O 40 Adsorption an Oberflächen IV

Zeit: Dienstag 10:45–13:00 Raum: TU EB202

O 40.1 Di 10:45 TU EB202

CO adsorption on Ag and Co nanoparticles monitored by SFG and TDS — •Frank Höbel, Günther Rupprechter, and Hans-Joachim Freund — Fritz-Haber-Institut, Faradayweg 4-6, 14195 Berlin

CO adsorption on Al_2O_3 supported Ag nanoparticles and Nb_2O_5 supported Co nanoparticles was studied by sum frequency generation (SFG) vibrational spectroscopy from ultrahigh vacuum (UHV) to 100 mbar, at temperatures from 90 K to 450 K. Under UHV conditions CO binding energies and coverages were examined by thermal desorption spectroscopy (TDS).

Under UHV CO adsorbs on silver only at temperatures below 60 K. Adsorption studies at higher temperature therefore require higher gas pressure, e.g. terminal CO was detected at 50 mbar and 150 K. Results of CO adsorption on a Co-Nb_2O_5 Fischer-Tropsch model catalyst under reaction conditions will be presented.

O 40.2 Di 11:00 TU EB202

Alloy surface segregation in reactive environments via density-functional theory and atomistic thermodynamics — •John Kitchin, Karsten Reuter, and Matthias Scheffler — Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin

The chemical and materials properties of an alloy surface depend sensitively on its detailed surface composition and structure, which in turn can differ substantially from the one of the bulk alloy due to segregation of one species to the surface. Concerning the alloy function e.g. in catalytic or corrosive environments, this surface segregation can furthermore depend on the partial pressures and temperatures in the surrounding, if one alloy component interacts more strongly with a gas-phase species than the other. Instead of solely predicting the chemical and materials properties on the basis of the formal bulk composition, this requires a theory that explicitly considers the effect of the reactive environment.
As a first step in this endeavor, we are extending the concepts of *ab initio atomistic thermodynamics* to address segregation in binary transition metal alloys in the presence of a reactive gas phase. We apply the approach to the (111) surface of Ag_3Pd in an O_2 atmosphere, and find that contrary to the situation in ultra-high vacuum, Pd segregates to the surface at high oxygen pressures. We discuss the difficulties and possible inaccuracies of the *ab initio atomistic thermodynamic approach* with respect to the limited exploration of configuration space and the steps necessary to proceed beyond it.

O 40.3 Di 11:15 TU EB202

Hydrogen-induced relaxations in epitaxial Ni-films on Cu(001) — •W. Meyer[1], M. Krause[1], A. Klein[1], S. Müller[1], L. Hammer[1], K. Heinz[1], D. Sander[2], and J. Kirschner[2] — [1]Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle/Saale

We have investigated the atomic structure and morphology of epitaxial Ni-films on Cu(001) in the coverage regime 2-12 monolayers (ML) as well as their changes upon hydrogen adsorption. Quantitative Low-Energy Electron Diffraction (LEED) and Scanning Tunnelling Microscopy (STM) were applied in-situ. The STM studies show layer-by-layer growth in the coverage range up to 5 ML while thicker films exhibit an increased roughness. The LEED structure determinations reveal a tetragonal distortion (-3.1% on average) of the hydrogen-free Ni-films very close to the predictions of elastic theory (-3.2%). For all coverage values the first layer spacing is reduced even further (by -4.5%). Yet, by adsorption of 1 ML of hydrogen it increases to a value larger than that of deeper spacings whereas the latter are rather unaffected, i.e. the films subsurface tetragonal distortion remains.

The LEED fit allows to detect also the hydrogen atoms. They reside in the 4-fold hollow sites at 0.3 Å above the top Ni layer. It has been proposed that these H-induced changes are also decisive for the accompanied spin reorientation-transition from in- to out-of-plane [1].
[1] D. Sander, W. Pan, S. Quazi, J. Kirschner, W. Meyer, M. Krause, S. Müller, L. Hammer, K. Heinz, Phys. Rev. Lett., in press

O 40.4 Di 11:30 TU EB202

Formation of Fe Clusters on Superstructured Al_2O_3 Films on $Ni_3Al(111)$ — •Anne Lehnert, Regis Decker, Katharina Franke, Stefano Rusponi, and Harald Brune — IPN, EPF Lausanne, Switzerland

Common industrial catalysts consist of small metal particles dispersed on oxide surfaces. In order to prepare a model system to study systematically the catalytic properties as a function of size, shape, and composition, we grow a well-ordered Al_2O_3 film on $Ni_3Al(111)$. The alumina film is known to exhibit a long-range ordered superstructure, partly of electronic origin.

On top of the oxide layer we deposit iron. By using STM, we investigate the formation of iron clusters in dependence of several parameters, such as coverage, deposition and annealing temperature.

O 40.5 Di 11:45 TU EB202

Nanostrukturiertes Eisenwachstum auf einem Aluminiumoxidfilm auf $Ni_3Al(111)$ — •Aleksander Krupski, Stefan Degen, Marko Kralj, Conrad Becker und Klaus Wandelt — Institut für Physikalische und Theoretische Chemie, Wegelerstr. 12, 53115 Bonn

Ein bei einer Temperatur von 1000 K in einer Sauerstoffatmosphäre auf einer $Ni_3Al(111)$-Oberfläche gewachsener doppellagiger Aluminiumoxidfilm weist eine hexagonale Überstructur der Gitterkonstante 2,40 nm auf [1] und erweist sich dadurch als Templat für nanostrukturiertes Eisenwachstum. Die mittels eines Metallverdampfers im UHV bei Raumtemperatur aufgewachsenen Eisenschichten wurden mit Rastertunnelmikroskopie bei Raumtemperatur sowie bei 23 Kelvin untersucht. Es findet ausschließlich Clusterwachstum statt, und die Nukleation der Cluster wird von der Oxidüberstruktur bestimmt. Die aufgewachsenen Cluster besetzen genau die Gitterpunkte dieser hexagonalen Überstructur. In früheren Experimenten wurde bereits Mangan und Vanadium auf den gleichen Oxidilm aufgewachsen [2]. Die Ordnung der Eisencluster ist nicht ganz so gut wie diejenige der Vanadiumcluster, aber deutlich besser als die der Mangancluster. Bei sehr niedrigen Eisenbedeckungen konnte der Templateffekt, den der Oxidfilm auf die Eisennukleation ausübt, deutlich gezeigt werden. Weiterhin wurden tunnelspektroskopische Messungen an einzelnen Eisenclustern durchgeführt, deren Interpretation sich aufgrund der Komplexität des Systems als schwierig erwiesen hat.

[1] A. Rosenhahn et al., J. Vac. Sci. Technol. A 18 (2000) 1923.
[2] C. Becker et al., New J. Phys. 4 (2002) 75.

O 40.6 Di 12:00 TU EB202

Adsorption of superheavy elements on metal surfaces using relativistic density functional theory — •Cristina Sarpe-Tudoran[1], Josef Anton[1], Valeria Pershina[2], and Burkhard Fricke[1] — [1]Institut für Physik, Universität Kassel, D-34109 Kassel, Germany — [2]Gesellschaft für Schwerionenforschung, D-64291 Darmstadt, Germany

The production of isotopes with half-lives of up to 30 min. for element 112 justifies chemical experiments. Using the gas-phase-chromatography technique the adsorption energy of element 112 on an Au surface is aimed to be measured. The theoretical prediction is very complicated. We present here an ab initio embedded-cluster relativistic density functional calculation of this quantity for the element 112 and for its homologue Hg on an Au(100) surface.

Different clusters were designed, corresponding to a top-, hollow-, and bridge-position of the adsorbate relative to the metal lattice in order to check at which position the ad-atom is adsorbed. We present the potential energy curves and the corresponding values of the binding energies and bond lengths. The geometry of the cluster was kept unchanged during the self-consistent calculations.

Our analysis shows that the adsorption energy of element 112 on a gold surface is about 0.12 eV smaller than the corresponding value for the adsorption of Hg on the same surface. This result offers a benchmark to the experimentalist for this value, which is helpful in designing the chemical experiment with element 112.

O 40.7 Di 12:15 TU EB202

Observation of two states of Ce adparticles on Ag(100) — •Markus Ternes, Marina Pivetta, François Patthey, and Wolf-Dieter Schneider — Institut de Physique des Nanostructures, École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

We report on intriguing experimental results obtained with a scanning-tunneling microscope after evaporation of a small amount of Ce on a Ag(100) surface at low temperature (5K). Some adparticles (about 5%) can be switched from their initial state, where they appear large and with featureless dI/dV spectra around E_F, to a state where they appear smaller and with a narrow dip at the Fermi level in the dI/dV spectra. The latter is tentatively interpreted as a Kondo resonance with a Kondo temperature of about 30K. This observation may be related to a change in the 4f electron-valence band hybridization when passing from one state to the other.

O 40.8 Di 12:30 TU EB202

Coverage-dependent adsorption phases of Cs on Cu(111) — •Thomas von Hofe, Jörg Kröger, and Richard Berndt — Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098 Kiel

While the adsorption structure of several alkali metals on noble metal surfaces is well examined, little is known about Cs on Cu(111). We report about atomically resolved STM images of Cs on Cu(111) with coverages $0 < \Theta \leq 0.25\,\mathrm{ML}$ at 9 K. Depending on coverage, we observe four incommensurate rotated and a commensurate phase similar to Cs on Ag(111). We explain the observed rotation angles of the incommensurate phases with a model by McTague and Novaco [1] which was originally developed to explain adsorption structures of argon on graphite.

[1] J.P. McTague, A.D. Novaco, Phys. Rev. B **19**, 5299 (1979)

O 40.9 Di 12:45 TU EB202

Alkali Intercalation in Transition metal dichalcogenides via Steps — •Claudia Ramirez[1], Rainer Adelung[2], Lutz Kipp [3], and Wolfgang Schattke[1] — [1]Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, Leibnizstrasse 15, 24098 Kiel, Germany — [2]Technische Fakultät, Christian-Albrechts-Universität zu Kiel, Kaiserstrasse 2, 24143 Kiel, Germany — [3]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel,Leibnizstrasse 19, 24098 Kiel, Germany

The aim of this work was to understand how alkali metal atoms intercalate into transition metal dichalcogenides (TMDCs). To this end, a detailed investigation into the geometrical and electronic effects on TMDCs caused by adsorption and intercalation of alkali atoms was carried out by means of ab initio density-functional theory. The question of whether the alkali atoms can reach the van der Waals gap from the plain surface through the atomic planes was addressed. Because of the huge energy barrier involved in this process (3.81 eV), this type of intercalation can be excluded. The high value of the barrier suggests that the most probable path of intercalation must be through the edges or defects of the crystal such as steps or dislocations. The diffusion of Li adatom across and along two different steps, $(10\bar{1}0)$ and $(\bar{1}2\bar{1}1)$, was studied. STM experiments favor mainly the two step here considered. A model of alkali intercalation into TMDCs was obtained, namely via a $(10\bar{1}0)$ step.

This work was supported by the Deutsche Forschungsgemeinschaft (DFG), Forschergruppe FOR 353.