

O 49: Metal Substrates III: Structure, Epitaxy and Growth

Time: Wednesday 10:30–12:30

Location: H5

O 49.1 Wed 10:30 H5

Internal space analysis of a dodecagonal oxide quasicrystal and its approximants — ●SEBASTIAN SCHENK¹, STEFAN FÖRSTER¹, and WOLF WIDDRA^{1,2} — ¹Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany — ²Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle, Germany

Two-dimensional oxide quasicrystals (OQC) with 12-fold symmetry have recently been derived from ultrathin perovskites on Pt(111) substrates [1,2]. They exhibit a tiling generated from quadratic, triangular, and rhombic elements of equal side length. By lifting the atomic coordinates of the tiling to a four-dimensional hyperspace, the structural properties of these monolayer structures are fully captured. The projection of the four-dimensional coordinates onto the so-called internal space allows a detailed analysis of the long-range ordering of the quasicrystal and a more precise differentiation between quasicrystals and their periodic approximant structures. Two different measures for the strength of the approximant structures will be given. As a tool for distinguishing defective quasicrystals from complex large unit cell periodic structures, the point distribution in the internal space and the phason strain matrix are discussed.

[1] S. Förster et. al., *Nature* **502**, 215 (2013)

[2] S. Schenk et. al., *J. Phys.: Condens. Matter* **29**, 134002 (2017)

O 49.2 Wed 10:45 H5

Electronic structure and property of ZnO/Ag(111): A combined study of UPS, LEED and STM — ●TING-CHIEH HUNG and KARINA MORGENSTERN — Chair of Physical Chemistry I, Ruhr-University of Bochum, Germany

Zinc Oxide (ZnO) is a broad bandgap semiconductor, which is widely used as a catalyst. Therefore, the properties of ZnO have been investigated extensively. However, the microscopic views and properties of ZnO ultrathin film supported by metal single crystal have remained unexplored. We investigate the shifting and broadening of the surface state of Ag(111) with increasing ZnO coverage by ultraviolet spectroscopy (UPS). The UPS surface state results reveal an increasing intensity of the ZnO peak with increasing ZnO coverages, while the intensity of the Ag peak decreases. The low energy electronic diffraction (LEED) pattern shows the orientation of ZnO(0001) on Ag(111) with a lattice constant of (335 ± 1) pm. We also confirmed the Moiré pattern of ZnO(0001) on Ag(111) [1] by our room temperature scanning tunneling microscopy (STM). Further STM results will be presented in this talk.

[1] Q. Pan et al, *Catalysis Letters*, 2014, 144(4), 648-655.

O 49.3 Wed 11:00 H5

Structure analysis of ultrathin NaCl-layers on various metallic substrates — ●KIRA KOLPATZECK, EBRU EKICI, VIJAYA BEGUM, MARKUS GRUNER, ROSSITZA PENTCHEVA, and ROLF MÖLLER — Faculty of Physics and Center of Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

The electronic decoupling of single atoms, molecules or clusters from a metallic substrate gains in importance whenever radiative transitions shall be observed. Moreover, for various surface science methods, such as scanning tunneling microscopy, a non-vanishing surface conductivity is necessary. To combine those two requirements ultrathin insulating layers come into play. We have studied the growth of ultrathin NaCl films with various thicknesses on several copper and gold substrates by low-energy electron diffraction (LEED) and scanning tunneling microscopy (STM) at low temperatures (8 K and 80 K). As well-known from literature [1] the evaporation of NaCl onto a clean Cu(111) surface at room temperature leads to the growth of rectangular monolayer NaCl islands on top of a continuous NaCl film, which covers the surface partially. If the NaCl is deposited onto the heated copper surface, the formation of nanowires associated with dislocation lines is observed in our measurements. The study of evaporated NaCl on Au(110) also reveals two distinguishable superstructures, resulting from different arrangements of the interface atoms.

[1] R. Bennewitz, et al., *Surf. Sci.* **438**, 289 (1999).

O 49.4 Wed 11:15 H5

Helical interdigitation of alpha-L polyalanine investigated by

ambient STM — ●NGUYEN THI NGOC HA¹, YOSSIL PATILTE², and CHRISTOPH TEGENKAMP^{1,3} — ¹Technische Universität Chemnitz — ²Department of Applied Physics, Hebrew University of Jerusalem, Israel — ³Leibniz Universität Hannover, Germany

Polyalanine (PA) has an alpha-helix conformation, which is maintained by hydrogen bonds formed by backbone N-H and C=O groups of the amino acid located three or four residues earlier along the protein sequence. PA has gathered recently a lot of interest as the propagation of electrons along the helical backbone structure comes along with spin polarization of the transmitted electron. Self-assembly of PA molecules on HOPG substrate form two types of hexagonal structures: after showing a hexagonal structure with a next-neighbor distance of around 2.0nm, finally a well-ordered structure with closer lattice parameter (1.2nm) is found. This closed package structure is formed by the interdigitation between adjacent PA molecules due to the formation of additional hydrogen bonds from their helical back-bones and can be kinetically controlled by increasing the deposition temperature. The ordering within helical film refers to new ordering mechanism and can most likely explain the coherence in the electronic transport and high efficiency for the current induced spin selectivity [1] [1] R. Naaman, D. H. Waldeck, *Annu. Rev. Phys. Chem.* **66**, 263-81, 2015.

O 49.5 Wed 11:30 H5

Formation of PtRu surface alloy on Ru(0001) substrate: A kinetic Monte Carlo study — ●DAVID MAHLBERG and AXEL GROSS — Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Deutschland

Optimising the reactivity and selectivity of a specific catalytic reaction by the rational design of heterogeneous catalysts requires a comprehensive understanding of the factors underlying their reactivity and stability. A precise control of surface properties then allows to improve the performance of catalysts. In particular bimetallic surfaces offer the possibility to tailor their catalytic properties by deliberately modifying their composition and/or structural arrangement, which depends on the mixing ratio of the two metal elements.

We have studied the stability of PtRu/Ru(0001) surface alloys by kinetic Monte Carlo simulation using first-principles electronic structure calculations in order to derive the barriers for vacancy diffusion. Thus the structure formation of surface alloys on macroscopic time scales and mesoscopic length scales as a function of composition and temperature can be monitored for varying Pt concentrations. We will analyse the dependence of the diffusion barriers on the particular arrangement of the surface alloy based on the interaction between the constituents.

O 49.6 Wed 11:45 H5

Unexpected surface structure of the Rashba system Te/Ag(111) — ●TILMAN KISSLINGER¹, MAXIMILIAN ÜNZELMANN², HENDRIK BENTMANN², FRIEDRICH REINERT², THOMAS FAUSTER¹, ALEXANDER SCHNEIDER¹, and LUTZ HAMMER¹ — ¹Lehrstuhl für Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg — ²Lehrstuhl für Experimentelle Physik VII, Julius-Maximilians Universität Würzburg

Materials with Rashba-split bands are of interest for the use in spintronics and are intensively studied by experiment and theory [1].

Especially the systems prepared by depositing one third of a monolayer of Pb, Bi, Te or Sb on Ag(111) and Cu(111), which are considered to be substitutional surface alloys, show a Rashba splitting for which the strength strongly depends on the outward relaxation of the guest atoms [2]. However, for the Te/Ag(111) system the Ag₂Te surface alloy structure was never proven so far.

Upon deposition of 0.33 ML of Te on Ag(111) at temperatures between 90 K and 1000 K (and annealing to at least 373 K) we observe the formation of a $(\sqrt{3} \times \sqrt{3})R30^\circ$ -structure. STM measurements reveal a perfectly ordered surface phase with terraces of the width of several thousands of Angströms. Our quantitative LEED-I(V)-analysis shows that the surface is a TeAg honeycomb layer, where the atoms occupy hcp sites of the Ag(111) substrate. This finding is supported by atomically resolved STM measurements and DFT simulations.

[1] G. Bihlmayer et al., *New J. Phys.* **17** 050202 (2015)

[2] Gierz et al., *Phys. Rev. B* **81**, 245430 (2010)

O 49.7 Wed 12:00 H5

Revisiting the O/Cu(111) system (again): Looking through the lens of theoretical surface spectroscopy and microscopy —

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Oxidation of copper surfaces has been investigated for decades with the goal of understanding the rich surface phase space where oxygen interacts readily with copper under reactive conditions. Nevertheless, a systematic and thorough characterization of metal-supported Cu surface oxides is currently far from complete due to their structural complexity and sensitivity to the growth conditions. Here, we survey and study the various possible ultrathin oxidic structures of Cu using first-principles density-functional theory (DFT) calculations. Namely, we report the DFT-derived surface core-level shifts (CLS) and simulated scanning tunneling microscopy (STM) images (where the orbitals of the STM tip are explicitly considered) for various oxidic O/Cu structures, as well as those containing surface defects. Here, we provide a first-principles microscopic picture of the O/Cu(111) system to interpret and explain the structural ambiguities reported in recent CLS and STM experiments.

O 49.8 Wed 12:15 H5

Electronic and atomic structure of Bi(111) and anomalous be-

haviour after ion bombardment — •KUANYSH ZHUSSUPBEKOV¹, BRIAN WALLS¹, ANDREY IONOV^{1,2}, SERGEY BOZHKO^{1,2}, RAIS MOZHCHIL², KILLIAN WALSH¹, and IGOR SHVETS¹ — ¹School of Physics and Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College Dublin, Dublin 2, Ireland — ²Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Russia

Defects in a surface crystal structure of layered materials lead to a local break of surface translational symmetry and can modify the surface states. In this work, Bi(111) surfaces cleaved at low temperature and ion etched are investigated by Low-Energy Electron Diffraction (LEED), X-ray Photoelectron Spectroscopy (XPS), Ultraviolet Photoelectron Spectroscopy (UPS), Scanning Tunneling Microscopy (STM) and Spectroscopy (STS) techniques. STM measurements on the Bi(111) crystal demonstrated different heights of the steps (mono- and bi-layered steps). Furthermore, STS revealed that these steps have slightly different electronic properties, likely correlated to the cleavage breaking covalent (mono-layer) vs Van der Waals (bi-layer) bonds. The Bi(111) surface after ion etching at 110 K and room temperature reveals anomalous behaviour of the surface crystal structure: it results in the formation of flat mono- and bi-layer terraces and surface periodicity as observed by LEED even after continuous ion sputtering. Analysis of the electronic density of states near the Fermi level measured by UPS did not observe a noticeable difference at the Fermi edge.