O 30: Metal & Semiconductor substrates: Structure, epitaxy and growth – Poster

Time: Monday 18:00–20:00 Location: P2

O 30.1 Mon 18:00 P2

Structural analyses for S and Te on transition metal chain-like phases on the Ir(100) substrate — •Eric Engel, Alexander Wegerich, and M. Alexander Schneider — Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

The magnetic properties of one-dimensional transition metal oxide chains Ir(100)-(3×1)-MO_2 (M = Mn, Fe) [1,2] may in the case of Mn be tuned by changing the number of oxygen atoms in the chain structure [3]. Here, we present our attempts to replace O by S and Te and the quantitative LEED-IV analyses of the resulting structures.
Dosing H_2S to the MnO_2 or FeO_2 chains leads to the formation of a dominant $c(2 \times 2)$ superstructure. The structural analyses reveal with Pendry R-factors $R_P < 0.11$, that reduced transition metal chains remain as ordered (3×1) structures in the surface layer. The true unit cell of the system is hence a $c(6 \times 2)$ but with only little deviations in the S adsorbate layer from a $c(2 \times 2)$.
For Te, MO_2 chains were reduced in H_2 first, followed by Te deposition. In the case of 1/6 ML Te on the Ir(100)-(3×1)-$FeIr_2$ a (3×2)-Te superstructure emerges, where the Te atoms take positions on pure Ir hollow sites between the Fe-chains ($R_P = 0.123$). For 1/2 ML Te a dominant $c(2 \times 2)$ superstructure appears, again with only slight influences of the metal chains in the Ir(100) surface adsorbate positions.
[1] P. Ferstl et al., Phys. Rev. Lett. **117**, 046101 (2016)
[2] M. Schmitt et al., Phys. Rev. B **100**, 054431 (2019)
[3] J. Qi et al., Phys. Rev. B **107**, 060409 (2023)

O 30.2 Mon 18:00 P2

Structure of Standing Tetracyanoethylene Molecules on Cu(111) and Cu(100) — •Lorenz Brill[1], Jonas Brandhoff[1], Christoph Wachter[2], Roman Forker[1], Oliver T. Hofmann[2], and Torsten Fritz[1] — [1]Friedrich Schiller University Jena, Germany — [2]Graz Universtiy of Technology, Austria

Tetracyanoethylene (TCNE) has been predicted to go through a standing-lying transition on Cu(111) depending on the deposition conditions. However, only disordered growth with a mix of standing and lying molecules has been observed in the past. Here, we present the first evidence of well ordered structures of standing TCNE molecules grown on Cu(111) and Cu(100), observed by low energy electron diffraction and scanning tunneling microscopy. We compare the obtained structures to predictions calculated in thermodynamic equilibrium.

O 30.3 Mon 18:00 P2

Quantitative sputter depth profiling: LEIS measurements and SDTrimSP simulations on silicon oxide — •Julian Pichler, Camil Bocaniciu, Alper Tunga Celebi, and Markus Valtiner — Technische Universität Wien, Wiedner Hauptstr. 8-10, Vienna, 1040, Austria

Precise surface characterization is crucial in semiconductor devices, to guarantee highest quality and optimal device fabrication.

This involves identifying defects, accurate handling of layers and surface contaminations, as well as determining elemental concentrations. This study focuses on a combined interpretation of Low Energy Ion Scattering Spectroscopy (LEIS) measurements on silicon oxide by quantification with references and Monte Carlo simulations with the SDTrimSP code [1]. We calculate surface erosion rates from simulations to deduce layer thicknesses in target materials, under consideration of atomic intermixing effects induced by sputtering.

For silicon oxide on pure silicon we find good quantitative agreement in sputtering depth profiles between LEIS measurements and SDTrimSP simulations for oxide layer thicknesses around 2 nm. We provide an estimation of layer thicknesses within a few Ångstrom and demonstrate intermixing at the interface induced by sputtering.

References [1] Mutzke et al., SDTrimSP Version 6.00, IPP report (2019)

O 30.4 Mon 18:00 P2

Should Doping be illegal at inorganic/organic Interfaces — •Aleksey Sokolov, Christoph Wachter, and Oliver T. Hofmann — Institute of Solid State Physics, Graz University of Technology, Graz, 8010, Austria

Organic/inorganic-semiconductor interfaces are central to the performance of devices such as organic light-emitting diodes and photovoltaic cells. The geometric arrangements of the molecules at the interface, known as polymorphism, heavily influence the properties of the interface, such as ionization energy, electron affinity, and charge mobility. Which arrangement molecules assume under given deposition conditions is governed by a variety of factors, such as the molecular size and shape, the intermolecular interactions as well as the molecule-substrate interactions, particularly the adsorption-induced charge-transfer. The amount of charge transfer, however, is critically determined by the substrate's doping concentration. Although there are now successful methods in predicting stable polymorphs, the role of the substrate doping for the interface polymorphism is not sufficiently understood. In this work, we use density functional theory in combination with the machine learning-driven structure search method SAMPLE to investigate how doping-induced charge transfer influences the thermodynamically stable phases of the example of F4TCNQ on ZnO. The results give insight into the interplay between doping, charge transfer, and interface structure, which can be used to generalize the effects in similar systems.