O 69: Metal Substrates: Clean Surfaces

Time: Friday 10:15–11:45 Location: H41

O 69.1 Fri 10:15 H41

First-principles based prediction of composition and substitutional ordering in the $Pt_{25}Rh_{75}$(100) surface — •Philipp Welker, Ole Wieckhorst, and Stefan Müller — Universität Erlangen-Nürnberg, Lehrstuhl für Festkörperphysik, Staudtstr. 7, D-91058 Erlangen, Germany

The clean (100) surface of the disordered $Pt_{25}Rh_{75}$ alloy shows a strong tendency towards Pt segregation. Whereas the segregation profile is well known from both, STM- and LEED-investigations [1,2], only little progress has been made in understanding the energetics that lie behind the observed segregation behaviour. We find almost the same Pt enrichment in the first layer as already predicted for the (111) surface [3]. This result can be explained in terms of the difference in surface energies of the two components, being almost the same for both the (111) and the (100) surface. However, the underlying layers in the (100) surface consist mainly of Rh, in contrast to the (111)-surface that shows an oscillatory depth profile. The difference in the layer dependent Pt concentration can be explained by the segregation energies, i.e. the energy gain for the exchange of a Pt atom from the bulk with a Rh atom from the surface. Moreover, the combination of density functional theory (DFT) and cluster expansions with Monte-Carlo-simulations allows for the prediction of the temperature dependence of the substitutional ordering behaviour in the $Pt_{25}Rh_{75}$(100) surface.

[1] E. Platzgummer et al., Surf. Sci. 419 (1999) 236.
[2] E. L. D. Hebenstreit et al., Surf. Sci. 441 (1999) 441.
[3] S. Müller et al., Appl. Phys. A 82 (2006) 415.

O 69.2 Fri 10:30 H41

Influence of defects in the NiAl(100) surface on structure and energy — •Kerrin Dössel, Daniel Lerch, Stefan Müller, and Klaus Heinz — Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr.7, D-91058 Erlangen

The ordered B2-phase of NiAl is stable over a wide composition range around the 1:1 stoichiometry. Therefore, atomic defects such as vacancies or antisites must exist, whose concentration - especially at grain boundaries and surfaces - may heavily influence the stability of the alloy with respect to segregation phenomena. We studied the atomic structure and energetics of the NiAl(100) surface in view of the existence of vacancies and antisites by first-principles calculations and quantitative Low-Energy Electron Diffraction (LEED). The influence of defects on the surface formation and structure and their correlation to segregation will be discussed by use of DFT-based results. The enthalpy of surface formation and the surface structure have been calculated using Density Functional Theory for the ideal surface as well as for different defect types and configurations. The results will be compared to the best-fit structure resulting from our LEED structure analysis.

O 69.3 Fri 10:45 H41

Image-potential states examined by a "Display-Type Analyzer" — •Matthias Gubo and Thomas Fauster — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

The Rydberg-like series of image-potential states is a prototype system for loosely bound electrons at a metal surface. The electronic structure and the femtosecond dynamics of these states are studied by energy- and time-resolved two-photon photoemission.

A two-dimensional, multi-angle energy analyzer is used for electron detection. It consists of an ellipsoidal mirror low pass filter, a retarding field high pass filter, microchannel plates as an area detector and an image processing system for data acquisition [1].

The image-potential states on the clean Cu(001) surface were successfully imaged. The results are in good agreement with previous measurements using hemispherical analyzers. Several methods to analyze the multidimensional data sets are discussed.

[1] D. Rieger, R. D. Schnell, W. Steinmann und V. Saile, Nucl. Instr. Methods 208 (1983) 777

O 69.4 Fri 11:00 H41

Real-space observation of the Kondo-effect on deeply burried Co-Atoms — •Alexander Weismann, Martin Wenderoth, and Rainer Ulbrich — IV. Physikalisches Institut Universität Göttingen; Friedrich Hund Platz 1; 37077 Göttingen

Isolated Co Atoms beneath the Cu(100) surface were prepared by simultaneous deposition of host-metal and impurity-compound under UHV-conditions. Scanning Tunnelling Spectroscopy performed at 6K shows highly anisotropic bulk Friedel-oscillations around the impurities which can be detected even for impurity depths of 15 ML. Due to the real-space properties of the single electron propagator, which depends decisively on details of the host-metals Fermi-surface, the electron density is only influenced in narrowly defined directions from the impurity (electron focusing). A distinct phase-shift of the LDOS-oscillations can be observed around zero bias as a direct consequence of the Kondo resonance of the Co impurity. dI/dU(U) spectra exhibit Fano-lineshapes with a spatially dependent asymmetry. These can be observed only within the regions of high LDOS-modulation while no spectral feature is present directly above a deep Co-Atom.

O 69.5 Fri 11:15 H41

Electron pair emission from surfaces excited with photons and electrons — •Frank Oliver Schumann, Carsten Winkler, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik

It has been shown theoretically that the double photoemission (DPE) intensity from an electronic system consisting of independent electrons vanishes. A non-zero DPE intensity requires electron-electron interaction. However, apart from the simultaneous ejection of two electrons upon photon absorption, another pathway of pair emission exists. It is possible that the photon is absorbed by a single electron. This electron eventually scatters from another electron, which can also lead to pair emission. The question arises to what extent the total coincidence intensity comes from a DPE process. We have addressed this issue by studying the pair emission from a Cu(111) surface excited by 50 eV photons as well as primary electron of 45 eV, which means that the maximum sum energy of the emitted pair is in both instances 40 eV. The experiments were performed with a time-of-flight spectrometer using two channelplate detectors with delay line anodes. As pulsed light source we used the BESSY storage ring in the single-bunch mode. For in-house experiments we employed a pulsed electron gun. We find that the 2D-energy distributions for photon excitation are markedly different from those obtained from electron excitation. Qualitatively this can be understood by the selection rule for double photoemission. Hence, the DPE intensity comes from the absorption of a photon followed by the ejection of an electron pair.

O 69.6 Fri 11:30 H41

Die elektronische Struktur der Ni(111) Oberfläche — •Kai-Felix Braun — Freie Universität Berlin, Arnimallee 14, 14195 Berlin

Mit Hilfe von Rastertunnelspektroskopie wurde bei tifen Temperaturen die Ni(111) Oberfläche untersucht. Punkt- und Flächenspektroskopie wurden auf der reinen und mit Einzelatomen bedeckten Oberfläche aufgenommen. Die Auswertung im Fourierraum ergibt eine hohe Auflösung eines Oberflächenzustandes. Feinstruktur und Aufspaltungen werden diskutiert. Lebensdauern der Oberflächenelektronen wurden über das Abklingverhalten der reflektierten Elektronenwellen an einer Stufenkante bestimmt. Die vergleichbar kleinen Werte sind nicht symmetrisch zur Fermienergie.Eine Oberflächenresonanz unterhalb des Oberflächenzustandes konnte nur an der Stufenkante beobachtet werden.