O 6: Metal Substrates: Clean Surfaces

Time: Monday 11:15–13:00 Location: MA 005

O 6.1 Mon 11:15 MA 005

Imaging phonon excitation with atomic resolution — •Heiko Gawronski and Karina Morgenstern — Institute of Solid State Physics, Department of Surface Science, Leibniz University Hannover, Appelstr. 2, D-30167 Hannover, Germany

Scanning tunneling microscopy (STM), inelastic tunneling spectroscopy (IETS), and d^2I/dV^2-mapping at low temperature are used to investigate vibrations of Au(111) and Cu(111). The low energy peaks in the IET-spectra at 9 meV on Au(111) and 21 meV on Cu(111) are attributed to phonons at surfaces. This phonon energy on Au(111) is not influenced by the different stacking of the surface atoms, but it is considerably influenced by different atomic distances within the surface layer. In addition, the spatial variation of the phonon excitation is measured in d^2I/dV^2-maps on Au(111). These display a novel type of atomic resolution that is explained in terms of site specific phonon excitation probabilities.

O 6.2 Mon 11:30 MA 005

Diffraction and crystal symmetry in electron pair emission from surfaces — •Frank O. Schumann, Carsten Winkler, and Jürgen Kirschner — Max-Planck-Institut f\"{u}r Mikrostrukturphysik, Weinberg 2 , 06120 Halle, Germany

We have investigated the electron pair emission from a Cu(111) surface excited with a primary electron beam of 30.7 eV kinetic energy via a coincidence time-of-flight experiment. The movement of two interacting particles can be described within the so-called two-body problem, where it is shown that the motion of the center-of-mass can be separated from the relative motion. We adopt this notation in our presentation of the data. If we focus on the motion of the center-of-mass, we compute the sum of the in-plane momentum of the pair. Plotting the coincidence intensity as a function of the sum momentum gives a two-dimensional distribution, which displays intensity peaks, if a reciprocal lattice vector is added to the sum momentum of this electron pair and not to the individual electrons. This highlights the fact that the pair as the whole experiences diffraction at the surface. This in turn means that the electrons must be interacting. The interaction within the pair is described by the relative motion. The intensity distribution of this motion reveals the six-fold symmetry of the surface. Both features are only observed, if the valence band electron comes from the vicinity of the Fermi level, where the Cu(111) surface exhibits a Shockley surface state. For an explanation of our observations this electronic state is important.

O 6.3 Mon 11:45 MA 005

Relaxations at the Ag(001) surface: A LEED study — •Michael Huth, Wolfram Münchgesang, Karl-Michael Schindler, and Wolf Widdra — Martin-Luther Universität Halle-Wittenberg, Institut für Physik, Halle, Deutschland

For low-energy electron diffraction a new approach of data recording and postprocessing has been developed. The improved I(V) curves for Ag(001) show low intensity features and additional fine structure of high intensity peaks. By comparing experimental and calculated I(V) curves significant relaxations of the top two layer distances have been determined. The relaxations found basically confirm recent theoretical predictions [1]. Detailed analysis shows that I(V) curves exhibit a strong dependence on the angle of incidence and show that small deviations from normal incidence can remove essential structures from the I(V) curves.

[1] J.-M. Zhang, Y. Shu, K.-W. Xu, Sol. Stat. Comm. 137 (2006) 441

O 6.4 Mon 12:00 MA 005

How Au(100) and Pt(100) reorganize themselves: Large-scale surface reconstructions studied by all-electron DFT — •Paula Havu[1], Ville Havu[1], Patrick Rinke[1,2], Volker Blum[1], and Matthias Scheffler[1,2] — [1]Fritz-Haber-Institut, Berlin, Germany — [2]University of California at Santa Barbara, CA 93106, USA

Pt(100) and Au(100) show large-scale quasi-hexagonal, often called (5×20), surface reconstructions that are intimately linked to the external surface conditions (temperature, absorbates, electrochemistry). The reconstruction energy of Pt(100) is known from a careful calorimetric measurement [1], but earlier first principles studies of both surfaces have so far so far restricted to simpler (5×1) models that neglect the long range aspect of the reconstruction. We here use the new numerical atom centered orbital based all-electron code FHI-aims [2] to determine the full (5×20)-reconstructed surface structure, by means of density functional theory (DFT) calcluations. We compare our results to full-potential LAPW results for older (5×1) models. The full surface reconstruction is investigated both in DFT-LDA and -GGA (PBE functional), both to uncover the precise relaxation mechanism, and to compare quantitatively to the experimental reconstruction energy. [1] Y. Y. Yeo, C. E. Wartnaby, D. A. King, Science **268**, 1731-1732 (1995). [2] V. Blum *et al.*, The FHI-aims project, www.fhi-berlin.mpg.de/aims/

O 6.5 Mon 12:15 MA 005

determination of the DOS in Nb(110) from scanning tunneling spectroscopy — •Stefania C. Bobaru, Berndt Koslowski, and Paul Ziemann — Institut für Festkörperphysik, Universität Ulm, D-89069 Ulm, Germany

We investigate the electronic structure of Nb(110)/Al2O3(0001) by means of Scanning Tunneling Spectroscopy (STS) at 6.2 K. To enable a comprehensive analysis of the local electronic structure of niobium, we employ standard I-V as well as I-z and dI/dz-z spectroscopy. The experimental results will be discussed in the framework of a recently developed method for recovering the electronic density of states (DOS) from STS data [1]. Based on the one-dimensional WKB approximation this method should enable recovering the DOS of the sample semi-quantitatively, and it should allow principally a deconvolution of tip and sample DOS. In this contribution we first elucidate the effect of data evaluation on the recovered DOS separating contributions from the bulk and the surface. We then try to deconvolute the DOS of tip and sample at least partially by comparing I-V data and differential barrier measurements taken at different locations of the sample with the same tunneling tip.

References:

[1] B. Koslowski, Ch. Dietrich, A. Tschetschetkin, P. Ziemann, Phys.Rev. B 75, 035421 (2007).

O 6.6 Mon 12:30 MA 005

Surface electronic structure of Y(0001): A consistent picture — •Michael Budke, Juliet Correa, and Markus Donath — Physikalisches Institut, WWU Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

The photoemission (UPS) spectra of the (0001) surfaces of rare earth single crystals like Sc, Pr, Y, Gd, Tb, Ho and Er show an intense feature at about 10 eV binding energy. Its sensitivity to the degree of surface order led to the acronym "surface order dependent state"(SODS) in the literature [1]. For more than 20 years it remains an unsolved puzzle why the SODS was not observed in photoemission data obtained from clean rare-earth thin films grown on W(110) or Mo(110). On the one hand, experiments performed on rare earth single crystals are known to suffer from inherent impurities. On the other hand, thin films grown on W(110) or Mo(110) are of higher purity but not as well ordered as single crystals due to the considerable lattice mismatch between substrate and film. In our contribution, we give a consistent picture of the surface electronic structure of Y(0001) that explains the differences between single-crystal and thin-film UPS data. Furthermore, we provide evidence that the SODS is in fact due to carbon contamination, and not, as believed for more than 20 years, an indicator for a well prepared, highly ordered surface.

[1] S.D. Barrett, Surface Science Reports **14**, 271 (1992).

O 6.7 Mon 12:45 MA 005

Efficient ab-initio based modelling of segregation profiles in metal alloys for arbitrary bulk concentrations — •Tobias Kerscher and Stefan Müller — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen

As shown recently [1], the combination of density functional theory (DFT) with cluster expansion methods and Monte-Carlo simulations is a powerful tool to model surface segregation in binary metal alloys. However, the predicted surface properties are then restricted to the in-plane lattice parameter defined by the bulk concentration of the alloy. Indeed, a change of the bulk concentration demands the re-calculation of all atomic configurations via DFT being the most time-consuming

factor in the used approach. We will present a cluster-expansion Hamiltonian which provides universal and volume-corrected bulk energetics for all bulk concentrations, and simultaneously, minimizes the number of DFT calculation which have to be performed. This is demonstrated for the [100] direction of the bulk systems $Pt_{25}Rh_{75}$ and $Pt_{50}Rh_{50}$. Our results are in quantitative agreement with experimental measurements.

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