O 87: Metal Substrates: Structure, Epitaxy and Growth

Time: Thursday 10:30–13:00 Location: WIL C307

Invited Talk O 87.1 Thu 10:30 WIL C307

Structure and redox dynamics of ultrathin ceria films and nanostructures — •Jan Ingo Flege — Institute of Solid State Physics, University of Bremen, Bremen, Germany — MAPEX Center for Materials and Processes, University of Bremen, Bremen, Germany

Cerium oxide is of considerable importance for a wide range of technological applications including, e g., energy harvesting, storage, and conversion, chemical sensing, and heterogeneous catalysis. Epitaxially grown ceria thin films and nanostructures represent important model systems allowing for the investigation of their peculiar materials properties using surface science methodology. In this presentation, I will focus on the growth and characterization of cerium oxide ultrathin films and microparticles on transition metal surfaces and the subsequent monitoring of their structural and chemical modifications in reactive environments using low-energy electron microscopy and related methods. Starting from the frequently employed ceria(111)/Ru(0001) inverse model catalyst [1], it will be demonstrated that nanoscale structural transformations that occur upon chemical reduction, thermal annealing, or reoxidation can be followed in real-time. Furthermore, it will be shown that in situ probing during epitaxial growth facilitates a deeper understanding of the prevailing mechanisms, which may be exploited to selectively synthesize ceria(001) nanostructures and microparticles [2, 3] for model catalytic studies.

[1] D. C. Grinter et al., Appl. Catal., B 197, 286 (2016).
[2] J. Höcker et al., J. Phys. Chem. C 120, 4895 (2016).
[3] J. I. Flege et al., Nanoscale 8, 10849 (2016).

O 87.2 Thu 11:00 WIL C307

Growth and Magnetism of Fe Thin Films on Rh(111) — •Matthias Vogt, Nicolai Seubert, Martin Schmitt, Jeannette Kemmer, and Matthias Bode — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We present a growth study of monolayer and bilayer Fe films on Rh(111) monitored by scanning tunneling microscopy. The arrangement of the Fe layers on the surface can be influenced to a certain extent by varying the post-annealing temperature, but Fe tends to form high islands with small terrace size under these conditions. Large flat Fe terraces were only observed when the sample was heated during evaporation. Whereas the first layer seems to grow pseudomorphic, the second layer exhibits zig-zag–shaped arrays, which seem to be suppressed in areas with high defect densities. They share many aspects with the Fe double-layer on Ir(111) reported previously [1] and resemble a periodic herringbone pattern. For the Fe double-layer on Rh(111) the periodicities amount to about 1.58 nm between the ribs and about 14.5 nm from backbone to backbone. The results of measurements performed with magnetically coated probe tips will be presented and discussed to identify the underlying Fe spin structure.

[1] P.-J. Hsu *et al.*, Phys. Rev. Lett. **116**, 017201 (2016).

O 87.3 Thu 11:15 WIL C307

Spectroscopic observation and molecular dynamics simulation of Ga surface segregation in liquid Pd-Ga alloys — •Mathias Grabau[1], Jannis Erhard[2], Nicola Taccardi[3], Sandra Krick Calderon[1], Andreas Görling[2], Peter Wasserscheid[3], Christian Papp[1], and Hans-Peter Steinrück[1] — [1]Physikalische Chemie II, Friedrich-Alexander Universität Erlangen-Nürnberg (FAU) — [2]Theoretische Chemie, FAU — [3]Chemische Reaktionstechnik, FAU

Pd-Ga alloys with 0.8, 1.8 and 4.7 at.% of Pd were examined as a function of temperature between 400 and 750 K using angle-resolved x-ray photoelectron spectroscopy (XPS). The Pd surface concentration is found to depend on temperature. This is explained by the transition from a liquid phase to a two-phase system, consisting of a buried solid Ga_5Pd phase and a liquid Pd-Ga alloy, which leads to Pd depletion of the liquid phase. In the liquid phase, Pd was depleted from the vacuum/liquid interface, as deduced from the comparison of XPS data obtained in 0 and 80° emission; this observation is independent of temperature and Pd concentration of the liquid phase. It is interpreted as an inhomogeneous depth distribution function of Pd, that is, Pd depletion in the topmost layer and enrichment in the next layer. In line with experiment, a DFT-based molecular dynamics simulation (MD) shows interfacial stratification of Ga and an inhomogeneous Pd distribution along the surface normal. The experimental data was evaluated by using a rigid layer model leading to excellent agreement with the results of the MD simulation. We acknowledge the financial support by the Cluster of Excellence 'Engineering of Advanced Materials'.

O 87.4 Thu 11:30 WIL C307

Correlogram Correlation for Surface Topology Evaluation by White Light Interferometry — •Ilia Kiselev[1], Michael Drexel[1], Egor Kiselev[2], and Michael Hauptmannl[1] — [1]Breitmeier Messtechnick GmbH, Englerstr. 24, 76275 Etlingen — [2]Physikalisches Institut, Karlsruhe Institut of Technology, Wolfgang-Gaede-Str. 1, 76131 Karlsruhe

Established methods to gauge the surface height by the white light interferometry do not use the full Information contained in a correlogram. As the result, the envelope evaluation methods suffer from susceptibility to noise, whereas the phase methods are prone to the *2-pi ambiguity*. The suggestion here is to determine the surface position via the correlation of the local correlogram with a reference correlogram. It is easy to see that the method is to be the most stable to noises of different kinds: it benefits using the complete correlogram information. Theoretical Cramer-Rao estimations as well as evaluations of measured data samples demonstrates the prevalence of the method. Tolerance to noise of this method is by more than one order of magnitude higher, than that of the envelope methods and exceeds that of the phase method; available data which indicates the 2-pi jumps by phase method provide smooth results by this one. Another advantage of the suggested method is the immediate availability of a suitability criterion for a local correlogram * the correlation coefficient with the reference one.

O 87.5 Thu 11:45 WIL C307

Diffusion properties of lithium and magnesium studied using DFT: growth phenomena and the effect of an electric field — •Markus Jäckle[1,2] and Axel Gross[1,2] — [1]Helmholtz Institut Ulm - Elektrochemische Energiespeicherung, 89069 Ulm, Germany — [2]Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany

The formation of dendrites poses a significant problem with respect to the performance and safety of batteries as it can lead to short-circuits during battery operation. Metal growth processes are intimately linked to diffusion behaviour. Therefore, we have extended our initial theoretical first-principles study of the self-diffusion properties of lithium, sodium and magnesium [1] by investigating a broader variety of diffusion processes. Thereby we intend to contribute to a better understanding of this phenomenon which may help avoiding battery failure due to dendrite growth.

According to our new calculations, the previously established picture of an inhomogeneous lithium surface and a homogeneous magnesium surface [1] is still correct. Our new results suggest a significant influence of the across-step diffusion barrier, which will be elucidated in the presentation.

[1] M. Jäckle and A. Groß, J. Chem. Phys. **141**, 174710 (2014).

O 87.6 Thu 12:00 WIL C307

Metallic Nanopore Arrays as Ideally Nanostructured Electrode for Supercapacitors — •Huaping Zhao, Ranjith Vellacheri, Min Zhou, Yang Xu, and Yong Lei — Institut für Physik & IMN MacroNano* (ZIK), Technische Universität Ilmenau, Ilmenau, Germany

Supercapacitors have attracted great interest as an electrical energy storage system because of their high power density, fast charge-discharge rate, and excellent cycle stability. Besides the active materials themselves, the electrode structure also plays an important role in determining the charge storage capability and rate capability of supercapacitors. Considering that the energy storage of supercapacitors is through either ionic adsorption-desorption or fast and reversible surface redox reactions at the electrode/electrolyte interface, a promising supercapacitor electrode should have large specific area to realize high charge storage capability. Meanwhile, it should provide shorter ion diffusion path and lower electron transfer resistance that enable the achievement of high rate capability. Here, we demonstrate metallic nanopore arrays fabricated using a two-step replication process from

porous anodic alumina membrane as an ideally nanostructured electrode for supercapacitors. With metallic nanopore arrays as supercapacitor electrode, the large specific surface area could ensure high capacitance, while the highly oriented and stable nanoporous structure can facilitate ion transport, thus high charge storage capability and high rate capability of supercapacitor were achieved simultaneously.

O 87.7 Thu 12:15 WIL C307

Low temperature bias-assisted RF-sputtering process for heteroepitaxial growth of iridium (100) on sapphire (11-20) — Frank Meyer[1], Eduard Reisacher[1], Johannes Preussner[1], Andreas Graff[2], Alexander Fromm[1], Lukas Gröner[1], and •Frank Burmeister[1] — [1]Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg i. Br., Germany — [2]Fraunhofer-Institut für Mikrostruktur von Werkstoffen und Systemen IMWS, Halle, Germany

Heteroepitaxially grown iridium (100) on sapphire (11-20) is one of the most promising systems for large scale heteroepitaxial diamond growth [1]. However, due to the high melting point of iridium (2466°C) and low adatom mobility, in various e-beam or sputter deposition experiments, epitaxial growth has only been observed at substrate temperatures above 600°C. Very recently, Tolstova et al. [2] were able to significantly reduce the temperature necessary for growing epitaxial platinum and gold films on MgO by using RF-sputtering with an additionally applied substrate bias. In this study we investigated the influence of the additional substrate bias on the growing Ir film. Crystallinity and morphology were characterized using X-ray diffraction and electron backscattering diffraction. We found that in the first seconds of the deposition process, an additional substrate bias creates a thin iridium seeding layer, which enables epitaxial growth of iridium (100) on sapphire (11-20) already at temperatures slightly above 300°C. [1] Z. Dai et al., Appl. Phys. Lett., 82, 3847 (2003) [2] Y. Tolstova et al. Scientific Reports 6, 23232, (2016)

O 87.8 Thu 12:30 WIL C307

Transformation of the Pt(001)-hex to a smooth and clean Pt(001)-(1x1) — Rene Hammer[1], Florian Schumann[1], •Oliver Krahn[1], Stefan Förster[1], Klaus Meinel[1], and Wolf Widdra[1,2] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [2]Max-Planck Institut für Mikrostrukturphysik, D-06120 Halle, Germany

The quasihexagonal reconstruction of the (001) surfaces of gold and platinum have been under intense investigation for decades. Yet the non-reconstructed (1x1) structure is important for particular applications. Here, we study by STM, SPA-LEED and HREELS the structural transformation of the Pt(001)-hex to an unreconstructed (1x1) surface by gas adsorption. The lifting of the hex occurs along the reconstruction rows. Surplus Pt atoms are pushed on top of the surface leading to one-dimensional chains growing along [110] at low temperatures (77 K). These chains decay into islands at room temperature and result in a roughening of the Pt(001)-(1x1) surface. Surface smoothing by intralayer diffusion above 150 °C fails because the hex layer recovers from the islands. Island growth is only attained by step edge diffusion at around 100 °C promoting a Smoluchowski ripening of the islands. When island size reaches 10 nm, Ostwald ripening at 350 °C can be applied. This leads to a smooth surface with large two-dimensional islands. Finally an annealing process at 150 °C in O_2 atmosphere results in a well-ordered and adsorbate-free (1x1) surface.

O 87.9 Thu 12:45 WIL C307

Electron energy loss spectroscopy with parallel readout of energy and momentum — •F. C. Bocquet[1,2], H. Ibach[3], J. Sforzini[1,2], S. Soubatch[1,2], and F. S. Tautz[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA), Fundamentals of Future Information Technology — [3]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich, 52425 Jülich, Germany

Electron Energy Loss Spectroscopy (EELS) has been a very successful technique for the past three decades for studying elementary excitations at surfaces (e.g. vibrational modes, phonons, plasmons) and providing sub-meV resolution [1]. In this work, we demonstrate that the combined use of a hemispherical electron analyzers equipped with a multichannel plate (MCP) as detector, together with a modified version of the conventional double monochromator allows a faster detection of electron in the off-specular geometry. We show the first results obtained on the phonon dispersion of clean Cu(111) [2]. The full dispersion curve has been obtained in a single 7-minutes long measurement, which is a clear improvement with respect to standard spectrometer that would require several hours of acquisition.

References [1] H. Ibach, J. Elec. Spec. Relat. Phenom. 64 819 (1993) [2] H. Ibach, et al. submitted (arXiv:1611.09709)