

O 97: Nanostructured Surfaces and Thin Films

Time: Friday 10:30–12:30

Location: S053

O 97.1 Fri 10:30 S053

High-quality Ru(0001) thin films by magnetron sputter deposition for ceria inverse model catalysts — ●MEIKEL WELLBROCK, MARC SAUERBREY, JAN HÖCKER, MARCO SCHOWALTER, JON-OLAF KRISPONEIT, JENS FALTA, and JAN INGO FLEGE — Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee, 28359 Bremen

The investigation of model systems in heterogeneous catalysis with surface science methods typically requires the use of single crystal substrates. Offering enhanced experimental flexibility at lower costs, thin films prepared by magnetron sputter deposition, an industrially scalable process, represent an attractive alternative. In this study, high-quality, 80 nm thin Ru(0001) films were sputter-deposited on *c*-plane sapphire and then employed as substrates for the subsequent growth of cerium oxide for surface catalysis. After thermal treatment, atomic force microscopy (AFM) and low-energy electron microscopy (LEEM) showed the Ru thin films to be atomically flat over several micrometers, superior to commercially available Ru single crystals. Sequentially, ceria was grown by evaporation of metallic Ce in an oxygen ambient at elevated temperature and monitored *in situ* by LEEM. Contrary to the studies involving single crystal substrates, large, triangular, and smooth CeO₂(111) islands were observed to nucleate exclusively at randomly distributed v-shaped surface defects (v-pits), determining their azimuthal orientation. Together with the narrow height distribution as revealed by *ex situ* AFM, these microparticles represent a well-suited model system for the study of surface chemical reactions over ceria inverse model catalysts.

O 97.2 Fri 10:45 S053

Investigation of monolayer-thick ZrO₂ films created by sputter deposition — ●PETER LACKNER, JOONG-IL J. CHOI, ULRIKE DIEBOLD, and MICHAEL SCHMID — Institute of Applied Physics, TU Wien, Vienna, Austria

Investigating zirconia (ZrO₂) is challenging due to its high band gap. As an insulator it is not accessible to measurement methods relying on electronic conduction, such as scanning tunneling microscopy (STM), at room temperature. To circumvent this issue, ultrathin ZrO₂ films can be studied [1]. However, the very low vapor pressure of zirconium makes deposition slow when using evaporation in ultrahigh vacuum (UHV). We therefore present an UHV-compatible sputter source similar to [2], which can be used to deposit ZrO₂ thin films of any desired thickness.

By variation of film thickness and annealing temperature a continuous and well-ordered film can be produced. We present STM, LEED and XPS results on ZrO₂ films with a thickness of one to 7.5 monolayers. On Rh(111), different surface reconstructions are observed for every layer up to five monolayers. Films with a thickness of five or more monolayers show stripes on the surface, which are indicative of bulk-terminated monoclinic or tetragonal ZrO₂.

[1] Meinel *et al.*, Phys. Rev. B 74, 235444 (2006).

[2] Mayr *et al.*, Rev. Sci. Instrum. 84, 094103 (2013).

O 97.3 Fri 11:00 S053

Microstructure of Yttrium Oxide Deposited by Reactive RF Magnetron Sputtering with Different Oxygen Inlet Flux — ●YIRAN MAO, JAN ENGELS, ANNE HOUBEN, JAN COENEN, MARCIN RASINSKI, JONATHAN STEFFENS, and CHRISTIAN LINSMEIER — Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung - Plasmaphysik, 52425 Jülich, Germany

Yttria (Y₂O₃) is a well-known ceramic material extensively used in industry and material science applications. Reactive magnetron sputtering is one of the methods to produce Y₂O₃ coatings. The influence of the oxygen inlet flux on the Y₂O₃ film microstructure grown by reactive radio-frequency magnetron sputtering was investigated. The oxygen inlet flux showed a hysteresis behavior effect on the deposition rate. With a low oxygen flux, the so called metallic mode process with a high deposition rate (up to 1.4 *m/h) was achieved, while with a high oxygen flux, the process was considered to be in the reactive mode with low deposition rate (~20 nm/h). The metallic mode layers represented a mixture of different crystal structures including the metastable monoclinic phase and the stable cubic phase, while the reactive mode products showed a pure monoclinic phase structure. Comparing the reactive mode layers, the metallic mode layers showed dense

structures with less porosity. Annealing at 600 °C for 15 h caused a phase transformation from monoclinic phase to cubic phase for both reactive mode and metallic mode. For metallic mode layers, cracks are formed due to the thermal expansion coefficient difference between Y₂O₃ and the substrate which was not seen in reactive mode.

O 97.4 Fri 11:15 S053

Comparative study of amorphous hydrogenated carbon (a-C:H) layers on Si (100) and high-density polyethylene (HDPE) — ●CHRISTIAN B. FISCHER, ALBERTO CATENA, and STEFAN WEHNER — Department of Physics, University Koblenz-Landau, 56070 Koblenz, Germany

Silicon and high-density polyethylene (HDPE) have been gradually covered by thin a-C:H films with acetylene-plasma to study the inter-layer forming behavior between the base material and carbon coating. Two different carbon coatings, one with indirect (f-type) and one with direct (r-type) deposition, were realized. Surface characteristic studies by atomic force microscopy (AFM) showed an unexpected similar morphology for both types and materials. The analysis of average height and area for single evolving grains over uniformly textured protrusions at the bottom revealed a smaller amount of carbon deposition for the f-type than for the r-type to obtain similar morphologies independently of the chosen basic material. The average grain area increases for all f- and r-depositions. The average grain height increases in the beginning and approaches a level with nearly constant height. Furthermore, the values of the average grain heights are correlated to the values of the average grain areas and are localized in a limited area, indicating a given regularity throughout the different carbon depositions.

O 97.5 Fri 11:30 S053

Remote plasma treatment as a method to improve the surface conductivity of bipolar plates for fuel cells — ●TATIANA FEDOSENKO-BECKER^{1,2}, NICOLAS WÖHRL¹, VOLKER BUCK¹, and MARIO GILLMANN³ — ¹University of Duisburg-Essen, Duisburg, Germany — ²University of Wuppertal, Wuppertal, Germany — ³ZBT GmbH - The fuel cell research center, Duisburg, Germany

Fuel cells are promising alternative energy sources, therefore they have recently earned scientific interest. However they are not without deficiencies, since during fabrication of carbon/polypropylene (PP) composite bipolar plates (BP) the PP is enriched at the surface reducing the electrical conductivity and the efficiency of the fuel cells. The surface conductivity can be improved by selectively etching the PP from the surface by plasma treatment, using the plasma source CYRANNUS by iplas in remote mode. A detailed investigation of the properties of BP, of plasma processes during the treatment and the influence of the process parameters was done.

It was shown that plasma treatment of BP is a suitable method to decrease the surface resistance without causing mechanical damage to the surface. The most suitable experimental parameters for this task were found. Using FTIR and Raman spectroscopy it was shown that PP and nanocrystalline graphite is removed from the surface. The experimental parameters, such as plasma chemistry, pressure, treatment time, distance from plasma, which provide the best conductivity of the BP, were found.

O 97.6 Fri 11:45 S053

Study of Solid Electrolyte Interphase layer in Sodium-Ion Batteries — ●LIANG-YIN KUO¹, PAYAM KAGHAZCHI¹, and BING-JOE HWANG² — ¹Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin, Germany — ²Department of Chemical Engineering, National Taiwan University of Science and Technology, No.43, Sec. 4, Keelung Rd., Taipei 106, Taiwan

Sodium (Na)-ion batteries are considered as alternative to Li-ion batteries. Sodium is abundance in the earth's crust and the distribution of sodium mineral salts is widespread. In this work, we present a combined *in situ* surface-enhanced Raman spectroscopy (*in situ* SERS) and density functional theory (DFT) study on the solid electrolyte interphase (SEI) layer over the surface of Sn anodes in Na-ion batteries. Our *in situ* SERS measurements show that the main components of the SEI layer during Na-ion insertion/extraction are Na₂O (peaks around 479 cm⁻¹ and 597 cm⁻¹) and Na₂CO₃ (peak around 1080 cm⁻¹). Afterwards, we will discuss our DFT results on electronic and atomic

structure as well as the mechanism of Na diffusion through Na₂O and Na₂CO₃.

O 97.7 Fri 12:00 S053

Chemical vapor deposition and infiltration for the production of tungsten fiber reinforced tungsten composite material —

•MARTIN AUMANN¹, JAN WILLEM COENEN¹, HANNS GIETEL², TILL HOESCHEN², JOHANN RIESCH², KLAUS SCHMID², RUDOLF NEU², and CHRISTIAN LINSMEIER¹ — ¹Forschungszentrum Juelich GmbH, Institut für Energie- und Klimaforschung, 52425 Juelich — ²Max-Planck-Institut für Plasmaphysik, 85748 Garching

Due to its high melting point, high corrosion resistance and its preferable properties in terms of hydrogen retention, tungsten is a promising candidate in future nuclear fusion devices. However, the mechanical behavior of tungsten is crucial, as it is inherently brittle at room temperature. As possibility to overcome this brittleness, a composite material can be formed, which shows pseudo-ductility and therefore avoids catastrophic failure of the material. A possibility to produce such a Wf/W-composite is chemical vapor deposition and chemical vapor infiltration, where tungsten is deposited on thin tungsten wires through the reaction of WF₆ and H₂. With ongoing infiltration time, pores are formed between the fibers, which decrease in size through the chemical reaction. For better process understanding, a pore model was established, which solves the mass balance inside the pore and the resulting pore diameter simultaneously. It shows a significant difference in diameter for longer infiltration times. This behavior shall be

investigated in experiments with an experimental pore, which is similar to the simulated one. Furthermore also kinetic investigations on the chemical surface reaction are carried out to increase the process understanding.

O 97.8 Fri 12:15 S053

Simulation of oblique angle deposition — •CHRISTOPH GRÜNER, JENS BAUER, STEFAN MAYR, and BERND RAUSCHENBACH — Leibniz-Institut für Oberflächenmodifizierung, Permoserstraße 15, 04318 Leipzig, Germany

Computer simulations are a powerful tool to study thin film growth phenomena. Here, application of simulations focuses on understanding and controlling atomistic processes during glancing angle deposition in order to create nanostructures with unique new physical properties and functionalities. Ballistic deposition models are used to describe kinetics and morphology of film growth [1]. Such simulation outcomes depend strongly on the implementation of the sticking process and the choice of the simulation grid geometry [2]. Focusing on glancing angle deposition, different issues of simple grid based simulations are studied. Shape and tilt angle of the deposited nanostructures are investigated as well as the porosities of the complete films. The benefit of using cluster particles is discussed.

[1] A.-L. Barabasi and H.E. Stanley, *Fractal Concepts in Surface Growth*, Cambridge Univ. Press, Cambridge 1995

[2] B. Tanto, C. F. Doiron, and T.-M. Lu, *Phys. Rev. E* 83 (2011), 016703