O 68: Semiconductor substrates: Epitaxy and growth

Time: Thursday 10:30–13:00 Location: H42

O 68.1 Thu 10:30 H42

Dimer Flipping at the MOVPE-prepared P-rich GaP(100) Surface — •Peter Kleinschmidt, Henning Döscher, Sebastian Brückner, Anja Dobrich, Oliver Supplie, Christian Höhn, and Thomas Hannappel — Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

The structure of the P-rich GaP(100) surface has been known for some time, showing a p(2x2)/c(4x2) reconstruction. The surface is terminated by alternating buckled phosphorus dimers stabilized by one hydrogen atom per dimer. The STM image of this surface consists of zigzag dimer chains where neighbouring chains can be aligned in phase as well as out of phase to each other. The in-phase configuration results in a p(2x2) surface unit cell, while the out-of-phase configuration corresponds to a c(4x2) unit cell.

We prepared the P-rich GaP(100) surface in a commercial MOVPE system and employed a dedicated transfer system, which enables contamination-free transfer from the MOVPE environment to UHV and, using a mobile transfer chamber, to various surface analysis systems including STM. The quality of our STM images enabled us to compare successive images, revealing in some locations flipping of the P-dimers and therefore of the surface reconstruction. This process requires shifting of the H-termination between the P-atoms in the respective dimer. It could be thermally activated, not dissimilar to the dimer flipping on the clean Si(100) surface, where the flipping cannot be resolved at room temperature by STM, or tip-induced, similar to systems where manipulation of surface atoms can be achieved.

O 68.2 Thu 10:45 H42

Real Time Measurements of Surface Diffusion in a Multi-Reconstruction System: Ag/Si(111) — •Dirk Wall[1], Ingo Lohmar[2], Kelly Ryan Roos[3], Joachim Krug[2], Michael Horn-von Hoegen[1], and Frank-Joachim Meyer zu Heringdorf[1] — [1]Fakultät Physik und Center for Nanointegration Duisburg-Essen (CeNIDE), Universität Duisburg-Essen, 47057 Duisburg, Germany — [2]Institut für Theoretische Physik, Universität zu Köln, 50937 Köln, Germany — [3]Department of Physics, Bradley University, Peoria, Il 61625, USA

Photoemission Electron Microscopy (PEEM) is used to study the thermal decay (750-850°C) of Ag islands grown on Si(111) surfaces. During decay, Ag atoms are expelled from the island edges and migrate over the surface. Due to continuous desorption, a coverage gradient forms around each island. Depending on local Ag coverage, two different concentric reconstructions form. These reconstructed "isocoverage zones" are imaged with PEEM. A simple continuum model is presented explaining the dynamic decay of the islands for multi-reconstruction systems. Using this model, we extract diffusion parameters for the specific areas in one simple desorption experiment. We demonstrate that the imaging of these reconstructed "isocoverage zones" constitutes a unique experimental method for directly imaging diffusion fields in epitaxial systems. The general applicability of this imaging technique is demonstrated by the decay of other metal islands on Silicon surfaces of various orientations.

O 68.3 Thu 11:00 H42

Microscopic picture of hydrogen on the (MO)VPE-preparation of Si(100) — •Anja Dobrich, Henning Döscher, Sebastian Brückner, Peter Kleinschmidt, Oliver Supplie, Christian Höhn, and Thomas Hannappel — Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner Platz 1, 14109 Berlin, Germany

The preparation of Si(100) in the (MO)VPE environment usually involves hydrogen as carrier gas and as by-product from precursors. Hydrogen is suggested to have a crucial impact on the step structure of the silicon surface. To study the complete microscopic picture of the Si(100) surface we observed the (MO)VPE-preparation in situ with reflection anisotropy spectroscopy (RAS) and with a variety of surface-sensitive UHV-based techniques using a contamination-free (MO)VPE to UHV transfer system. Correlation between these results led to the conclusion that the surface is covered with hydrogen, in form of monohydrides and the surface is completely terminated with monohydrides. FTIR-spectroscopy in an attenuated total reflection (ATR) configuration served to perform surface-sensitive measurements of silicon-hydrogen bonds. This is in agreement with results from LEED and STM, which indicated that the surface unit cell consists of dimers. While our results were in agreement with the existence of H-Si-Si-H dimers, ATR spectroscopy did not reveal to what extent dangling bonds of the surface silicon atoms were saturated with hydrogen. Therefore we carried out tip-induced H-desorption by STM, which evidenced complete H-termination of the surface.

O 68.4 Thu 11:15 H42

Structural and electronic properties of MnGa monolayers on wurzite GaN(0001) surface — •Kangkang Wang, Abhijit Chinchore, Meng Shi, and Arthur Smith — Ohio University, Athens, OHIO, U.S.A.

Ferromagnetic (FM) metal/semiconductor bilayers are of great interest due to their importance in novel spintronics applications, such as spin injection and spin light-emitting diodes[1]. It has been reported[2] that delta-MnGa, a FM alloy with curie temperature higher than room temperature (RT), can be grown epitaxial on top of w-GaN(0001) with sharp interface and controllable magnetism. Using molecular beam epitaxy, we deposit up to 3 monolayers (ML's) of Mn onto w-GaN(0001) "1x1" surface, which forms Mn(x)Ga(1-x) with x varying from 0 to ~0.6. Mn-induced surface reconstructions and formation of Mn(x)Ga(1-x) crystalline phases are observed by reflection high-energy electron diffraction (RHEED), Auger electron spectroscopy as well as in-situ RT-STM. The data suggests large-period reconstructions upon deposition of <0.25ML Mn and quick formation of delta-MnGa at ~1 ML of Mn. Structural and electronic properties at representative stages will be presented, as well as possible magnetic properties of MnGa ML's. This work has been supported by DOE (Grant No.DE-FG02-06ER46317) and NSF (Grant No.0730257). Equipment support from ONR is also acknowledged.

[1] S.A.Wolf et al, Science 294, 1488 (2001)

[2] E.Lu et al, Phys.Rev.Lett. 97, 146101 (2006) K.K.Wang et al, Mater.Res.Soc.Symp.Proc.1118-K06-06 (2009)

O 68.5 Thu 11:30 H42

Characterization of copper-metallized ZnO and brass surfaces with STM, SEM and XPS — •Vadim Schott[1], Zhinong Wang[1], David Silber[1], Franziska Traeger[1], Alexander Birkner[1], Martin Kroll[2], Ulrich Köhler[2], and Christof Wöll[1,3] — [1]Chair of physical chemistry I, Ruhr-Universität Bochum, Germany — [2]Experimental Physics IV, Surface Science Group, Ruhr-Universität Bochum, Germany — [3]Institute of functional interfaces, Karlsruhe Institute of Technology, Germany

The metal-substrate interaction is of particular importance for a better understanding of the methanol synthesis process using Cu/ZnO containing catalysts. Scanning tunneling microscopy (STM) and scanning electron microscopy (SEM) was used to investigate the topography of the copper-metallized ZnO and brass surfaces. Addionally x-ray photoelectron spectroscopy (XPS) reveals information about the chemical composition and the oxidation states of surface atoms. Our ultrahigh vacuum (UHV) apparatus allows STM-, SEM-Imaging and XPS measurements at the same sample position. The initial preparation of the ZnO single crystals is done by cycles of Ar-sputtering (E=800eV) and annealing up to 700°C. Then Cu is deposited by molecular beam epitaxy (MBE). In this work we focus on the growth of Cu on the different ZnO surfaces, diffusion of Cu into ZnO and the feasibility of brass formation. The next step of our research is the characterization of brass single crystals. After initial preparation of the crystals and additional oxidation ZnO layers are growing on the surface. The orientation of this ZnO layer was determined using pyridine as a probe molecule.

O 68.6 Thu 11:45 H42

Analysis of Anti-Phase-Domains for GaP Heteroepitaxie on Si(100) by LEEM — •Benjamin Borkenhagen[1], Henning Döscher[2], Gerhard Lilienkamp[1], Peter Kleinschmidt[2], Anja Dobrich[2], Sebstian Brückner[2], Ulrike Bloeck[2], Thomas Hannappel[2], and Winfried Daum[1] — [1]Institute of Energy Research and Physical Technologies, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin

Anti-phase disorder in polar epilayers on non-polar substrates is one

of the major obstacles to overcome during the growth of III-V/Si heterojunctions, e.g., for multi-stack solar cells. As a model system, thin heteroepitaxial GaP films were grown on Si(100) substrates with metal-organic vapour phase epitaxy (MOVPE). Despite the use of stepped single-domain Si(001)(2x1) substrates, the complete prevention of anti-phase domains (APD) in the GaP layer is still an unsolved problem. We have applied low energy electron microscopy (LEEM) to retrieve APDs in the main phase matrix. APDs and main phase can be distinguished by dark-field LEEM using specific diffraction spots for imaging. The results are in good agreement with TEM images of identically prepared samples. In contrast to TEM, LEEM needs no further sample preparation and allows for non-destructive investigations. A further advantage is the possibility to analyze large sample areas and find scattered defects. LEEM can also be applied to study the initial growth of such films and to inspect defect formation from the beginning.

O 68.7 Thu 12:00 H42

Symmetry and Shape of Reconstructed Two-dimensional Nanostructures — •Bert Voigtländer, Konstantin Romanyuk, and Vasily Cherepanov — Institute of Bio and Nanosystems (IBN-3), Forschungszentrum Jülich, 52425 Jülich, Germany, and JARA-Fundamentals of Future Information Technology

We show that the symmetry of the shape of reconstructed 2D islands (nanostructures) on reconstructed surfaces can deviate from both the symmetry of the underlying substrate and the symmetry of the reconstruction. Only an analysis of the symmetry of the *combined system* of reconstructions on substrate and island and of the substrate lattice can deduce predictions for the island shapes (equilibrium shape or steady state growth shape). In explicit case studies we analyze the symmetry of islands on simple cubic (100), fcc(100), fcc(110) and diamond lattice (111) surfaces and present predictions for the expected island shapes. We introduce a general method for the symmetry analysis of the combined system. Our symmetry analysis includes as a special case also the symmetry of any kind of epitaxial reconstruction domain surrounded by a reconstruction at a surface.

O 68.8 Thu 12:15 H42

Surface electronic structure and morphology of epitaxial $CuInSe_2$ — •Andreas Hofmann — Helmholtz-Zentrum Berlin für Materialien und Energie, Institut für Ladungsträgerdynamik (E-I4)

Solar cells based on chalcopyrite absorbers reach the highest efficiencies of all thin-film devices. However, the best laboratory cells still lag dramatically behind the theoretical energy conversion limit. So far, calculations for the surface reconstructions and electronic properties exist [1,2], but experimental data on crystalline material is sparse. Therefore, our approach is to study epitaxial $CuInSe_2$ films as a model system with surface analytic techniques.
Samples of different orientation and stoichiometry were prepared by molecular beam epitaxy, the analysis was performed in-situ in a dedicated UHV system. LEED measurements confirmed the c(4x2) surface for near-stoichiometric $CuInSe_2$(112) which was also predicted by calculation [1]. For the copper-depleted surface, however, a (1x1) structure is found. Angle-resolved photoemission data obtained for the (001) surface showed a good agreement with the band structure from DFT [2]. The morphology of surface with different orientation was investigated with scanning tunnelling microscopy.

[1] S.B. Zhang et al., Phys. Rev. B **57**, 9642 (1998)
[2] S.B. Zhang and S.-H. Wei, Phys. Rev. B **65**, 081402 (2002)

O 68.9 Thu 12:30 H42

Evolution of the surface reconstructions during the growth of an InAs wetting layer on GaAs(001)-c(4×4) — •Holger Eisele, Jan Grabowski, Christopher Prohl, Britta Hoepfner, and Mario Daehne — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, D-10623 Berlin

We studied the growth of the first monolayer of InAs on the GaAs(001)-c(4×4) surface using a combined UHV-MBE-(RHEED)-STM setup, which provides atomically resolved images of the growth surfaces. For a coverage below about 2/3 of an monolayer of deposited InAs we observe single signatures of the deposited material at the GaAs(001)-c(4×4) surface. The number of these signatures is proportional to the amount of deposited InAs. They occur first at the domain boundaries and further at the hollow sites of the GaAs(001)-c(4×4) reconstruction. At a coverage of about 2/3 of a monolayer an abrupt phase transition occurs in the RHEED. Also the STM images changes completely from the c(4×4) reconstruction to a flat topmost layer, showing an (n×3) periodicity along [110] direction. The detailed analysis of this layer exhibits an in-line (4×3) reconstruction alternating with a brick-lined c(4×6) reconstruction, shifted to each other along the [-110] direction by the insertion of an (6×3) surface unit cell. The stoichiometry of the (4×3) could be determined to $In_{2/3}Ga_{1/3}As$ for the topmost layer and the complete structural model for this surface reconstruction can be given, due to comparison of the STM images with DFT-calculations. On top of this layer, the InAs grows in pure stoichiometry and forms chains and 2D islands with $\alpha 2(2\times4)$ and $\beta 2(2\times4)$ reconstructions.

O 68.10 Thu 12:45 H42

In situ RAS Analysis of MOVPE prepared GaP/Si(100) heterointerfaces — •Oliver Supplie, Henning Döscher, Sebastian Brückner, Anja Dobrich, Peter Kleinschmidt, Christian Höhn, and Thomas Hannappel — Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

For high-quality optoelectronic devices built on III-V/Si(100) heterostructures, it is crucial to reduce the defect concentration induced by the heterointerface. As an extremely surface sensitive optical probe, reflectance anisotropy spectroscopy (RAS) can be applied *in situ* in the MOVPE environment. Utilizing RAS, we monitor and characterize the growth of thin GaP layers on a silicon substrate as a model system for III-V/Si(100) heterostructures.
Since RA spectra of the homoepitaxial GaP(100) and heteroepitaxial GaP/Si(100) show characteristic deviations, it is necessary to distinguish the different origins of the RAS signal contributions. Homoepitaxial spectra change with measurement conditions and surface reconstructions. Buried heterointerfaces lead to additional reflections and interference affecting both the reflectance and anisotropy signal. We correct this interference with an empirical method. At III-V/Si(100) heterointerfaces, anti-phase disorder and strain may affect the RAS signal as well. Potentially the interface itself is anisotropic. Applying multiple thin film optical models and reflection simulations, we separate the surface and interface dielectric anisotropy from our measured RAS data.