O 80: Epitaxy and growth: Metals and semiconductors I

Time: Thursday 15:00–17:00 Location: WIL C307

O 80.1 Thu 15:00 WIL C307

Strain aspects of the atomic structure of the InAs wetting layer grown on GaAs(001)-c(4×4) — •Christopher Prohl, Jan Grabowski, Britta Höpfner, Mario Dähne, and Holger Eisele — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin

InAs/GaAs is the model system for III-V-semiconductor quantum dots and is also a well-known example for the Stranski-Krastanow growth mode in epitaxy. As shown before by scanning tunneling microscopy (STM) investigations of molecular beam epitaxy (MBE) grown samples, the InAs wetting layer evolution on GaAs(001)-c(4×4) can be separated into three phases before quantum dot occurrence: signatures of InAs on GaAs-c(4×4) for low coverages, an $In_{2/3}Ga_{1/3}As$-(4×3) reconstructed monolayer at about 0.67 ML, and different InAs-(2×4) reconstructions forming on top of the latter. In this talk, a closer look at the surface strain of the identified atomic surface structures will be taken. The strain situation of the different growth regimes will be discussed in detail. For this purpose, mainly the bond lengths defining the stress situation will be considered.

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O 80.2 Thu 15:15 WIL C307

Anion-enhanced self-diffusion on Au(100) — •Mostafa Mesgar, Payam Kaghazchi, and Timo Jacob — Institut für Elektrochemie, Universitüt Ulm, Albert-Einstein-Allee 47, 89069 Ulm

Surface phenomena, such as thin film growth, corrosion and crystal growth, are determined by the diffusion of atoms on surfaces. Although several experimental and theoretical studies already focused on the adatom diffusion, much less is known about how possible coadsorbates might influence diffusion barriers or even migration mechanisms, which could lead to modifications in the surface morphology. Performing large-scale density functional theory (DFT) studies we have investigated the anion-modified self-diffusion on Au(100). We investigated the adsorption and various migration mechanisms of Au atoms on clean [1] and Cl-covered Au(100) with and without surface defects (e.g. steps, kinks, or vacancies). Our studies indicate that in both systems (i.e. clean and Cl-covered) the exchange mechanism, is the most favorable mechanism. Further, we find that for all diffusion processes the presence of co-adsorbed Cl decreases the diffusion barriers, which should result in faster Ostwald ripening. Based on our DFT results the next aim will be to generate a reactive forcefield for Au-Au and Au-Cl interactions,[2] which coupled with kinetic Monte-Carlo will allow for large-scale simulations, providing macroscopic quantities (e.g. diffusion coefficients) readily comparable to experiments.

1. K. Pötting, W. Schmickler, T. Jacob, *Chem. Phys. Chem.*, **11**, 1395 (2010). 2. D. Fantauzzi, J. A. Keith, A. C. T. van Duin, T. Jacob, *Phys. Rev. B*, **81**, 235404 (2010).

O 80.3 Thu 15:30 WIL C307

Growth of atomically flat Zn films on ZnO(0001) surface — •Hao Zheng, Natalia Schneider, and Richard Berndt — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

Transition metal/oxide heterostructures have been investigated as model catalyst. Owing to the largely different surface energies of these materials, three-dimensional metal islands usually form on oxide surfaces. On semiconductors, flat metal films are obtained by a two-step growth method involving low temperature deposition followed by room temperature annealing. Up to now, there are no reports of similar results on oxide surfaces. Here we present scanning tunnelling microscopy data from atomically flat Zn films on ZnO(0001) obtained by a simple one step growth. Subtle variations of the apparent height of the Zn surface are observed, which resemble structures observed from the ZnO(0001) surface underneath. This observation is discussed in terms of tunnelling to quantum well resonances of the Zn films. Support by the DFG via SFB 855 is acknowledged.

O 80.4 Thu 15:45 WIL C307

The Interaction of Copper with a Rhenium$(10\bar{1}0)$ **Surface** — •Daniel Przyrembel and Klaus Christmann — Institut für Chemie und Biochemie, Freie Universität Berlin

Ultrathin Cu films have been deposited in UHV on a Re$(10\bar{1}0)$ surface between 650 K and 800 K and studied by means of MEED, LEED and TPD. Two desorption states are observed between 1000 K and 1180 K. The low temperature α state exhibits zeroth order desorption kinetics, the high temperature β state shows first-order desorption for low Cu coverages shifting to zeroth order with increasing coverage. *In-situ* observation of the MEED (0,0) beam intensity during Cu deposition shows only one maximum that coincides with the saturation of the β TPD peak and a LEED (1×1) structure. No other LEED structures were observed in the investigated coverage range in contrast to the behaviour of Au and Ag [1,2]. Linear superposition of the LEED I,V curves from the clean Re surface and the closed Cu layer reproduces the respective I,V curves for all Cu coverages in that range. Together with the data for Au and Ag on Re$(10\bar{1}0)$ and for Au, Ag and Cu on Re(0001) [3] these findings suggest: (i) On Re$(10\bar{1}0)$ Cu grows in a Stranski-Krastanov mode. (ii) The closed Cu layer is a *bilayer* with two atoms per unit mesh. (iii) The bilayer is formed from two-dimensional islands with local (1×1) structure that show a temperature dependent phase transition towards a two-dimensional lattice gas.

[1] C. Pauls and K. Christmann, J. Phys.: Condens. Matter **21** (2009) 134012; [2] A. Vollmer, Ph.D. thesis, FU-Berlin (1999); [3] R. Wagner, D. Schlatterbeck, K. Christmann, Surf. Sci. **440** (1999) 231-251.

O 80.5 Thu 16:00 WIL C307

Initial stages of the ion-beam assisted epitaxial GaN film growth on 6H-SiC(0001) — •Lena Neumann[1], Jürgen Gerlach[1], Thomas Höche[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

The influence of the nitrogen ion-to-gallium atom flux ratio (I/A ratio) on the early stages of gallium nitride (GaN) nucleation and thin film growth directly on super-polished 6H-SiC(0001) substrates is studied. Ultrathin GaN films below 15 nm were formed using the ion-beam assisted molecular-beam epitaxy (IBA-MBE) technique. The deposition process was performed at a constant substrate temperature by evaporation of gallium using a conventional effusion cell and irradiation with hyperthermal nitrogen ions from a constricted glow-discharge ion source. The nitrogen ion flux was kept constant and the selection of different I/A flux ratios was done by varying the Ga flux. The GaN growth was determined by in situ reflection high energy electron diffraction and scanning tunneling microscopy measurements. The film microstructure was investigated by transmission electron microscopy. A strong dependence of the resulting film morphology and topography as a function of the Ga deposition rate could be observed. A three-dimensional island growth mode is favoured at I/A ratio >1. At higher Ga deposition rates (I/A ratio <1) the formation of islands developed through early coalescence into two-dimensional growth with the coalescence thickness being about 12 to 30 monolayers of GaN.

O 80.6 Thu 16:15 WIL C307

AES/LEED/I(V) LEED investigation of ultrathin Pb and In layers deposited on Ni(001) and Ni(111) faces — •Katarzyna Miśków and Aleksander Krupski — Institut of Experimental Physic, University of Wrocław, Wrocław, Poland

Properties of ultrathin indium and lead layers deposited on Ni(001) and Ni(111) faces at temperature between T = 150 K and T = 950 K and coverage up to 6 ML have been studied by AES-t, LEED and I(V) LEED. For In/Ni(111), Frank-van den Merwe and Stranski-Krastanov type of growth is observed for temperature below and above 450 K, respectively. In case of In/Ni(001), below T < 600 K it seems that Volumer-Weber or Simultanoeous Multilayers type of growth plus Simultanous Multilayers type of growth. For the adsorption of Pb on Ni(001) only Volumer-Weber type of growth is observed. Two different indium structures have been found for (001) and (111) faces of nickel. For In/Ni(001) the p(2x2) structure has been observed for temperature between 600 K and 950 K. At about 950 K, reconstruction of the p(2x2) structure to c(2x2) one takes place. In case of In/Ni(111) the p(2x2) structure has also been observed, but for temperature between 450 K and 850 K. At about 900 K reconstruction of the p(2x2)

structure to the p(3x3)R30 one is observed. In case of Pb/Ni(001) only the c(2x2) structure has been observed. Indium makes surface alloy on both nickel crystal faces upon annealing while for lead, only desorption process is observed. The atomic structure and relaxation of the clean Ni(111) surface were investigated with the use of experimental I(V) LEED profiles and theoretical TensErLEED calculations.

O 80.7 Thu 16:30 WIL C307

Epitaxial growth of Group IV materials by Chemical Vapor Deposition for Germanium Metal Oxide Semiconductor devices — •Benjamin Vincent, Roger Loo, and Matty Caymax — imec, Kapeldreef 75, B-3001 Leuven, Belgium

Over the past 5-10 years, germanium has attracted a lot of interest to replace Silicon as a high carrier mobility material in future p-Metal Oxide Semiconductors transistors. This paper reviews developments of epitaxial Group IV materials (silicon, germanium, tin and alloys) by means of Reduced Pressure Chemical Vapor Deposition for use as Channel, Gate stack and Source/Drain in high performance Germanium transistors. We will first describe Germanium growth on standard Silicon wafers. Selective epitaxial growth within Shallow Trench Isolation structures allows seamless integration of Germanium channels in Si platform with a significant defect reduction down to levels required for state-of-the-art VLSI technology. Next we will focus on the most successful passivation approach for Germanium MOS interfaces by means of ultrathin epitaxial Si capping layers. This moves the problem of gate stack formation from a germanium surface to a silicon surface. We will discuss novel extremely low temperature CVD processes involving innovative precursors, and impacts of point defects, strain relaxation and Silicon-Germanium intermixing on Germanium device performance. Finally, the implementation of Germanium-Tin alloys in embedded Source/Drain regions in Germanium transistors will be proposed as an innovative architecture to implement strain in Germanium channels.

O 80.8 Thu 16:45 WIL C307

Ab-initio study on the temperature dependence of adsorbate-induced segregation in C/$Pt_{25}Rh_{75}$(100) — •Tobias C. Kerscher and Stefan Müller — Technische Universität Hamburg-Harburg, Institut für Keramische Hochleistungswerkstoffe, Denickestr. 15, 21073 Hamburg, Germany

Understanding the adsorbate-induced segregation of alloy surfaces is essential for catalytic surfaces. An interesting example is the C/$Pt_{25}Rh_{75}$(100) system: In comparison to the clean surface [1,2], even a small amount of carbon impurities leads to a considerable decrease in the Pt concentration of the top layer [1]. Previously, our first principles study of the coupled surface–adsorbate system was restricted to $T = 0$ K, where density functional theory shows that this change in segregation is driven by the antagonism between the segregation energies of Pt and Rh, and their binding energies to C. Now, we use an ab-initio-based cluster expansion in the framework of the UNCLE code [3] to investigate the $T > 0$ K temperature behaviour of the system by means of Monte Carlo simulations. We discuss the substitutional ordering of both the carbon adsorbate layer and the four topmost surface layers of $Pt_{25}Rh_{75}$(100) as a function of temperature and concentration. Our predictions are compared to experimental data in a quantitative manner.

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[1] E. Platzgummer *et al.*, Surf. Sci. **419** (1999), 236.
[2] P. Welker *et al.*, J. Phys.: Condens. Matter **22** (2010), 384203.
[3] D. Lerch *et al.*, Model. Simul. Mater. Sci. Eng. **17** (2009), 055003.