O 90: Metals and semiconductors: Epitaxy and growth

Time: Friday 10:30–12:30 Location: A 060

O 90.1 Fri 10:30 A 060

Role of pulse control and material parameters on submonolayer pulsed-laser depositions — Martin Mašín and •Miroslav Kotrla — Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, 182 21, Praha 8, Czech Republic

Pulsed laser depositions is the promising experimental method for nanostructuring of oxide, and also metallic thin films [1]. However, its theoretical understanding on the microscopic level is still insufficient. Recently, we performed Monte Carlo simulation motivated by a Fe/Mo system to analyze the temperature dependence of island density in the case of reversible growth [2]. In this work, we present our study of the dependence of the island density on varying characteristics of pulses: different chopping frequencies, and different duration of pulses. We also compare two regimes of pulse frequency variation: with a constant average flux and with a constant pulse intensity. In the former case, we found that low frequency increases the island density highlighting the recently found anomaly in the Arrhenius plot [2]. In the latter case, we observe, in contrary, that higher frequency leads to a higher island density. Increase of pulse length causes decrease of island density, leading to molecular beam epitaxy results. Moreover, we analyzed dependence on material parameters. The increase of a diffusion barrier for monomers shifts the whole Arrhenius curve to higher temperatures, and increase of binding energy moves a position of plateaus to higher temperatures. Our results allow to optimize pulse deposition.

[1] P. O. Jubert, O. Fruchart and C. Mayer, Phys. Rev. B , 64 (2001) 115419. [2] M. Mašín, M. Kotrla: Europhys. Lett. 90 (2010) 18006.

O 90.2 Fri 10:45 A 060

Atomic structure of Fe on Ir(001) - (1x1) — •Marco Corbetta, Zhen Tian, Yiqi Q. Zhang, Alvaro Augusto Leon Vanegas, Safia Ouazi, Dirk Sander, and Jürgen Kirschner — Max Planck Institute, Halle (Saale), Germany

The correlation between structural and magnetic properties of Fe monolayers makes it a particularly interesting system to investigate the impact of lattice strain on film structure, morphology and magnetism. We study the Ir(001) - (1x1) surface by STM with a W tip obtaining atomic resolution. We then deposit 0.6 ML of Fe at 300 K and we observe a (3x3) periodicity on one layer height Fe islands at 8 K in STM constant current images. This suggests the formation of a coincidence structure where three Ir-Ir atomic distances along the [110] crystallographic direction correspond to two bcc Fe-Fe atomic distances in the same direction. The difference in length between three Ir-Ir (8.145 A) and two Fe-Fe (8.105 A) atomic distances is only +4 pm and this makes our model a reasonable proposition. After deposition of 1.2 ML of Fe we observe a (1x1) contrast by STM on the closed first Fe monolayer, in agreement with earlier studies [1]. The analysis reveals a nearest neighbour spacing of the Fe monolayer which corresponds to that of the Ir substrate. Our findings could be ascribed to a structural rearrangement within the Fe deposit with increasing Fe coverage. [1] V. Martin, W. Meyer, C. Giovanardi, L. Hammer, K. Heinz, Z. Tian, D. Sander and J. Kirschen, Phys. Rev. B 76, 205418 (2007).

O 90.3 Fri 11:00 A 060

Characterization of Pt_xCu_1-x alloys on Pt(111) surfaces as model catalysts for core shell nanoparticles. — •Stephan Beckord, Albert K. Engstfeld, and R. Jürgen Behm — Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany

Core-shell nanoparticles consisting of a bi- or multialloy core enclosed by a layer of a pure metal often show interesting catalytic properties. One example are PtxCu1-x alloy core Pt shell particles, which show an increased catalytic reactivity towards the oxygen reduction reaction [1] or the water gas shift reaction [2] compared to the respective monometallic particles.

To study the effect of the Pt_xCu_1-x core on the Pt shell, we prepared nanostructured bimetallic planar model surfaces under ultra high vacuum (UHV) conditions, by evaporation of Cu on a Pt(111) surface followed by annealing for (surface) alloy formation. Subsequent deposition of a Pt monolayer film results in a model system closely resembling the structure of a bimetallic core-shell nanoparticle. The resulting surfaces were characterized by scanning tunneling microscopy (STM) and auger electron spectroscopy (AES) to elucidate the composition, morphology and the distribution of the different species in the surface. From these data we will determine the dominant factors for surface alloy formation. [1] *R. Strivastava, P. Mani, N. Hahn, and P. Strasser, Angewandte Chemie, 46, 8988 (2007). [2]*J. Knudsen, A. U. Nilekar, R. T. Vang, J. Schnadt, and F. Besenbacher, J. Am. Chem. Soc. 120, 6485 (2007).

O 90.4 Fri 11:15 A 060

Taking (different) sides - Zn and Ga on different Pd-facets — •Werner Stadlmayr, Christoph Rameshan, Simon Penner, Bernhard Klötzer, and Norbert Memmel — Institute of Physical Chemistry, University of Innsbruck, Innsbruck, Austria

Pd/Zn- and Pd/Ga-catalysts have been proven to be interesting candidates for methanol-steam-reforming ($CH_3OH+H_2O \rightarrow CO_2+3H_2$)[1]. Using thin films of Zn and Ga on Pd-substrates, we investigated them regarding their alloying, structure as well as catalytic behaviour. We comment on the trends in thermal stability and give a comprehensive overview of the structural findings so far. In particular we find that both the films and alloys derived from the (110)-facets are more stable than those derived from the (111)-facets. Furthermore, Zn-films have a stronger tendency for surface alloy formation than Ga-films, while such a simple relationship does not hold for the decomposition of the alloys. Concerning catalytical properties, we show that properly prepared Pd/Zn-alloys exhibit CO_2-selectivity, while no such selectivity can be found for Pd/Ga-alloys.

[1] N. Iwasa and N. Takezawa, Top. Catal. **22**, 3-4 (2003)

O 90.5 Fri 11:30 A 060

Core shell model electrodes: Pt terminated mono- and multilayer CuPt alloys supported on Ru(0001) single crystals. — •Albert K. Engstfeld and R. Jürgen Behm — Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany

Core shell particles consist of a metal A rich shell and a bi- or multialloy core, showing different catalytic activity compared to pure metal particles. An interesting example are Pt enclosed alloy particles containing Cu, Co and Pt, having a much better activity towards oxygen reduction than pure Pt.[1] The effect is mainly attributed to a change of the electronic structure of the shell due to lattice strain within the alloy core.

To study the strain effect we focus on the preparation of mono and bilayer Cu/Pt alloys on Ru(0001) single crystal surfaces under ultra high vacuum conditions, characterized by scanning tunnelling microscopy. From the atom distribution within the alloy we will discuss the dominant factors for alloy formation, in view of the different size of the atoms and difference in their intermetallic bonding. Furthermore, we will elucidate the surface segregation behaviour of Pt in the bilayer alloy during the alloying process.

[1] R. Strivastava, P. Mani, N. Hahn, and P. Strasser, Angewandte Chemie, 46, 8988 (2007)

O 90.6 Fri 11:45 A 060

Growth study: ultrathin GaN films on 6H-SiC(0001) — •Lena Neumann[1], Jürgen Gerlach[1], and Bernd Rauschenbach[1,2] — [1]Leibniz Institute of Surface Modification (IOM), D-04318 Leipzig, Germany — [2]University Leipzig, Institute of Experimental Physics II, D-04103 Leipzig, Germany

Ultrathin gallium nitride (GaN) films were deposited using the ion-beam assisted molecular-beam epitaxy (IBA-MBE) technique. The influence of the nitrogen ion to gallium atom flux ratio (I/A ratio) at different substrate temperatures during the early stages of GaN nucleation and thin film growth directly on super-polished 6H-SiC(0001) substrates was studied. The deposition process was performed by evaporation of Ga and irradiation with hyperthermal nitrogen ions from a constricted glow-discharge ion source. The GaN growth in N- and Ga-rich regimes was investigated by *in situ* reflection high energy electron diffraction (RHEED) and scanning tunnelling microscopy (STM) measurements. The results show, that the I/A ratio has a major impact on the properties of the resulting ultrathin GaN films. The growth mode, the surface roughness, the degree of GaN coverage of the substrate and the polytype mixture depend notably on the I/A ratio.

At the substrate temperature of 700 °C and the I/A ratio less than 1.6 the formation of islands developed through rapid coalescence into two-dimensional growth. A three-dimensional island growth mode is favoured at lower Ga fluxes, so that the I/A ratio > 1.6. The increase of the islands diameter to height ratio with the I/A ratio increasing was observed.

O 90.7 Fri 12:00 A 060

Investigation of the three layer system MgO/Fe/GaAs(001) — •Dominique Handschak[1], Tobias Lühr[1,2], Frank Schönbohm[1,2], Sven Döhring[2], Christoph Keutner[1,2], Ulf Berges[2], and Carsten Westphal[1,2] — [1]TU-Dortmund, Experimentelle Physik I — [2]DELTA, TU-Dortmund

We report a synchrotron high-resolution x-ray photoemission (XPS) and photoelectron diffraction (XPD) study of the three layer system MgO/Fe/GaAs(001). The interface of Fe/GaAs is interesting because it is a semiconductor-ferromagnetic junction, being an interesting model system for research to spintronics. Magnesium oxide is a very efficient insulator which is used especially in TMR-components. Both interfaces have a strong influence on the efficiency of the contributing effects. In this study we report on the preparation process of the three layer system with a GaAs reconstructed surface. The structure of each layer could be clarified with core level high-resolution spectra and diffraction patterns.

O 90.8 Fri 12:15 A 060

XPD-pattern analysis of MgO/Fe/GaAs(001) by means of Genetic Algorithms — •Tobias Lühr[1,2], Dominique Handschak[1], Frank Schönbohm[1,2], and Carsten Westphal[1,2] — [1]Fakultät Physik - TU Dortmund, Otto-Hahn-Str.4, D 44221 Dortmund, Germany — [2]DELTA - TU Dortmund, Maria-Goeppert-Mayer-Str. 2, D 44227 Dortmund, Germany

Thin films of iron on gallium arsenide are of great relevance in current research. This system forms a semiconductor-ferromagnetic junction. For this reason it becomes interesting for spintronic devices. An insulating layer like magnesium oxide on this system offers the possibility of growing additional layers for technical applications (e.g. TMR-components). We investigated the three layer system MgO/Fe/GaAs(001) by means of angle-resolved photoelectron diffraction (XPD) for determining the structure of the individual layers and interfaces. For this task it is necessary to compare the experimental data sets to simulated diffraction patterns of several model structures. In the face of endless possible structures we developed a genetic algorithm that generates and optimizes such model structures in order to fit the experimental data sets. We show the functionality of the algorithm, and the results of the MgO/Fe/GaAs(001) structure determination.