O 48: Metal & Semiconductor substrates: Structure, epitaxy and growth

Time: Tuesday 14:30–16:00 Location: HSZ/0204

O 48.1 Tue 14:30 HSZ/0204

Electric-field induced formation of a two-dimensional adatom gas on cryogenic Li(110) — Shyam Katnagallu[1], Samuel Mattoso[1], Huan Zhao[1,2], Se-Ho Kim[1,3], Jing Yang[1], Baptiste Gault[1,4], •Christoph Freysoldt[1], and Jörg Neugebauer[1] — [1]MPI for Sustainable Materials, Düsseldorf Germany — [2]State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an, China — [3]Department of Materials Science and Engineering, Korea University, Seoul, Korea — [4]Department of Materials, Royal School of Mines, Imperial College London, UK

The field evaporation behavior of Li at 60 K in atom probe tomography (APT) shows very inhomogeneous distribution on the detector hit map with hot-spot sites accounting for thousands of evaporations, implying an unusual high surface mobility. We therefore investigated the ad-atom energetics and diffusion behavior on the prototypical Li(110) surface in the presence of the very high fields (10^{10} V/m) by density-functional theory. Two key effects are found to jointly explain the experimentally observed behavior. Firstly, free ad-atoms become energetically favorable over kink sites at fields above 10 V/nm, making sizeable ad-atom densities in thermodynamic equilibrium. Secondly, the ad-atom diffusion barrier vanishes at $\sim$11 V/nm due to a degeneracy of the on-top and bridge sites. We suggest that a highly dynamic adatom gas forms, that enables efficient transport to evaporation hotspot sites. Our static calculations are corroborated by molecular dynamics simulations, that show the spontaneous ad-atom emission from a kink-site enabled by the field.

O 48.2 Tue 14:45 HSZ/0204

Structural analysis of the interaction of $\mathrm{H_2S}$ with the $\mathrm{FeO_2}$ chain phase on Ir(100) — •Alexander Wegerich, Eric Engel, and M. Alexander Schneider — Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

On the Ir(100) surface, a self-organised growth of oxide chains of the form Ir(100)-(3 × 1)-$\mathrm{MO_2}$ (M = Mn, Fe, Co and Ni) can be observed. These transition metal oxide chains are shifted by half an Ir(100) lattice constant with respect to the iridium rows [1]. Furthermore, it is possible to reduce these oxide chains to an Ir(100)-(3 × 1)-$\mathrm{MIr_2}$ (M = Mn, Fe, Co and Ni) surface alloy by annealing under $\mathrm{H_2}$ atmosphere, now with the reduced chains aligned to the Ir rows [2].

Using quantitative LEED-IV analyses, STM and DFT, we examine whether the iron oxide chain phase can be structurally changed and/or tuned by reaction with S, the only other non-metallic chalcogen. In contrast to oxygen, sulphur does not create a Ir(100)-(3 × 1)-$\mathrm{FeS_2}$ chain-like phase, but a c(6 × 2) superstructure. Prepared by annealing the $\mathrm{FeO_2}$ chains under a $\mathrm{H_2S}$ atmosphere, the oxide chains are reduced and sulphur adsorbes on them. The so-formed c(6 × 2) can be interpreted as a c(2 × 2)-S adphase on the Ir(100)-(3 × 1)-$\mathrm{FeIr_2}$ chains.

[1] P. Ferstl et al., Phys. Rev. Lett. **117**, 046101 (2016)

[2] P. Ferstl et al., Phys. Rev. B **96**, 085407 (2017)

O 48.3 Tue 15:00 HSZ/0204

STM study of surface evolution and phase stability in Sn/Pt(111) systems — •Qing Shi, Fumio Komori, Masaki Mizuguchi, and Toshio Miyamachi — Nagoya University, Nagoya, Japan

The formation of $\mathrm{Pt_3Sn}$ surface alloys on Pt(111) is of considerable interest for applications in catalysis and topological electronics. Depositing Sn on Pt(111) followed by annealing offers a route to realize atomically flat, single-crystalline $\mathrm{Pt_3Sn}$(111) surfaces suitable for detailed surface studies. Here, we reveal how the annealing process directly controls the surface morphology and local electronic structure in Sn/Pt(111) systems by scanning tunneling microscopy and spectroscopy (STM/S).

In the lower-temperature regime ($<$ 400 K), where a Sn overlayer is stabilized, Sn atomic layers preferentially attach to step edges. The STS measurements indicate that the Sn overlayer is metallic due to hybridization with the Pt substrate. Upon annealing to higher temperatures, the surface undergoes Pt-Sn alloying, leading to the formation of a Pt3Sn phase across the surface. This transition is accompanied by pronounced island coarsening, morphological rounding, and an increase in local disorder, driven by thermally activated atom processes. Equilibrium shape analysis of the alloy islands reveals nearly isotropic step free energies, indicating minimal energetic differences between alternating A- and B-type step edges. Spectra acquired on the $\mathrm{Pt_3Sn}$ terraces show a high density of states near the Fermi level, corresponding to contributions from both bulk and surface electronic states.

O 48.4 Tue 15:15 HSZ/0204

Enhanced thermal switching of an azobenzene derivative via metal doping on graphitic surfaces. — •Nidhi Rawat[1], Hariom Birla[2], and Thiruvancheril G. Gopakumar[3] — [1]Indian Institute of Technology Kanpur, Kanpur, India — [2]Indian Institute of Technology Kanpur, Kanpur, India — [3]Indian Institute of Technology Kanpur, Kanpur, India

The thermal isomerization (switching) of azobenzene derivatives is often limited by high activation barriers, limiting efficient switching between trans and cis configurations induced by heat. In this study, we first examined the thermal induced switching of pristine azobenzene-based thin films and observed no isomerization upon heating. Upon introducing a metal dopant into the films, several morphological changes are observed, across varying molecular coverages, upon heating confirming that thermal switching is readily induced in the doped films. The analysis of the morphology and microscopic structure of the film is analysed using AFM and STM. These results clearly demonstrate that metal doping can effectively modulate the energy barrier and facilitate thermally driven molecular switching. This approach offers a promising pathway to tailor the isomerization dynamics of molecular systems, providing new opportunities for the development of thermally responsive devices.

O 48.5 Tue 15:30 HSZ/0204

Evolution of surface superstructures on altermagnetic MnTe thin films — •Marco Dittmar, Franziska Beisler, Hannes Haberkamm, Lena Hirnet, Maximilian Ünzelmann, and Friedrich Reinert — Exp. Physik VII and Würzburg-Dresden Cluster of Excellence ctd.qmat, Universität Würzburg, Germany

MnTe has recently attracted significant attention as a workhorse altermagnet, where real space spin arrangements give rise to symmetry-driven, momentum-dependent spin splitting without net magnetization. In terms of basic research as well as for enabling high-quality interfaces in potential devices, the investigation of the surface atomic structure of MnTe becomes very important. In this talk, we present an electron diffraction surface analysis of epitaxially grown MnTe thin films, highlighting the factors that govern their surface atomic structure. In particular, we discuss how variations in Te flux and surface evaporation conditions guide the formation and stability of different surface reconstructions, we have found experimentally.

O 48.6 Tue 15:45 HSZ/0204

Atomic structure of MBE-grown Ta-Ge alloy on Ge(001). — •Suhani Singh[1], David Sommers[1], Patrick Strohbeen[2], Yi-Hsun Chen[1], Javad Shabani[2], Arkady Fedorov[1], and Peter Jacobson[1] — [1]School of Mathematics and Physics, University of Queensland, St. Lucia, Queensland 4072, Australia — [2]Center for Quantum Information Physics, Department of Physics, New York University, New York, New York 10003, USA

Tantalum-germanium (Ta-Ge) alloys are a promising option for superconducting devices.[1] Here, we study the atomic-scale structure and thermal evolution of an MBE-grown Ta-Ge alloy film on Ge(001) using scanning tunnelling microscopy (STM) and synchrotron-based soft x-ray photoemission (XPS). A series of annealing steps between 673 K and 873 K smoothed the initially corrugated surface and enabled atomic-resolution STM. Short anneals at 873 K, reveal three-fold symmetric surface domains. Longer anneals at 873 K led to the appearance of square lattice consistent with Ta(100), coexisting with more corrugated regions. Further temperature increase made the surface progressively rougher and difficult to image. Synchrotron-based XPS shows higher temperature annealing produces a Ge-rich surface, suggesting Ta migrates into the bulk. These preliminary results map out how thermal processing affects the Ta-Ge surface and will guide strategies to obtain cleaner, sharper superconductor-semiconductor interfaces.

[1] Patrick J Strohbeen et al. *Molecular beam epitaxy growth of superconducting tantalum germanide*. Applied Physics Letters 124, 9 (2024).