O 7: Metal Substrates: Adsorption I

Time: Monday 11:15–12:45 Location: H39

O 7.1 Mon 11:15 H39

Ground state search via cluster-expansion for a multi-site adsorption scenario: H in the Ir(100)-5×1-H phase — ●Daniel Lerch, Ole Wieckhorst, Andreas Klein, Lutz Hammer, Stefan Müller, and Klaus Heinz — Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D- 91058 Erlangen

Upon H adsorption the (quasi-)hexagonal 5×1-reconstruction of Ir(100) is lifted and a recently discovered hydrogen induced Ir(100)-5×1-H surface is formed [1]. Thereby, our density functional theory calculations have shown that there is a clear preference for H to adsorb on bridge sites. Within the 5×1 unit cell of the surface, six bridge sites can be found which are energetically relevant. Obviously this constitutes a very large configuration space when trying to determine the ground state configuration for the adsorption of more than one adsorbate per 5×1 unit-cell, or configurations with larger periodicities than the unit-cell. A sensible approach for the treatment of large configuration spaces is the cluster-expansion (CE). Its application to multisite adsorption systems has now been implemented successfully within our CE code UNCLE and used to determine the ground states for the adsorption of up to 1.2 ML H on Ir(100)-5×1-H. This is the first case where the CE formalism has been applied successfully to a problem with multiple adsorbate sites. The results from both DFT and CE will be presented along with experimental findings.
[1] L. Hammer et al. *PRL* **91** (2003) 156101

O 7.2 Mon 11:30 H39

Surface stress change during H-induced surface reconstruction on Ir(100) — ●Zhen Tian[1], Wei Pan[2], Dirk Sander[1], and Jürgen Kirschner[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, — [2]Department of Physics, National Chung Cheng University, Taiwan

Adsorption induced surface reconstructions are in some cases associated with a corresponding surface stress change [1]. In this work, we performed stress measurement during hydrogen exposure that induces structural reonstruction from Ir(100)-(5×1)hex to Ir(100)-(5×1)H surface[2]. We combine stress measurements by the crystal curvature technique with LEED experiments to investigate the correlation between the surface stress change and surface reconstruction. The change in surface stress is measured while introducing onto Ir(100)-(5×1)hex surface at room temperature. The surface stress starts to decrease once hydrogen is offered and gradually saturates when the amount of hydrogen reaches 4 langmuir. The total surface stress change is - 1.75 N/m. We find a linear relation between the surface stress change and the intensity ratio of LEED spots during the reconstruction, which suggests that the surface stress change is directly correlated with the structural transition.
[1] M. J. Harrison, D. P. Woodruff, and J. Robinson, D. Sander, W. Pan, and J. Kirschner, Phys. Rev. B 74, 165402 (2006).
[2] L. Hammer, W. Meier, A. Klein, P. Landfried, A. Schmidt and K. Heinz, Phys. Rev. Lett. 91, 156101 (2003).

O 7.3 Mon 11:45 H39

Surface phase transition in H/W(110) achieved by tuning the Fermi surface nesting vector by Hydrogen loading — Yoichi Yamada, ●Wolfgang Theis, and Karl-Heinz Rieder — Freie Universität Berlin, Berlin, Germany

At a hydrogen coverage of one monolayer, W(110) is known to exhibit a Fermi nesting in its electronic surface states with an incommensurate nesting vector of 0.9 Å^{-1} and a resulting phonon anomaly. Here we show that additional H-adsorption allows a controlled tuning of the nesting vector. As the nesting vector approaches the commensurate value of 1.0 Å^{-1} the phonon anomaly becomes more pronounced, finally disappearing as the surface reconstructs from a clean surface c(2x2) to a p(8x2) superstructure. The gradual change in the nesting vector is attributed to an energetic shift of the surface state as the surface is loaded with additional hydrogen.

O 7.4 Mon 12:00 H39

Dispersion of the O(2x1) Cu(110) surface phonons — ●Klaus Brüggemann and Harald Ibach — IBN-3 Forschungszentrum Jülich , Leo-Brandt-Str. , D-52428 Jülich

In the past the O(2x1) Cu(110) surface was investigated by serveral groups(1) with the main focus on the formation of the (2x1)superstructure built by the CuO-Chains. In this work we present the measurements of the dispersion of the CuO surface phonons. The surface of the Cu single crystal was oxidized with 6 Langmuir Oxygen so that it was fully covered with 1ML of CuO. After annealing to 660K the energy loss spectra of the ordered layer were measured by an HREELS Spectrometer (2) built in our Institute. The scattering plane of the electron beam laid along the [001] and [1-10] directions. In that way we were able to determine the dispersion of the suface phonons along Gamma to Y and Gamma to X of the Brillouin zone. It turned out that the phonon vibration could be tracked at an electron energy of ca. 50eV. In the Gamma to Y direction we measured a TO mode starting at a wavenumber of 750 1/cm in Gamma and ending with 690 1/cm in Y. In the Gamma to X direction was a LO mode starting at 400 1/cm in Gamma and ending with 370 1/cm in X.
(1)H.Ibach et al., Phys. Rev. B 72, 245408 (2005) ; K. Kern et al., Phys. Rev. Lett. 67, 855 (1991) ; O.Skibbe et al. Phys. Rev. B 66, 235418 (2002)
(2)H. Ibach, Electron Energy Loss Spectrometers, Springer Series in Optical Sciences Vol. 63 (Springer, Berlin 1991)

O 7.5 Mon 12:15 H39

Enhanced erosion rate by adsorbates in grazing incidence ion bombardment applications — ●Alex Redinger[1] and Thomas Michely[2] — [1]I. Physikalisches Institut, RWTH Aachen University, 52056 Aachen, Germany — [2]II. Physikalisches Institut, Universität Köln, 50937 Köln, Germany

Noble gas ion bombardment not only causes erosion, but is also known to efficiently remove adsorbates from the retracting surface. However, little is known about the interaction between the impinging ions and the adsorbates and its consequences for the eroding surface. In order to gain more insight into the effects the surface morphology of Pt(111) was investigated by scanning tunneling microscopy after 5 keV Ar$^+$ ion bombardment at an angle of 83° to the surface normal. During the ion bombardment at 550 K the substrate has been exposed to different oxygen partial pressures. At 550 K oxygen adsorbs dissociatively on Pt(111) with a small sticking probability. The analysis shows that for small ion fluences the amount of removed material varies by an order of magnitude in dependence of the oxygen partial pressure. Subsequent annealing experiments were performed to take into account the subsurface damage. The origin of the dependence of the erosion rate on oxygen partial pressure is traced back to an adsorbate induced suppression of surface channeling.

O 7.6 Mon 12:30 H39

Adsorption of Molecules Studied by Collision-energy-resolved Electron Spectroscopy with He*(2^3S) Metastable Atoms: Benzenes, Acetonitrile, and Acetic Acid on the Ag(110) at 80K — ●Andriy Borodin[1,2], Naoki Kishimoto[1], Koichi Ohno[1], and Michael Reichling[2] — [1]Department of Chemistry, Graduate School of Science, Tohoku University, Aramaki, Aoba-ku, Sendai 980-8578, Japan — [2]Department of Physics, University Osnabrueck, Barbarastr. 7, 49076 Osnabrueck, Germany

The interaction between metastable atoms and surfaces can be utilized for electron spectroscopy on surfaces (MIES). This technique is characterized by an extremely high surface sensitivity. Such a technique applied to the gas phase is also widely known as the 2D-PIES method, which provides information on the collision energy dependence of the ionization cross section for interaction between the He*(2^3S) atom and a target. In the presented work we show results of the 2D-method applied to acetonitrile, acetic acid, and benzenes adsorbed on Ag(110).

A strong collision-energy dependence of the band intensities was found for acetonitrile. The C-N group is attractive towards He*(2^3S), especially in a multilayer film, while He*(2^3S)-interaction with CH$_3$-group has a rather neutral character. The intermolecular interaction in adsorbed films was studied for the acetic acid. The acetic acid dimers were found to be formed even in a sub-monolayer film at 80 K. Moreover, the adsorption of C_6H_6, C_6H_5OH, and C_6H_5SH was investigated. Flat adsorption was detected by the collision-energy-resolved technique for films with thickness of about 0.5 ML and 2 ML.