O 61: Poster Session V: Oxide and insulator surfaces: Structure, epitaxy and growth I

Time: Wednesday 10:30–12:30 Location: P

O 61.1 Wed 10:30 P

High Pressure Oxidation of Copper on Au(111) - A Route towards Bulk-like Cuprous Oxide Films — •Alexander Gloystein[1], Claudine Noguera[2], Jacek Goniakowski[2], and Niklas Nilius[1] — [1]Carl von Ossietzky University, Institute of Physics, D-26111 Oldenburg, Germany — [2]CNRS-Sorbonne University, UMR 7588, INSP, F-75005 Paris, France

As low-pressure oxidation is inefficient to grow Cu2O films of more than monolayer thickness, Cu slabs were oxidized on Au(111) at 50 mbar of oxygen. The procedure results in bulk-like Cu2O films with (111) termination, as concluded from XPS, LEED and STM. Their surface shows a (sqrt3 x sqrt3)R30° reconstruction, also known from bulk crystals. Using DFT, it is assigned to an array of Cu4O nanopyramids that occupy every third Cu-O six ring of the bulk-cut (111) surface and remove the majority of its dangling bonds. Electronically, the films exhibit a p-type conductance behavior with the valence-band maximum located directly at EF. At high temperature, the films decay into Cu2O(111) crystallites and a Cu3O2 surface oxide, the latter resembling the Cu-O monolayer formed upon low-pressure Cu oxidation.

O 61.2 Wed 10:30 P

First-Principles Characterisation of the Diamond(110) Surface Oxygenation State — •Shayantan Chaudhuri[1], Samuel Hall[1], Benedikt Klein[1,2], Andrew Logsdail[3], Julie Macpherson[1], and Reinhard Maurer[1] — [1]University of Warwick, Coventry, United Kingdom — [2]Diamond Light Source, Didcot, United Kingdom — [3]Cardiff University, Cardiff, United Kingdom

Diamond is a material that possesses numerous properties and has applications in a variety of fields. When grown via chemical vapour deposition, the growth rate of the (110) face is typically much faster than the other two dominant crystallographic orientations: (111) and (100). Due to its fast growth rate, both polycrystalline and nanocrystalline diamond have been shown to have a predominant (110) texture. Despite the (110) surface having so much apparent importance, there has been a lack of both experimental and theoretical studies on this surface. Diamond surfaces are typically cleaned in a way prior to use that renders their surfaces oxygen-terminated, which can have numerous effects on the properties exhibited by the diamond. For this reason, it is important to be able to determine the oxygenation state of the (110) surface. Using density functional theory, we determine that the phase diagram of the diamond(110) surface is dominated by a highly stable phase of coexistent carbonyl and ether groups, while peroxide groups become more stable at lower temperatures and higher pressures. Our findings are corroborated by comparing simulated core-level binding energies and vibrational frequencies to experiment.

O 61.3 Wed 10:30 P

Surface reconstructions: challenges and opportunities for the growth of perovskite oxides — Giada Franceschi, Michael Schmid, Ulrike Diebold, and •Michele Riva — Institute of Applied Physics, TU Wien, Austria

Achieving atomically flat and stoichiometric films of complex multicomponent oxides is crucial for integrating these materials in emerging technologies. While pulsed laser deposition (PLD) can in principle produce these high-quality films, experiments often show rough surfaces and nonstoichiometric compositions.

To understand the cause, we follow the growth at the atomic scale from its early stages, using STM. We focus on $SrTiO_3$(110) and $La_{0.8}Sr_{0.2}MnO_3$(110) films. For both, the non-stoichiometries introduced during growth accumulate at the surface. As a result, their surface structure evolves along phase diagrams of surface structure vs. composition [1,2,3]. This can drastically degrade the surface morphology: pits develop on reconstructed areas with different sticking [4]; ill-defined oxide clusters nucleate when the non-stoichiometry introduced is too large to be accommodated in the surface by changing its structure. On the positive side, one can take advantage of the high sensitivity of surface structures to composition deviations to grow films with thickness of several tens of nanometers retaining atomically flat surfaces, and with stoichiometry control better than 0.1% [1].

[1] Phys. Rev. Mater. **3**, 043802 (2019). [2] J. Mater. Chem. A **8**, 22947 (2020). [3] arXiv:2010.05205 (2020). [4] Phys. Rev. Res. **1**, 033059 (2019).

O 61.4 Wed 10:30 P

Thermal (in)stability of the bulk-terminated $SrTiO_3$(001) surface — •Igor Sokolović[1], Giada Franceschi[1], Zhichang Wang[1], Jian Xu[1], Jiří Pavelec[1], Michele Riva[1], Michael Schmid[1], Ulrike Diebold[1], and Martin Setvín[1,2] — [1]Institute of Applied Physics, TU Wien, Vienna, Austria — [2]Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic

The assumption of bulk-terminated perovskite oxide surfaces is common in most studies in literature, mostly based on (1×1) diffraction patterns observed in LEED or RHEED. The same is true for the prototypical $SrTiO_3$(001) perovskite surface, but the only direct evidence of an unreconstructed $SrTiO_3$(001) surface comes from our previous study [1], where it was obtained by cleaving single crystals, and studying the atomically flat surfaces with ncAFM. These surfaces consist of both (1×1)-terminated SrO and TiO_2 terminations, each covered with intrinsic polarity-compensating point defects. Neither of these two terminations is stable upon heating to 500 °C in UHV as clearly shown by ncAFM, despite the (1×1) LEED pattern and no shifts in XPS [2]. The (1×1) termination was also not observed by ncAFM on TiO_2-terminated surfaces prepared by traditional wet-chemistry, which likewise exhibit the (1×1) LEED pattern [2]. These clear evidence that the (1×1) LEED diffraction patterns can originate from subsurface layers below a disordered surface should be taken into account, since the common assumption of a pristine and unreconstructed $SrTiO_3$(001) might not be warranted. [1] Sokolović *et al.*, Phys. Rev. Mater. 3, 034407 (2019), [2] Sokolović *et al.*, arXiv:2012.08831 (2020).

O 61.5 Wed 10:30 P

Role of apical oxygen in oxide thin films — •Judith Gabel[1], Matthias Pickem[2], Philipp Scheiderer[3], Marius Fuchs[3], Berengar Leikert[3], Martin Stübinger[3], Lenart Dudy[4], Jan M. Tomczak[2], Giorgio Sangiovanni[3], Karsten Held[2], Tien-Lin Lee[1], Michael Sing[3], and Ralph Claessen[3] — [1]Diamond Light Source, United Kingdom — [2]TU Wien, Austria — [3]Universität Würzburg, Germany — [4]Synchrotron SOLEIL, France

Owing to their complex phase diagram, transition metal oxides are an interesting playing field for fundamental research but also open up a gateway to novel electronic functionalities. Oxide thin films are of particular importance as they bring along additional parameters to tune the phase diagram. The films are commonly assumed to be stoichiometric and to have an abrupt surface. Using the example of the prototypical correlated metal $SrVO_3$, we demonstrate here that this description overlooks an essential ingredient, apical oxygen adsorbing at the surface, which has to be considered for an accurate description of oxide thin films. The oxygen adatoms, which form even under UHV, change the film stoichiometry and are shown to severely alter the intrinsic electronic structure. They can affect the doping level of the film as well as the energetic order of the atomic orbitals and may lead to the formation of an electronically and magnetically dead surface layer. We demonstrate that, in the presence of apical oxygen, the thickness-dependent metal-insulator transition observed in $SrVO_3$ can no longer be categorized as a purely bandwidth-controlled Mott transition as previously understood.

O 61.6 Wed 10:30 P

A Large Unit Cell Quasicrystal Approximant derived from $SrTiO_3$ on Pt(111): A LEED, STM and STS Study — •Oliver Krahn, Sebastian Schenk, Stefan Förster, and Wolf Widdra — Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

The discovery of a two-dimensional dodecagonal oxide quasicrystal (OQC) formed from $BaTiO_3$ on Pt(111) has pushed the field of ultrathin ternary oxides on metal supports [1]. The OQC structure is based on atomic arrangements in vertices of triangles, squares and rhombuses. Periodically repeated patches of the OQC tiling are known as approximants. In this contribution, we present the largest approximant observed so far, emerging in ultrathin $SrTiO_3$ on Pt(111), homogenously covering the entire substrate surface. As derived from low-temperature scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED), its unit cell spans an area of (44×43)Å^2. Inside the unit cell, 48 Ti atoms are seen by STM, which form the vertices of 48 triangles, 18 squares and 6 rhombuses. Interestingly, this structure can be understood as a unit cell doubling of a previously reported approximant resulting from a glide mirror symmetry [2]. Detailed studies of the electronic structure by scanning tunneling spectroscopy (STS) reveal the metallic behaviour of the film around the Fermi energy and the independence of the local electronic structure from different vertex configurations in the unoccupied states regime.

[1] S. Förster, O. Krahn et al., Phys. Status Solidi B **257**, 1900624 (2020)

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

O 61.7 Wed 10:30 P

Subtle differences between periodic and aperiodic 2D ternary oxides determined from photoemission spectroscopy

— •Loi Vinh Tran, Maniraj Mahalingam, Oliver Krahn, Stefan Förster, and Wolf Widdra — Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

The discovery of oxide quasicrystals (OQCs) in two-dimensional ternary oxides on metal support has triggered many studies in this field in recent years [1,2]. Here, for the first time, the single-phase preparations of approximants in a periodic hexagonal wagon-wheel structure (WW) and a six-membered ring (6Net) network structure are reported, which are known from mixed phases [3]. This enables a side-by-side comparison between the aperiodic OQC and two distinct periodic superstructures of the same material by means of X-ray, UV photoemission spectroscopy (XPS, UPS). These periodic structures together with the OQC system are distinguished in terms of stoichiometry, workfunction, and atomic density measured by XPS, UPS and STM. Changes in workfunctions from 3.8, via 4.0, to 4.2 eV for the OQC, WW, and 6Net structures, respectively, are observed. On the other hand, XPS reveals a decreasing Ba:Ti ratio for the same sequence of structures as well as the atomic density measured by STM. The implications of these observations on different structural properties of BaTiO3 will be discussed.

O 61.8 Wed 10:30 P

Charge Deposition on SrTiO3 as a Model for Spacecraft Surface Charging

— •Mirco Wendt[1], Franziska Dorn[1], Regina Lange[1], Jens Berdermann[2], Ingo Barke[1], and Sylvia Speller[1] — [1]Institute of Physics, University of Rostock, 18059 Rostock, Germany — [2]Institute for Solar-Terrestrial Physics, German Aerospace Center (DLR), 17235 Neustrelitz, Germany

Differential charging due to high energy particle bombardment is a common reason for hardware degradation and sensor errors in spacecrafts. As a model for studying charge accumulation and dynamics, we propose SrTiO3, a transparent oxide with charges deposited by utilising the electron beam of a scanning electron microscope (SEM). In a first step, we show that charges deposited on SrTiO3 (100) surfaces can be observed in ambient environment by force microscopy methods (AFM). Using a plate capacitor model [1], we also estimate the total deposited charge and charge density. To meet the conditions at medium earth orbit and to address more extended life times, in situ AFM-SEM studies in UHV environment are set up.

[1] A. Berkowitz, et al, Appl Phys Lett 74, 472 (1999)

O 61.9 Wed 10:30 P

Metal-supported two-dimensional ternary oxides: A case study of BaTiO$_x$ on Pd(111)

— •Friederike Wührl, Sebastian Schenk, Oliver Krahn, Stefan Förster, and Wolf Widdra — Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany

The discovery of a quasicrystalline phase in ultrathin films of BaTiO$_x$ (BTO) on Pt(111) opened a new field of research on ternary oxides on metal substrates [1]. The dodecagonal oxide quasicrystal (OQC) shows up in a two-dimensional wetting layer, for which atomically-resolved scanning tunneling microscopy (STM) images show the Ti subgrid decorating the vertices of three tiling elements with equal edge lengths: square, triangle and rhombus [2]. To elucidate the role of the substrate on the formation of OQCs, we report here on a growth study of ultrathin BTO films on Pd(111). Upon annealing in UHV at 930 K to 1030 K, reduced BTO forms long-range ordered two-dimensional layers encapsulating the Pd substrate. In these wetting layers a series of structures has been identified by means of STM and LEED. Depending on the preparation conditions, the different structures follow triangle-rhombus, triangle-square or in case of the largest ones triangle-square-rhombus tilings. They can be classified according to their atom density per unit area. Although the largest unit cell, which covers an area of $(2.6 \times 6.4)\,\mathrm{nm}^2$, host a complex triangle-square-rhombus tiling, an aperiodically ordered structure has not been detected on Pd(111).

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

[2] S. Förster *et al.*, Phys. Status Solidi B, 1900624 (2019)