O 34: Metal Substrates: Structure, Epitaxy and Growth

Time: Tuesday 18:15–21:00 Location: Poster A

O 34.1 Tue 18:15 Poster A

Emissivity of polished tungsten surfaces as a function of temperature, detection angle and wavelength — •Mate Puljiz, Sara Wanjelik, and Mathias Getzlaff — Institute of Applied Physics, University of Düsseldorf

The temperature of heated metallic surfaces in UHV chambers is usually measured by infrared pyrometry. Since metals cannot be regarded as black bodies, the material-dependent emissivity must be known in order to obtain accurate temperature data.

In this contribution, we report on the emissivity of a smooth polished tungsten surface with respect to its dependence on temperature, detection angle and wavelength. For this purpose, a temperature measurement using a W/Re thermocouple being in contact with the sample as reference was carried out simultaneously with a pyrometric measurement of the spectral radiance at wavelengths of 0.96 and 1.6 μm in a temperature range from 523 to 2473K. The sample was mounted rotatably in order to allow measurements for different detection angles. Subsequently, the emissivity was calculated using the measured data according to Planck's law. The results show a distinct angular dependence of the emissivity.

O 34.2 Tue 18:15 Poster A

Large potential steps at weakly interacting metal-insulator interfaces — •Menno Bokdam[1,2], Geert Brocks[1], and Paul J. Kelly[1] — [1]Faculty of Science and Technology and MESA+ Institute for Nanotechnology, University of Twente, Computational Materials Science, Enschede, The Netherlands — [2]Faculty of Physics, University of Vienna, Computational Materials Physics, Vienna, Austria

Potential steps exceeding 1 eV are regularly formed at metal|insulator interfaces, even when the interaction between the materials at the interface is weak physisorption. From first-principles calculations on metal|h-BN interfaces we show that these potential steps are only indirectly sensitive to the interface bonding through the dependence of the binding energy curves on the van der Waals interaction. Exchange repulsion forms the main contribution to the interface potential step in the weakly interacting regime, which we show with a simple model based upon a symmetrized product of metal and h-BN wave functions. In the strongly interacting regime, the interface potential step is reduced by chemical bonding.

O 34.3 Tue 18:15 Poster A

STM study of the preparation of superconducting Ta(110) surfaces — Thomas Eelbo, •Vladimir Zdravkov, and Roland Wiesendanger — Department of Physics, Scanning Probe Methods Group, University of Hamburg, Jungiusstr. 11a, D-20355 Hamburg, Germany

Exciting physics is expected on superconductor-ferromagnet interfaces [1]. Scanning tunneling microscopy/spectroscopy (STM/STS) has an great potential to study such systems due to it's lateral, energy and spin resolution capabilities. However, extreme sensitivity of STM/STS to surface contaminations requires a clean sample for reliable experiments. We explore possibilities to obtain clean and homogeneous Ta(110) surfaces which are characterized by STM/STS, by low-energy electron diffraction, and by Auger spectroscopy. In an early stage of the preparation we identify a surface reconstruction which is attributed to oxygen contaminants, favored by oxygen's high solubility and diffusivity within the Ta bulk crystal. We remove the oxygen from the surface by repeated cycles of high-temperature annealing in ultrahigh vacuum and Ar ion sputtering. Using this approach we succeeded in the preparation of surfaces with an effective contaminant-coverage of less than 5%.

[1] Stevan Nadj-Perge et al. , Science 346, 602(2014)

O 34.4 Tue 18:15 Poster A

Gold on Rhenium(10-10): A Combined STM and LEED Study — •Sebastian Schwede and Klaus Christmann — Inst. f. Chemie u. Biochemie FU Berlin

In complementing previous LEED and MEED experiments [1] we have performed an STM and LEED study on the growth of Au films on a Re(10-10) surface. While deposition at 300 K hardly leads to ordered growth, subsequent annealing to 850 K produces rectangular single-crystalline bilayer (BL) islands oriented parallel to the main crystal axes, with a size-dependent surface structure: islands with lengths between ca. 20 - 50 A exhibit a pseudomorphic (1x1) structure, while larger islands can no longer compensate the elastic strain caused by the lattice misfit and form (1xn) surface phases with n = 3, 4, 5. The Au diffusion seems to run via an intermediate precursor state located at and above the Au island edges. Films with Au coverages > 2 BL show a stable (1x8) structure that persists up to surprisingly high coverages of 30 BL. The STM images suggest a unique structural motif for all (1xn) phases that consists, in [0001] direction, of a bilayer line assembly with (n-1) Au bottom rows and (n-2) top rows, followed by an empty (vacant) row, a single Au row and another vacant row. In [1-210] direction the structure matches the Re - Re lattice spacing. [1] C. Pauls and K. Christmann J. Phys.: Condens. Matter 21 (2009) 134012

O 34.5 Tue 18:15 Poster A

Study of atomic layer deposition with scanning tunneling microscopy — •Zied Rouissi, Massimo Tallarida, and Dieter Schmeisser — Department of Applied Physics and Sensors,Brandenburg University of Technology, 03046 Cottbus, Germany

We present a work concerning the study of the initial steps of atomic layer deposition (ALD) with scanning tunneling microscopy (STM). We focus on the role of the substrates which has been often neglected.However, the detailed knowledge of precursor-substrate reactions is important for the understanding of how ALD proceeds. We report on the reaction of the Al-precursor, trimethyl-Al (TMA), on nanostructured surfaces such as Ag nanoclusters and nanostripes prepared by thermal evaporation on HOPG. We characterized the surface before and after one TMA adsorption pulse at room temperature, observing that the morphology of step edges changes after TMA creating a new terraces with a width of 7-10 nm, translated in the direction of the TMA deposition. This shows that, in case of a regular stepped surface, the substrate morphology would keep the same regularity with the translation in a direction privileged by the precursor absorption.

O 34.6 Tue 18:15 Poster A

Thermodynamics of Deposition Flux dependent Intrinsic Film Stress — Amirmehdi Saedi and •Marcel Rost — Kamerlingh Onnes Laboratory, Leiden University, P.O. Box 9504, 2300 RA Leiden, The Netherlands

The growth of polycrystalline films at temperatures above ˜0.2 of the melting temperature is accompanied by compressive stress development after film closure. Mysteriously, a significant part of this stress has a reversible nature: it disappears when the deposition is stopped and re-emerges upon resumption. It has been suggested that the variation of the surface chemical potential upon starting/stopping of the deposition may cause adatoms to diffuse in/out of the grain boundaries leading to the development/relaxation of the intrinsic compressive film stress. However, film growth involves a myriad of atomic processes such that the mystery is not yet solved and new mechanisms and ideas are still published frequently. Here we represent an analytical derivation, in which we address the variation of the chemical potential of the surface, the grain boundaries, and the film, that fully explains the magnitude of the reversible compressive stress using pure thermodynamic arguments. The tremendous stress levels observed in the experiments can indeed be explained by the flux induced density variations in the extremely dilute adatom gas on the surface.

O 34.7 Tue 18:15 Poster A

Temperature-dependent surface structure of *in-situ* cleaved $TlNi_2Se_2$ investigated by STM — •Martin Schmitt[1], Tobias Mauerer[1], Paolo Sessi[1], Hangdong Wang[2], Qianhui Mao[2], Minghu Fang[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Department of Physics, Zhejiang University, Hangzhou 310027, People's Republic of China

Recently, the Ni-chalcogenide $TlNi_2Se_2$ has been identified as a heavy-fermion multiband superconductor with a critical temperature T_C = 3.7 K [1]. We have investigated the temperature-dependent surface structure of *in-situ* cleaved $TlNi_2Se_2$ by means of low- and variable-temperature scanning tunneling microscopy. The cleaving process leads to large atomically flat (001) surfaces with typical terrace width

that exceed 100 nm. These terraces are separated by step edges which—in the vast majority of cases—are multiples of the Tl–Tl layer spacing, $d_{\mathrm{Tl-Tl}} = c/2 = 6.72$ Å. Our results indicate that the $TlNi_2Se_2$ surface structure at $T \leq 120$ K critically depends on the sample temperature during the cleaving process. Low-temperature cleavage leads to a surface which is dominated by a square-shaped ($\sqrt{2} \times \sqrt{2}$) superstructure and coexisting stripes of a (2×1) structure. In contrast, samples cleaved at room temperature exhibit a more irregular "worm-like" superstructure. Temperature-dependent STM data show an irreversible transition from the former to the latter at a temperature above of about 130 K upon heating.
[1] Hangdong Wang *et al.*, Phys. Rev. Lett.**111**, 207001 (2013).

O 34.8 Tue 18:15 Poster A

Structural sensitivity of medium energy intensity data in a LEED analysis — •Lutz Hammer, Pascal Ferstl, and M.Alexander Schneider — Solid State Physics, FAU Erlangen-Nürnberg

The crystallographic analysis of complex surface structures involves the quantitative determination of many structural parameters and hence requires a large experimental data base. For a full-dynamical LEED intensity analysis this means that either data sets taken at various angles of incidence have to be used or the energy range of the normal-incidence analysis has to be extended to significantly higher values. We investigated the implications of the second approach by comparing the structural sensitivity of low (50 - 300 eV) and high energy data sets (550 - 800 eV) obtained for different ordered phases of an oxidized or reduced cobalt submonolayer on Ir(100). As expected, the high energy data show a better sensitivity to structural details within deeply buried layers due to the larger penetration depth of the electron wave field. Although the relative scattering contribution of the surface layer is reduced, the the sensitivity towards structural changes at the very surface hardly diminishes. This compensation is caused by the smaller electron wave length at higher energies that provides an increased spatial resolution. The extension of the energy range thus also improves the reliability of the LEED analysis and may lead in favourite cases to structural uncertainties down to a single picometer.

O 34.9 Tue 18:15 Poster A

Oxygen interaction with Rhenium(10-10): A combined LEED and STM study — •Sebastian Schwede[1], Jörg Lenz[2], and Klaus Christmann[1] — [1]Inst. f. Chemie u. Biochemie FU Berlin — [2]Mantis Deposition GmbH. Mainz

A previous LEED and ARUPS study on the interaction of oxygen with a Re(10-10) surface [1] revealed a series of ordered oxygen phases, among others a c(2x4), a (1x5), a (1x4), and a (1x3) saturation phase. We have reinvestigated this system by means of scanning tunneling microscopy and focused on the growth mechanism and the surface morphology of the O-induced structures. The c(2x4) phase with an oxygen coverage of 0.25 contains one O atom that is located in the hcp site of the unreconstructed Re unit mesh, while a massive oxygen-driven surface reconstruction sets in as the (1xn) phases form for O coverages > 0.5. The (1x3)-2O saturation structure at a coverage of 0.67 can best be explained on the basis of a double-missing row reconstruction as proposed in recent DFT calculations [2]. [1] J. Lenz et al., Surf. Sci. 269/270 (1992) 410 [2] P. Kaghazchi and T. Jacob, Phys. Rev. B81 (2010) 075431

O 34.10 Tue 18:15 Poster A

Effect of Sr on the microstructure and properties of Mg-6Al alloy — •Tayebeh Nayeri and Sina Sadreddini — Department of Materials Science and Engineering, Science and Research Branch, Islamic Azad University, Tehran, Iran.

In this study, microstructures and properties of the Mg*Al alloy with strontium addition are studied. After the addition of strontium, structure analysis was performed to investigate phase evaluation. The potentiostate were also carried out in 3.5% Nacl solution with the results showing that the effect of adding strontium element to magnesium-aluminum alloys on corrosion behavior of this metal was strongly dependent on microstructure of the final alloy (e.g. grain size, type, intermetallic compounds, etc.).The major second phase included Al4Sr and Al2Sr, but the amount and morphology of these compounds was different in the alloys. The results indicated a reduction in the amount of Mg17 Al12 phase and corrosion rate as well as a rise in the resistance to cavitations.

O 34.11 Tue 18:15 Poster A

Initial stage of small molecular adsorption on Li metal: a DFT study — •Martin Callsen and Ikutaro Hamada — Global Research Center for Environment and Energy based on Nanomaterials Science (GREEN), National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

Reliable and efficient storage of energy in secondary batteries is the key for the advance of mobile communication and future electricity driven mobility technologies. Therefore research dedicated to the increase of the power density and the life time of Li based secondary batteries has recently gained a priority status. In order to design new and improved combinations of electrode and electrolyte materials, a comprehensive knowledge of the chemistry of Li is required. We will present density functional theory (DFT) calculations on the initial stage of adsorption of small molecules on low index Li surfaces in order to shed light on the reactivity of the Li electrode with electrolyte fragments.