

O 74: Oxide and Insulator Surfaces

Time: Wednesday 18:15–21:00

Location: Poster A

O 74.1 Wed 18:15 Poster A

Archimedean snub square tiling in a BaTiO₃ derived epitaxial film on Pt(111) — MARTIN TRAUTMANN¹, STEFAN FÖRSTER¹, FLORIAN SCHUMANN¹, CHRISTIAN TEICHERT^{1,2}, •KLAUS MEINEL¹, and WOLF WIDDRA^{1,3} — ¹Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — ²Institute of Physics, Montanuniversität Leoben, A-8700 Leoben, Austria — ³Max-Planck Institut für Mikrostrukturphysik, D-06120 Halle, Germany

Under specific conditions, ultrathin BaTiO₃ films on Pt(111) develop a 2D quasicrystalline structure of twelve-fold rotational symmetry which is composed by an aperiodic arrangement of triangular, quadratic, and rhombic tiling elements [1]. Searching for the basic mechanisms of its formation, a periodic approximant has been identified. It merely consists of the triangular and quadratic elements of the quasicrystal that arrange in a snub square tessellation. In vertex notation, this structure can be described as (3.3.4.3.4) pattern, which has already been considered by Kepler in his general analysis of Archimedean tilings [2]. Applying STM, LEED, and SPA-LEED, the corresponding lattice parameters and the epitaxy matrix with respect to the Pt(111) substrate are determined with high precision. STS indicates that Ti³⁺-O vacancy clusters are constituents of that structure similar to the case which has been deduced for the quasicrystal. The film structure found is an important additional nanoscale observation of the - hitherto rare - five-vertex motives in 2D interface tessellations.

- [1] S. Förster, et al., Nature 502, 215 (2013).
[2] J. Kepler, Harmonices Mundi, Johannes Planck, Linz (1619).

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Initial stages of epitaxy for the growth of ultrathin MgO layers on Fe₃O₄/MgO(001) — •TABEA NORDMANN¹, OLGA SCHUCKMANN¹, TIMO KUSCHEL², KARSTEN KÜPPER¹, and JOACHIM WOLLSCHLÄGER¹ — ¹Physics Department, Osnabrueck University, Germany — ²CSMD, Physics Department, Bielefeld University, Germany

Magnetite (Fe₃O₄) is a promising candidate for electrode material in magnetic tunnel junctions (MTJs) due to its theoretically predicted 100% spin polarisation at the Fermi edge. For high quality MTJs the crystalline structure of the tunneling barrier is as important as the structure of the magnetite. An interesting insulating material for MTJs consisting of magnetite is MgO because of the small lattice mismatch between magnetite and MgO of 0.3% and the symmetry filtering effect of MgO.

In this study the influence of the substrate temperature on the growth of MgO tunneling barriers (thickness 1-3 nm) on Fe₃O₄(001) films was investigated. Especially the growth mode and the quality of the crystalline structure of the MgO films were analyzed. The MgO films were deposited in several steps by reactive molecular beam epitaxy (RMBE). After each step x-ray photoelectron spectroscopy (XPS) and low energy electron diffraction (LEED) were performed. The analysis of the XPS measurements reveal island- and layer-plus-island growth at substrate temperatures between 25 °C to 200 °C and layer-by-layer growth at 250 °C. According to the LEED measurements the crystallinity of the MgO increases with the substrate temperature.

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Ab initio study of anatase and brookite phases doped with cerium — •LUKAS SOJKA¹, BARBORA KACEROVSKA¹, LENKA MATEJOVA², and DOMINIK LEGUT^{3,2} — ¹Nanotechnology Centre — ²Institute of Environmental Technology — ³IT4Innovations Centre, VSB-TU Ostrava, Ostrava, Czech Republic

TiO₂ is a well known photocatalyst [1], its efficiency in visible-light spectrum could be enhanced further. One way is to create oxygen vacancies or Ti³⁺ defects. Another way is by doping *e.g.* by lanthanides. Here we consider cerium doped TiO₂ in the anatase and brookite phases. Our results were obtained using *ab initio* calculations. The electronic structure and thermodynamical properties (enthalpy of formation) of Ce doped TiO₂ phases were investigated under pressure as motivated by experimental studies of processing of Ce-doped titania precursors by pressurized and supercritical fluids. Furthermore, the effect of doped cerium concentration on band gap and optical properties of titania was investigated. Two valences, *i.e.* Ce³⁺/Ce⁴⁺ were considered. The calculations were performed using the VASP code [2]

and the generalized gradient approximation [3] was used to account for exchange-correlation effects. The financial support of the Grant Agency of the Czech Republic (project reg. No. 14-23274S) is acknowledged. **References:**

1. D. O. Scanlon et al., Nature Mater. **12**, 798 (2013).
2. G. Kresse, J. Furthmüller, J. Comput. Mater. Sci. **6**, 15 (1996).
3. J.P. Perdew, K. Burke, M. Ernzerhof, Phys. Rev. Lett. **77**, 3865 (1996).

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ZnO growth on c-plane sapphire: Insights from ab initio simulations — •MARC LANDMANN, EVA RAULS, and WOLF GERO SCHMIDT — Universität Paderborn, Germany

The layer quality of heteroepitaxial ZnO films, grown on the most common c-plane sapphire substrate suffers from the large lattice mismatch between both materials. In order to reduce the defect density of ZnO films, the introduction of MgO buffer layers turned out to be beneficial. [1] In addition, the MgO buffer-layer approach facilitates the polarity control of ZnO films grown on c-plane sapphire. Experimentally, a Zn-polar (+c) growth has been observed for MgO layer thickness greater than 3 nm. In contrast, an O-polar (-c) film growth has been observed for layer thickness less than 2 nm. [2] Here, we have studied the ZnO growth process on the sapphire c-plane surface with and without inclusion of MgO buffer layers of varying thicknesses by state-of-the-art density functional theory calculations. Our results provide new insights into the fundamental growth dynamics of ZnO films and the driving forces behind the ZnO surface polarity.

- [1] M. W. Cho, A. Setiawan, H. J. Ko, S. K. Hong, and T. Yao, Semicond. Sci. Technol. **20**, 13 (2005) [2] H. Kato, K. Miyamoto, M. Sano, and T. Yao, Appl. Phys. Lett. **84**, 4562 (2004)

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Electronic structure of cerium titanates - first-principles calculations — •BARBORA KACEROVSKA¹, LUKAS SOJKA¹, LENKA MATEJOVA², and DOMINIK LEGUT^{3,2} — ¹Nanotechnology Centre — ²Institute of Environmental Technology — ³IT4Innovations Centre, VSB-TU Ostrava, Ostrava, Czech Republic

Cerium titanates offer broad range of technological applications because of their optical and catalytic properties. Cerium titanate can form various phases, which depend on the oxidation state of cerium. In CeTiO₄ and CeTi₂O₆ compounds cerium is in the oxidation state Ce⁴⁺. The latter is a safe analogue to actinide-containing brannerite-like titanate phase (*e.g.* UTi₂O₆) used for nuclear waste storage. We have investigated electronic structure of these compounds as well as CeO₂ using *ab initio* calculations. For CeTiO₄ we considered both orthorhombic and monoclinic phases. Furthermore, the influence of pressure applied to Ce titanate phases on various properties was revealed. Electronic structure, thermodynamical and optical properties were calculated using the single-electron framework of density functional theory employed in VASP code [1]. For the exchange-correlation term the generalized gradient approximation was considered [2]. The financial support of the Grant Agency of the Czech Republic (project reg. No. 14-23274S) is acknowledged.

References:

1. G. Kresse, J. Furthmüller, Phys. Rev. B **54**, 11169 (1996).
2. J.P. Perdew, K. Burke, M. Ernzerhof, Phys. Rev. Lett. **77**, 3865 (1996).

O 74.6 Wed 18:15 Poster A

Influence of strain on the adsorption site of Au anions on epitaxial NaCl films — •WOLFRAM STEURER¹, BRUNO SCHULER¹, NIKO PAVLICEK¹, LEO GROSS¹, JASCHA REPP², IVAN SCIVETTI³, MATS PERSSON³, and GERHARD MEYER¹ — ¹IBM Research-Zurich, Switzerland — ²University of Regensburg, Germany — ³University of Liverpool, UK

We present a detailed experimental and theoretical study of Au adatoms adsorbed on 2–10 ML thick NaCl films grown on Cu(111), Cu(100), and Cu(311) surfaces. Atomically-resolved scanning tunneling microscopy and atomic force microscopy images reveal a clear influence of lattice strain: Whereas Au anions adsorb in a site bridging two Cl atoms on unstrained and tensionally strained films, compressive strain shifts the energetically favored adsorption position to a site on

top of a chlorine atom. Using a simplified density-functional theory approach to handle charged adsorbates, we show that, apart from the interaction with the metal substrate, the stability of the on-top site strongly depends on the lattice mismatch between the NaCl film and the Cu substrate, indicating the possibility to engineer the adsorption

site of adsorbates by means of the film thickness and lattice parameter.

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