverage. Supported by Deutsche Forschungs-Gemeinschaft

[1] E. Platzgummer et al., Surf. Sci. 419, 236 (1999).

[2] S. Müller, M. Stöhr, O. Wieckhorst, Appl. Phys. A. 82, 415 (2006).

O 56.14 Thu 18:15 SCH A316

CuO: template and/or surfactant — •THORSTEN WAGNER, THOMAS BRANDSTETTER, MARTIN OEHZELT, and PETER ZEPPENFELD — Johannes Kepler Universität Linz, Altenberger Str. 69, A-4040 Linz, Österreich

The Cu(110) surface can be structured readily by adsorbing oxygen: If the coverage of oxygen is less than $\theta = 0.5$, the (2×1) reconstructed areas form stripes which are separated by unreconstructed copper areas. These stripes are uniformly distributed and parallel to the [001]-direction. To extend this one-dimensional template to a two-dimensional array we studied the adsorption of oxygen on a vicinal Cu(19191) surface by means of STM. The steps of this surface are perpendicular to the oxygen stripes. However, the formation of the oxygen reconstruction leads to step bunching and individual terraces are significantly broadened. Therefore the periodicity of the copper template is reduced.[1,2]

On the vicinal and the low index copper surface which were prestructured by the CuO stripe phase silver was adsorbed at 660K. Although more than a monolayer of silver was added, the total area covered by the CuO phase was preserved. By means of STM, PEEM, and AES we have determined that the step bunches (forming (111) facets on the vicinal surface) are covered by silver. The experimental results suggest that CuO is acting as a surfactant.

[1] T. Brandstetter et al., Phys. Rev. B 78 (2008) 075402

[2] T. Brandstetter et al., Phys. Rev. B 76 (2007) 245420

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In-situ X-ray Study of the Oxidation of vicinal NiAl(671) — •CLAUS ELLINGER, VEDRAN VONK, NAVID KHORSHIDI, ANDREAS STIERLE, and HELMUT DOSCH — Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, D-70569 Stuttgart

Vicinal surfaces with a regular stepped pattern are used to tailor the growth of oxide films or other epitaxial grown materials. In order to study the role of surface steps and kinks on the oxidation behaviour we investigated a vicinal NiAl(6,7,1) surface consisting of (110) terraces. It was chosen as the flat, oxidized NiAl(110) serves as important template for model catalysts and a tailoring of the ultra-thin alumina film

would open new ways for the growth of nano particles or nanowires. In the presented surface x-ray diffraction study we show that the regular stepped surface is preserved during the initial exposure of 10^{-6} mbar of oxygen at 540 K while the formation of large (110) facets is observed during the annealing process. Thereby the faceting is induced by the ordering of the alumina. In addition, the preferential oxide growth of one out of two possible twin domains is found, probably caused by stress relief at the step edges of the vicinal surface.

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Dissociative adsorption of methane on surface oxide structures of PdPt alloys — • Arezoo Dianat¹, Nicola Seriani², Man-FRED BOBETH¹, WOLFGANG POMPE¹, and LUCIO COLOMBI CIACCHI³ ¹Institute for Materials Science, Dresden University of Technology, Germany — ²Fakultät für Physik, Universität Wien, Austria -³Faculty of Production Engineering, University of Bremen, Germany Oxides of Pd and Pt are known for their high activity in the catalytic combustion of methane. It was reported that bimetallic Pd-Pt oxide systems exhibit higher activity for CH₄ combustion than PdO. To get some insight into the catalytic activity of PdPt we have studied the dissociative adsorption of CH₄ on oxidised PdPt surfaces using DFT. First, the stability of various surface oxides was investigated, including oxygen adsorbed on the surface, subsurface oxygen, and thin oxide films. As base structures for the thin oxide films we have chosen PdO(101)/Pd(100), α -PtO₂/Pt(111) and Pt₃O₄/Pt(100), which show small lattice misfit between film and substrate. Adsorption energies for oxygen on the PdPt surface and in subsurface positions are higher than on the monometals. For thin oxide films, doping of Pd or Pt results in lower mean oxygen binding energies compared to pure Pd and Pt oxide films. The decomposition of CH₄ to CH₃ and H has been found to be endothermic on metal surfaces, but it becomes exothermic on oxidised surfaces. Among the considered monometallic oxide structures, $Pt_3O_4/Pt(100)$ shows the highest CH_4 adsorption energy. For some of the bimetallic oxide configurations considered, the CH₄ adsorption energy was found to be higher than on the monometallic oxides.

O 56.17 Thu 19:00 SCH A316 The Interaction of Hydrogen with the Cobalt(0001) Surface — ZITA HÜSGES and •KLAUS CHRISTMANN — Institut für Chemie und Biochemie der FU Berlin, 14195 Berlin

We report latest data on the interaction of hydrogen with the hexagonal Co(0001) surface in the temperature range between 90 K and 600 K as obtained by means of LEED, thermal desorption spectroscopy (TDS) and work function change measurements. Expectedly, hydrogen adsorbs spontaneously and dissociatively with an initial sticking probability around 0,1. The H atoms form two binding states having desorption energies between 80 and 100 kJ/mole. Interestingly, H adsorption causes only a slight decrease of the work function between 10 and 17 meV near saturation ($^{\sim}$ 0.7 ML). Most notably, a H-induced c(2x2) LEED phase forms around half a monolayer coverage, similar to the H/Ni(111) system. T and coverage dependent LEED intensity measurements suggest a critical temperature of the ordered H phase of about 240 K and a strongly asymmetric phase diagram that points to a H honeycomb structure. Our data will be discussed and compared with previous work on Co(0001)/H and on Ni(111)/H.