O 36 Structure and dynamics

Time: Thursday 11:15–13:00 Room: WIL C207

O 36.1 Thu 11:15 WIL C207

Living on the Edge: Life and Death of Vacancies in Cu(100) — •Koen Schoots, Thomas H. Beuman, Marcel J. Rost, and Joost W.M. Frenken — Leiden Institute of Physics, Universiteit Leiden, Leiden, The Netherlands

We have used STM to investigate where surface vacancies originate and annihilate on Cu(100).

Because of the extremely high mobility of the surface vacancies, we have been forced to use tracer particles to follow the vacancy motion, in the form of In atoms, incorporated in the top layer. The "slide-puzzle"-diffusion of the vacancies makes the In atoms move through the surface, as has been reported in [1,2].

In the present study, we have employed tailor-made geometries, in which the In atoms were surrounded exclusively by upward or by downward steps. Our STM movies show a striking difference between these two cases, with differences in jump frequencies and average jump lenghts of more than one order of magnitude. These results show that vacancies are primarily created at the upper side of a step and can be formulated in analogy with the energetics of ad-atoms, in terms of an Ehrlich-Schwoebel barrier [3] for surface vacancies.

[1] R. van Gastel et al., Nature 408 (2000) 665, Phys. Rev. Lett. 86 (2001) 1562, Surf. Sci 521 (2002) 10, Surf. Sci. 521 (2002) 26.
[2] M.L. Grant et al., Phys. Rev. Lett. 86 (2001) 4588.
[3] G. Ehrlich et al., J. Chem. Phys. 44 (1966) 1039.

O 36.2 Thu 11:30 WIL C207

Lattice dynamics of an iron monolayer — •Marcel Sladecek[1], A. Chumakov[2], P.T. Jochym[3], J. Korecki[4,5], J. Lazewski[3], K. Parlinski[3], R. Röhlsberger[6], R. Rüffer[2], B. Sepiol[1], T. Slezak[4,5], N. Spiridis[5], S. Stankov[1,2], and G. Vogl[1] — [1]Institut für Materialphysik der Universität Wien, Wien, Austria — [2]ESRF, F-38043 Grenoble, France — [3]Department of Materials Research by Computers, Institute of Nuclear Physics, Polish Academy of Sciences, Cracow, Poland — [4]Faculty of Physics and Nuclear Techniques, AGH University of Science and Technology, Cracow, Poland — [5]Institute of Catalysis and Surface Chemistry, PAS, Cracow, Poland — [6]HASYLAB at DESY, Hamburg, Germany

Nuclear resonant scattering (Mössbauer spectroscopy with synchrotron radiation) allows the direct observation of the phonon density of states (DOS). The resonant feature of the method enables the selective investigation of the dynamics of an iron layer deposited at the surface or at an interface. The results of a systematic investigation of iron layers with thicknesses in the range from 40 ML down to 1 ML deposited on a W(110) substrate are presented and compared with bulk DOS and ab-initio calculations. The observed spectra, which are the first DOS spectra of an uncoated iron monolayer, show a phonon softening due to the broken translational symmetry and an inplane anisotropy.

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O 36.3 Thu 11:45 WIL C207

Dynamics of Heat Transport in Ultrathin Bi-Films on Si(001) Studied by Ultrafast Electron Diffraction — •Andreas Janzen, Boris Krenzer, Ping Zhou, Dietrich von der Linde, and Michael Horn-von Hoegen — Universität Duisburg-Essen, Institut für Experimentelle Physik, 47057 Duisburg

We used Ultrafast Electron Diffraction to study the surface temperature evolution following the intense fs-laser excitation (800 nm, 45 fs, 1.3 mJ/cm^2) of thin, epitaxial Bi(111)-films deposited onto Si(001)-substrates. Reflection high-energy electron diffraction patterns at 7 keV have been recorded in a laser pump-electron probe experiment with ps-time resolution. The transient surface temperature is determined utilizing the intensity drop due to the Debye-Waller effect and comparing the transient diffraction spot intensity with a static calibration measurement. The cooling of a 6 nm thick Bi-film is much slower ($\tau = 640$ ps) than expected for purely diffusive bulk-heat conduction. For the smooth, abrupt Bi/Si-interface, the acoustic mismatch model explains this effect in terms of total internal reflection of phonons at the interface: the phonons are trapped in the Bi-film. The dependence of the cooling rate on the Bi-film thickness and the transition to the regime of diffusive heat transport will also be addressed.

O 36.4 Thu 12:00 WIL C207

First-principles based ground-state analysis of Co subsurface segregation in CoAl(111) — •Christian Riedl, Ole Wieckhorst, Stefan Müller, Lutz Hammer, and Klaus Heinz — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen

As recently shown [1,2], the segregation profile of B2-ordered CoAl surfaces is controlled by tiny off-stoichiometries (Co antisite atoms). By applying the combination of density functional theory with the cluster expansion method and genetic algorithms we present the surface stability diagram of CoAl(111) considering the energetics of thousands of geometrically fully relaxed surface structures. It turns out that Al-Co-Co-Co layer stacking is clearly the most stable configuration in agreement with our earlier DFT and quantitative LEED analysis [2]. We discuss the electronic structure providing reasons for the stability of the Al-Co-Co-Co layer stacking. Furthermore, subsequent Monte-Carlo-simulations allow for the determination of the temperature dependent segregation profile up to the 7th layer as well as for an analysis of substitutional ordering at the surface.

[1] V. Blum et al, Phys. Rev. Lett. **89**, 266102 (2002)
[2] L. Hammer et al., Phys. Rev. B **71**, 075413 (2005)

O 36.5 Thu 12:15 WIL C207

Preparation and characterization of bimetallic AuPt/Pt(111) surface alloys - a quantitative STM study — •Andreas Bergbreiter, Harry E. Hoster, Eleonora Filonenko, and Rolf J. Behm — Department of Surface Chemistry and Catalysis, University of Ulm, D-89069 Ulm

Structures of atomically smooth and laterally equilibrated AuPt/Pt(111) surface alloys have been studied by UHV-STM. The alloys were prepared by Au island deposition onto a Pt(111) single crystal followed by annealing at 1000K. The Au fraction visible by atomically resolved STM images with chemical contrast is correlated to the respective amount of Au deposited on the Pt(111) single crystal prior to annealing. The known bulk immiscibility of AuPt is reflected in a tendency towards phase separation also in two dimensions. Across the whole concentration range, homoatomic bonds dominate the structure and cause the formation of larger homoatomic ensembles. For comparison with other systems, the short range order (SRO) was quantified by Warren-Cowley-parameters. In order to correlate the atomic distribution with adsorption properties and catalytic behaviour in further studies, the surface density of selected homoatomic adsorption sites were calculated.

O 36.6 Thu 12:30 WIL C207

First Principles based prediction of short range order at the $Pt_{25}Rh_{75}$ (111) surface — •Markus Stöhr, Ole Wieckhorst, and Stefan Müller — Universität Erlangen-Nürnberg, Lehrstuhl für Festkörperphysik, Staudtstr. 7, D-91058 Erlangen, Germany

The disordered $Pt_{25}Rh_{75}$(111) alloy surface shows a strong tendency towards Pt segregation. Although the segregation profile and atomic position in the near surface layers are well known by earlier STM and LEED studies [1,2], the reasons for the observed behaviour are widely unknown. We have used the combination of density funtional theory (DFT) with cluster expansions and Monte-Carlo-simulations to model the substitutional ordering behaviour of the $Pt_{25}Rh_{75}$ (111) surface. This approach allows for the determination of the segregation profile, being in good agreement with the experimental data [1,2]. Moreover our approach gives access to the detailed short range order behaviour of the surface, as well as to the geometric structure of the surface.

[1] E. Platzgummer, M. Sporn, R. Koller, S. Forsthuber, M. Schmid, W.Hofer, P. Varga, Surf. Sci. 419 (1999) 236.
[2] E. L. D. Hebenstreit, W. Hebenstreit, M. Schmid, P. Varga, Surf. Sci. 441 (1999) 441.

O 36.7 Thu 12:45 WIL C207

Investigation of kinetic effects in the PtAu/Ru system. — •Eleonora Filonenko, Harry Hoster, and R.J. Behm — Department of Surface Chemistry and Catalysis

In order to explain the catalysic properies of well defined PtAu films,

the behaviour of both metals was investigated in PtAu films deposited on the Ru(0001)monocrystal surfaces. The effect of heating temperature, ratio of both metals and sequential evaporation on the kinetic processes were studied in the model system PtAu/Ru by means of STM analysis. PtAu films were prepared by means of sequential evaporation and annealed. The non-miscibility of Pt and Au on Ru was proved by the carried out experiments, which agrees with the behavior of PtAu alloy in volume. Results are compared with a system PtAu/Pt(111) and discussed.