

O 32: Metal Substrates I

Time: Tuesday 10:30–12:30

Location: H42

O 32.1 Tue 10:30 H42

Energy transfer in inert gases-substrate interactions studied by Pt-SiO_x-Si chemo-electronic thin film devices — ●MICHAEL SCHEELE, IYEVGEN NEDRYGAILOV, ECKART HASSELBRINK, and DETLEF DIESING — Fakultät für Chemie, Universität Duisburg-Essen, 45117 Essen, Germany

Energy flow in chemical surface reactions comprise excitation and relaxation of reacting molecules as well as heating and electronic excitation of the substrate. On the other hand, molecules can also take up energy from a heated substrate. Both, energy loss of molecules to the substrate as well as energy take up from the substrate can be detected by means of chemo-electronic devices. These devices are thin film metal-semiconductor or metal-insulator-metal junctions with a top metal electrode of nanometer thickness acting as the substrate. The energy transfer from a heated metal film to a molecular beam of argon, helium or nitrogen can be monitored as a change of the device current driven by a constant bias voltage. The current changes can be a result of a temperature difference across the device. The sensitivity of the device can be tuned by the magnitude and the polarity of the bias voltage and the base temperature of the device.

O 32.2 Tue 10:45 H42

SPALEED and STM studies of the reconstructed Au(100) surface — ●RENE HAMMER¹, ANKE HÖFER¹, MARIO KIEL¹, KLAUS MEINEL¹, and WOLF WIDDRA^{1,2} — ¹Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — ²Max-Planck Institut für Mikrostrukturphysik, D-06120 Halle, Germany

The hexagonal reconstruction of Au(100) has been intensively studied over more than four decades [1]. Nevertheless, some issues regarding the top layer to substrate matching and alignment, respectively, are ambiguously reported. We quantitatively reinvestigated the system by combining the high resolving powers of SPALEED and STM. A Au(100) sample of excellent quality was used showing after cleaning two types of perfect c(26x48) superstructure domains. They are generated by the buckling of quasihexagonal top layers which are characterized by lattice vectors having the length of 0.9575a and 0.9630a, respectively, where a is the interatomic distance of Au(100). The former vectors exactly run along [011] or [01-1] whereas the latter ones deviate by 120.19° from that directions. Ar⁺ ion bombardment at elevated temperatures induced a rotation of the top layers up to angles of ± 0.89°. Sample annealing yields a turning back into the initial top layer alignment. The reorientation proceeds continuously, i.e. all angles between ± 0.89° are observed.

[1] D.G. Fedak and N.A. Gjostein, Surf. Sci. 8 (1967) 77; M.A. Van Hove et al., Surf. Sci. 103 (1983) 189; G.K. Binnig et al., Surf. Sci. 144 (1984) 321; P. Havu et al., Phys. Rev. B 82 (2010) 161418(R).

O 32.3 Tue 11:00 H42

Electron pair emission from Ag(100) — ●LUCIE BEHNKE¹, FRANK O. SCHUMANN¹, and JÜRGEN KIRSCHNER^{1,2} — ¹Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle/Saale — ²Institut für Physik, Martin-Luther-Universität, D-06120 Halle/Saale

A recent (e,2e) study on a Cu(100) surface revealed the importance of pair diffraction. A kinematic pair diffraction model described the results reasonably well. The approach is justified by current (e,2e) theory, which characterizes the in-coming and out-going electrons by LEED and time reversed LEED-states, respectively. To explore the validity of the kinematic model, the experiment was repeated with a Ag(100) crystal. We have systematically studied the electron pair emission from the surface as a function of the primary energy ($E_p = 30$ eV to 67 eV). An improvement to the previous experiment is the ability to measure the primary electron flux. This allows to determine the single/coincidence count rate per incoming electron. In addition, we identify contributions from valence states of different orbital characters. The spectra can be divided into three regions with the help of a theoretical band structure calculation. We focus now on the region near E_f , which has a low DOS. However, in the experiment high intensities were measured. Moreover, the relative spectral contribution from the electrons near E_f is strongly affected by the primary electron energy and display a non-monotonic behavior. The origin of these variations and the similarities and differences with respect to the Cu(100)

surface will be discussed.

O 32.4 Tue 11:15 H42

Electromechanical coupling coefficients of sp-bonded metals from first principles — ●ANJA MICHL^{1,2}, JÖRG WEISSMÜLLER^{1,3}, and STEFAN MÜLLER² — ¹Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — ²Institute of Advanced Ceramics, Hamburg University of Technology, Hamburg, Germany — ³Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany

Coupling between mechanical stress or strain of a surface and its electronic properties is relevant for a range of applications from sensors and actuators to heterogeneous catalysis. In experiment, coupling coefficients are determined via electrochemical experiments, e.g. by measuring the change in electrode potential upon applying tangential strain ϵ to the electrode surface. Theoretically, this coupling strength is obtained as the response of the electronic work function W to strain. Thus, we calculate strain response parameters $dW/d\epsilon$ for several sp-bonded metals from first principles using density functional theory. We find an increasing trend for the coupling coefficients with increasing number of valence electrons. For aluminum the sign is inverted leading to abnormal positive response parameters for all orientations considered. Due to the simple sp-bonded electronic structure of the investigated metals the homogeneous electron gas represents a suitable model system. Based on an analysis of the surface and volume contributions of the work function within the framework of this jellium model, we propose the unusual positive sign to be related to the high electron density of aluminum.

O 32.5 Tue 11:30 H42

Ab-initio modeling of electromechanical coupling at Si surfaces — ●SANDRA HOPPE¹, ANJA MICHL^{1,2}, JÖRG WEISSMÜLLER^{2,3}, and STEFAN MÜLLER¹ — ¹Institute of Advanced Ceramics, Hamburg University of Technology, Hamburg, Germany — ²Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — ³Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany

Electrochemical experiments have revealed a linear dependence of the electrode potential E of metal surfaces on an applied strain ϵ . This electromechanical coupling is characterized by the response parameter $\partial E/\partial \epsilon = \text{const} =: \zeta$. As the potential of zero charge of an electrode surface in electrolyte is closely linked to its work function W in vacuum, ζ is accessible via ab-initio calculations of $\partial W/\partial \epsilon$. The response of the work function to strain has been investigated experimentally and in theory for various metals. In order to gain further insight into the influence of the electronic structure on the work function strain response, we have calculated coupling coefficients for silicon surfaces. Density functional theory with the HSE screened hybrid exchange-correlation functional was applied to obtain accurate Si band structures. In contrast to most metal surfaces, the magnitude of the response parameters does not increase with packing density for Si. This phenomenon is discussed regarding the strongly directional covalent semiconductor bonds and their distortion under applied strain.

O 32.6 Tue 11:45 H42

Fe₃Al surfaces in dry and humid oxygen atmosphere — ●AFSHIN IZANLOU, MIRA TODOROVA, MARTIN FRIÁK, and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

The elastic and corrosion properties of iron-aluminides make them interesting candidates for high temperature applications, but the degradation of these properties at room temperature and in the presence of hydrogen hinder their utilisation. Aiming to understand the mechanisms and interactions, which have such negative impact on the properties of these materials, we study the low-index surfaces of Fe₃Al in dry and humid oxygen environment, combining density-functional theory with thermodynamic considerations. We find mixed terminated surfaces, i.e. containing both Fe and Al, to be most stable and a marked preference for oxygen adsorption in an aluminium rich environment. This result correlates nicely with the observation that Al₂O₃ is the thermodynamically stable oxide, when these surfaces come into contact with oxygen. Water, on the other hand, favours adsorption on

Fe, on which it adsorbs with the oxygen end. Consequences for the corrosion behaviour and protection of these surfaces will be discussed.

O 32.7 Tue 12:00 H42

Interactions of oxidizing species with the Mg(0001) surface: the role of electrostatic contributions — •SU-TING CHENG, MIRA TODOROVA, and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung GmbH

The adsorption of oxidizing species {N,O,F, Cl} on the Mg (0001) surface were studied using density functional theory. We observe a negative adsorbate-induced work function change and an increase in the binding energy with increasing adsorbate coverage, both of which fail to comply with common expectations regarding the adsorption of electronegative elements on a metal surface. Analysing the electronic structure we are able to explain these changes in terms of a redistribution of electrons at the surface, which lowers the surface dipole. We find a correlation between the efficient embedding of the electronegative adsorbates into the electron spill-out from the Mg surface and the size of the adsorbate atoms. The special reduction of the electron spill-out furthermore causes a decrease in the electrostatic energy which dominates the binding energy within the studied adsorption system. The impact of these unusual trends on metal corrosion will be discussed.

O 32.8 Tue 12:15 H42

Joint DFT and STM/LEED investigation of oxygen adsorption on Ir(100)-1x1 — •ANJA MICHL^{1,2}, PASCAL FERSTL³, TOBIAS SCHMITT³, LUTZ HAMMER³, M. ALEXANDER SCHNEIDER³, and STEFAN MÜLLER² — ¹Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — ²Institute of Advanced Ceramics, Hamburg University of Technology, Hamburg, Germany — ³LS f. Festkörperphysik, Universität Erlangen-Nürnberg, Germany

We explore the structure and stability of oxygen overlayers on Ir(100)-1x1 by combining first-principles calculations using density functional theory (DFT) with LEED and STM. The energetics of various ordered superstructures with different adsorption sites and coverages θ are used to construct a surface phase stability diagram. Apart from the well-known (2x1)-br superstructure and a (hypothetical)(1x1)-br phase, we identify two more ground states, which are also characterized by oxygen atoms exclusively occupying bridge positions: a (3x1)-br structure at $\theta = 0.33$ ML and a (4x1)-3br with 3 O-atoms per unit cell at $\theta = 0.75$ ML. Both new phases are verified by experiment, whereby the (3x1)-br structure could be prepared as single phase all over the surface, while the (4x1)-3br was found only as small patches of locally higher coverage within the (2x1)-br phase. Moreover, periodically arranged 1D domain walls with locally reduced oxygen coverage are observed with STM. We compare different models for the atomic structure of the domain walls based on a shifted row reconstruction mechanism of the underlying iridium substrate.