

## O 10: Semiconductor Substrates: Epitaxy and Growth

Time: Monday 13:15–16:45

Location: MA 042

O 10.1 Mon 13:15 MA 042

**Thickness-dependent structural investigation of thin GaN films by Photoelectron Diffraction** — ●CHRISTOPH RAISCH, ALEXEY SIDORENKO, HEIKO PEISERT, and THOMAS CHASSÉ — University of Tübingen, Institute of Physical Chemistry

Thin films of hexagonal gallium nitride have been grown on 6H-SiC by ion-beam assisted MBE. The thickness ranges from submonolayers to bulk-like samples of more than 100 monolayers. The samples were characterised by XPS, LEED and XPD. During growth, two different types of wetting layers were observed (i) a Ga metal wetting layer on the SiC substrate and (ii) a Ga metal wetting layer on top of the growing GaN film. They prove essential for the spreading wetting growth mechanism and were used to derive interface electronic parameters of the Ga/SiC and Ga/GaN Schottky barriers.

The substrate and the films have been examined by x-ray photoelectron diffraction XPD, a method capable of determining the local atomic structure of crystalline materials. By choosing different photoemission lines, the environments of gallium and nitrogen have been investigated separately and are compared to each other. The differences between Ga2p and Ga3d emission have been evaluated, with Ga3d photoelectrons being bulk sensitive while Ga2p photoelectrons are probing the surface. Features evolving with thickness are identified and interpreted. The experiments are supported by multiple scattering cluster calculations, showing clear trends with increasing film thickness. The simulations also allow the determination of the polarity of the films, which is found to be Ga-terminated for all samples.

O 10.2 Mon 13:30 MA 042

**Morphological and chemical characterization of thin heteroepitaxial Praseodymium sesquioxide films on Si(111)** — ●ANDREAS SCHAEFER<sup>1</sup>, VOLKMAR ZIELASEK<sup>1</sup>, THOMAS SCHMIDT<sup>2</sup>, ANDERS SANDELL<sup>3</sup>, JOACHIM WOLLSCHLÄGER<sup>4</sup>, JENS FALTA<sup>2</sup>, and MARCUS BÄUMER<sup>1</sup> — <sup>1</sup>Institut für Angewandte und Physikalische Chemie, Universität Bremen — <sup>2</sup>Institut für Festkörperphysik, Universität Bremen — <sup>3</sup>Department of Physics, University of Uppsala — <sup>4</sup>Fachbereich Physik, Universität Osnabrück

Among the rare earths Praseodymium oxides possess the highest oxygen mobility and a high oxygen storage capability. Due to this fact they are promising candidates for catalytic applications exploiting the variable valency of Pr. A simplified two dimensional model system of the oxide catalyst can be prepared on silicon substrates in an UHV environment to study the atomic details of oxygen transport and transfer when exposed to adsorbed molecules. Here we report on the growth and morphology of heteroepitaxial Pr<sub>2</sub>O<sub>3</sub> films at a low deposition rate on Si(111) which were investigated using Spot Profile Analysis of Low-Energy Electron Diffraction. In the initial stages of growth the specular diffraction spot exhibits a pronounced threefold symmetry most likely reflecting the formation of highly ordered islands of triangular shape as shown by STM. A roughening of the substrate surface is observed during growth of the initial Praseodymium oxide layer. Beyond these morphological studies, preliminary results of a first chemical characterization of the films with and without adsorbates (CO and oxygen) by XAS and XPS will be presented.

O 10.3 Mon 13:45 MA 042

**Combined electrical and chemical characterization of BaO thin films on Si(001)** — ●DIRK MÜELLER-SAJAK<sup>1</sup>, ALEXANDR COSCEEV<sup>2</sup>, HERBERT PFNÜR<sup>1</sup>, and KARL R. HOFMANN<sup>2</sup> — <sup>1</sup>Leibniz-Universität Hannover, Inst. f. Festkörperphysik — <sup>2</sup>Leibniz-Universität Hannover, Bauelemente der Mikro- und Nanoelektronik

In context with the search for alternative gate oxides on SiO<sub>2</sub> in CMOS technology, we have grown high-k BaO films at a thickness between 5 and 20 nm on clean Si(001) using molecular beam epitaxy of Ba metal in ambient oxygen pressure. Interface states and color centers were characterized by XPS and EELS while varying temperature and oxygen partial pressure during growth. For the electrical measurements, Si(001) has been pre-structured by optical lithography and BaO was only generated on small squares using a tungsten mask. After preparation, the films were capped with 250nm of Au and electrically characterized ex situ.

From capacity-voltage measurements on known areas of BaO windows, a dielectric constant of 30 was calculated. This means that for a

5nm BaO film corresponds to an equivalent oxide thickness (EOT) of 0.65 nm of SiO<sub>2</sub>. These measurements also show very low hysteresis (<5mV), and flatband voltages are close to that of the workfunction difference between Si and Au (+0.65eV). These results are encouraging in terms of the concentrations of fixed and mobile oxide charges both in the bulk and at the interface. The influence of different defects at the interface and within the BaO films will be discussed.

O 10.4 Mon 14:00 MA 042

**Photoelectron spectroscopy (XPS) studies on the system zirconium oxide on Si(100)** — ●FRANK SCHÖNBOHM<sup>1,2</sup>, CHRISTIAN FLÜCHTER<sup>1,2</sup>, DANIEL WEIER<sup>1</sup>, SVEN DÖRING<sup>1,2</sup>, PATRICK MEHRING<sup>1</sup>, ULF BERGES<sup>1,2</sup>, and CARSTEN WESTPHAL<sup>1,2</sup> — <sup>1</sup>Fakultät Physik - Technische Universität Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund, Germany — <sup>2</sup>DELTA - Technische Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, 44227 Dortmund, Germany

Because of the importance for industrial manufacturing we studied ultrathin ZrO<sub>2</sub> films on a Si(100)(2×1) reconstructed surface. We carried out XPS measurements of the Si 2p- and the Zr 3d-level and calculated the film thickness by the damping of the signal strength. Further XPS investigations were performed in order to examine the systems heat stability. The thermal behavior was investigated by annealing the sample at temperatures ranging from 500°C up to 750°C. A ZrO<sub>2</sub> film thickness of 11 Å on the Si(100) surface was thermally stable for temperatures up to 600°C. Above this temperature a new compound was found in the XPS spectra, chemically shifted by 3.7 eV. For temperatures higher than 750°C the ZrO<sub>2</sub>-signal disappeared completely from the surface and the structure of the new ZrSi<sub>2</sub> compound was then examined by a combined LEED, SEM and XPD investigation. The experiments indicated that ZrSi<sub>2</sub> forms islands on the surface. The experimental diffraction data were compared to simulations resulting in a first structure model of the islands.

O 10.5 Mon 14:15 MA 042

**The Influence of Carbon Contaminations in Silicon Epitaxy** — ●OLIVER SENFTLEBEN, PETER ISKRA, TANJA STIMPEL-LINDNER, DOROTA KULAGA-EGGER, IGNAZ EISELE, and HERMANN BAUMGÄRTNER — Universität der Bundeswehr München, Werner-Heisenberg-Weg 39, 85577 Neubiberg

Thermal desorption of the native oxide is a well-known process but leads to an increase in surface roughness and to the formation of SiC. HF treatment, however, leads to a strong carbon contamination of the surface. Both treatments influence subsequent epitaxial overgrowth differently, which will be shown throughout this contribution.

The influence of carbon contaminations on silicon epitaxy strongly depends on its distribution on the silicon surface. A rather homogeneous distribution still allows epitaxial layers of good quality. This will be shown by STM and SIMS. An even higher degree of carbon contamination after HF treatment still allows epitaxial layers of good electrical quality, evaluated by I-V measurements of CVD grown pin diodes with a very high amount of carbon at the interface, measured by SIMS.

Thermal desorption of the native oxide covered by carbon contaminants at temperatures between 800 °C and 900 °C lead to the formation of SiC, which acts as a nucleation site for the Si-monomer and to the formation of stable pyramidal structures with heights up to several 10 nanometers as well as polysilicon, which is demonstrated by STM, SEM and AES measurements. This causes a reduction of the epitaxial quality of subsequent layers.

O 10.6 Mon 14:30 MA 042

**Influence of an Ehrlich-Schwoebel barrier on growth oscillations during epitaxy in layer-by-layer mode** — ●CHRISTIAN HEYN — Institut für Angewandte Physik, Universität Hamburg, Germany

We study the mechanisms behind the damping of reflection high-energy electron diffraction (RHEED) oscillations during layer-by-layer growth of GaAs and AlAs. Experimental data are compared to results of both a kinetic Monte Carlo simulation as well as a rate equations based growth model. The rate model considers in particular reversible aggregation and interlayer migration. With the rate model, we find that the height of the Ehrlich-Schwoebel barrier for interlayer migration signif-

icantly influences the oscillation damping. Under consideration of an Ehrlich-Schwoebel barrier, the rate model quantitatively reproduces experimental oscillation damping as function of growth temperature and speed. Furthermore, the presence of an Ehrlich-Schwoebel barrier explains the more strongly damped oscillations during GaAs growth in comparison to AlAs. AlAs has a higher energy barrier for surface diffusion but a lower Ehrlich-Schwoebel barrier. From a quantitative analysis we obtain values of the Ehrlich-Schwoebel barrier height for GaAs of 0.134 eV and AlAs of 0.069 eV.

O 10.7 Mon 14:45 MA 042

**Investigation of a long-ranged ordered silicate adlayer on the 6H-SiC(0001) surface by LEED, AES and IPE** — ●NABI AGHDASSI, RALF OSTENDORF, and HELMUT ZACHARIAS — Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Straße 10, 48149 Münster

We have prepared well-ordered silicate adlayers on 6H-SiC(0001) surfaces by an ex situ hydrogen treatment at elevated temperatures. The generated surfaces appear to be fully passivated and therefore stable in ambient air. LEED patterns clearly feature a  $(\sqrt{3}\times\sqrt{3})R30^\circ$  periodicity which can be attributed to a long range order of the created oxide layers. Furthermore AES spectra exhibit a distinct  $O_{KLL}$  peak as well as a  $Si_{LVV}$  peak showing a typical oxidic-like shape that is indicating the presence of Si-O bonds on the surface. The unoccupied electronic states of the  $SiO_2/SiC$  interface are studied by inverse photoemission spectroscopy (IPE).

O 10.8 Mon 15:00 MA 042

**Optimized hydrogen bake as in-situ removal of residual oxide and carbon on silicon substrates for thin film deposition** — ●THOMAS ZILBAUER, PETER ISKRA, DOROTA KULAGA-EGGER, MARTIN SCHLOSSER, HELMUT LOCHNER, TORSTEN SULIMA, and IGNAZ EISELE — Universität der Bundeswehr München, Institut für Physik, Werner-Heisenberg-Weg 39, 85577 Neubiberg

The removal of carbon impurities and the native or chemical oxide from silicon substrates is an increasingly important issue for the fabrication of nanoscale semiconductor devices. Often a last in-situ cleaning step is necessary to prepare the partly recontaminated substrate surface after thorough wet chemical cleaning for a deposition process such as CVD, ALD or MBE.

Heating the substrate to temperatures above 800 °C in a hydrogen ambient leads to quick thermal desorption of the residual oxide. However, carbon impurities on the substrate may cause formation of stable silicon carbide at these elevated temperatures.

We demonstrate results from optimizing the hydrogen bake of a commercially available cluster tool for silicon substrates with different history of wet-chemical pre-treatment. The oxygen and carbon contamination are analyzed by secondary ion mass spectrometry (SIMS). Additionally, I-V-measurements of epitaxially grown p-i-n diodes are used to evaluate the cleaning results.

O 10.9 Mon 15:15 MA 042

**Impurity induced growth instabilities** — ●JÖRG MEGOW and FRANK GROSSE — Institut für Physik der Humboldt Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany

Growth instabilities can be utilized for the formation of semiconductor nanostructures, e.g. regular step bunches might be useful as templates for growth of quantum wires. A possible source for step bunching is the inclusion of small amounts of impurities during growth. The experimentally observed growth instability in the  $Si_{1-x}C_x/Si(118)$  system is explainable if the impurities (C) are nearly immobile and have reduced binding to the growing species (Si) [1].

We present kinetic Monte Carlo simulations for different growth scenarios. Special emphasis is given to the role of exchange processes leading to the incorporation of the impurities into subsurface sites. The resulting changes of the chemical ordering in the grown crystal are analyzed and related to changes in the step bunch distribution at the surface. The relation of the formation of three dimensional nanostructures on singular (001) surfaces and wetting behavior under different impurity concentrations is demonstrated.

[1] E.T. Croke *et al.* Appl. Phys. Lett. **77** 1310 (2000).

O 10.10 Mon 15:30 MA 042

**Strain Induced Pit Formation in Ge Layers on Si(111)** — ●KONSTANTIN ROMANYUK<sup>1</sup>, VASILY CHEREPANOV<sup>1</sup>, BERT VOIGTLÄNDER<sup>1</sup>, and JACEK BRONA<sup>1,2</sup> — <sup>1</sup>Institute of Bio- and Nanosystems (IBN 3), and cni — Center of Nanoelectronic Systems

for Information Technology, Research Centre Jülich, 52425 Jülich, Germany — <sup>2</sup>Institute of Experimental Physics, University of Wrocław, pl. Maxa Born 9, PL 50-204 Wrocław, Poland

When nanoscale Ge stripes are grown at Si step edges by step flow growth the formation of nanoscale pits in the one atomic layer thick Ge stripes is observed. This pit formation occurs in surfactant mediated epitaxy (Bi) when a small amount of Si is deposited and attaches as a small rim at the Ge stripes. As we will explain this nanoscale pit formation is driven by both, the energy gain when Ge leaves the Ge stripe and attaches to the thin Si rim terminating the Ge stripe, and the entropy gain due to SiGe intermixing at the step edges. While the direct vertical exchange would lead to a similar final state a high exchange barrier is involved. The pathway via pit formation involves a much lower exchange barrier.

O 10.11 Mon 15:45 MA 042

**Growth and arrangement of silicon and germanium nanowhiskers** — ●ANDREA KRAMER — Institut für Kristallzüchtung, Berlin

The growth of silicon and germanium nanowhiskers as well as their arrangement by pre-structuring of substrates will be discussed. Nanowhiskers are grown via vapor-liquid-solid (VLS) mechanism, which is a method based on solution growth within metal droplets, in an ultra-high vacuum chamber by molecular beam epitaxy (MBE). To obtain a defined positioning of metal droplets, and thus a regular arrangement of nanowhiskers, a reproducible process for the localization of single metal droplets in pre-structured nanopores was successfully developed. Silicon or germanium substrates are initially patterned with nanopores by focused ion beam (FIB) treatment. By adjusting metal evaporation rate and substrate temperature in the growth chamber, individual droplets are preferentially formed within the pre-structured pores. Subsequently, silicon or germanium is evaporated in order to form a solution with the metal and initiate the epitaxial growth of nanowhiskers on the substrate. The morphology of the processed samples has been investigated by scanning electron microscopy (SEM) and transmission electron microscopy (TEM). Results of whisker growth and arrangement will be presented.

O 10.12 Mon 16:00 MA 042

**Structure and morphology of graphene layers on SiC(0001)** — ●CHRISTIAN RIEDL<sup>1</sup>, CHARIYA VIROJANADARA<sup>1</sup>, CHRISTIAN AST<sup>1</sup>, ALEXEI ZAKHAROV<sup>2</sup>, KLAUS HEINZ<sup>3</sup>, and ULRICH STARKE<sup>1</sup> — <sup>1</sup>Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany — <sup>2</sup>MAX-Lab, Lund University, Box 118, Lund, S-22100, Sweden — <sup>3</sup>Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany

We report on the development of graphene layers on the 4H-SiC(0001) surface by high temperature annealing under ultra high vacuum conditions focusing on two issues: firstly, we analyze the precursor stage of graphitization, the  $(6\sqrt{3}\times 6\sqrt{3})R30^\circ$ -reconstruction. By means of low energy electron diffraction (LEED) and scanning tunneling microscopy (STM) we discuss the role of three observed phases with periodicities  $(6\sqrt{3}\times 6\sqrt{3})R30^\circ$ ,  $(6\times 6)$  and  $(5\times 5)$  for three different preparation conditions [1]. Secondly, the growth of epitaxial graphene is discussed in detail. Depending on tunneling bias and tip conditions STM micrographs show the graphene layers with atomic resolution and its long-range epitaxial relation to the underlying substrate [1]. We show that LEED pattern and intensities can be applied quantitatively to monitor the number of graphene layers during the preparation procedure. We correlate LEED fingerprints with angular resolved photoelectron spectroscopy (ARUPS) from HeII excitation, high resolution x-ray photoelectron spectroscopy (XPS) and low energy electron microscopy (LEEM).

[1] C. Riedl *et al.*, Phys. Rev. B, in print

O 10.13 Mon 16:15 MA 042

**Spatial variation of the Dirac-gap in epitaxial graphene** — ●LUCIA VITALI, CHRISTIAN RIEDL, ROBIN OHMANN, ULRICH STARKE, and KLAUS KERN — MPI for Solid State Research, Stuttgart, Germany

The unconventional electronic properties of graphene make it a promising candidate for the realization of novel nanoelectronic circuits which was first realized using single layer graphene samples produced by mechanical exfoliation. An alternative method has been established with the epitaxial growth of graphene on SiC basal-plane surfaces by thermal decomposition of the topmost SiC bilayers. The electronic structure of mono- and few-layer graphene on SiC shows the typical

linear dispersion of the  $\pi$ -bands at their crossing at the Dirac point. The opening of a gap as a function of the layer thickness and charge distribution can be observed by high-resolution photoemission experiments. However, the conditions and layer thickness required for the gap opening and the detailed values of gap size and Dirac energy shift are currently under debate. In the present communication we use scanning tunneling spectroscopy (STS) at low temperatures to obtain insight in the local electronic structure of mono- and bilayer graphene on SiC(0001). We show that already for the first graphene layer grown on top of the  $(6\sqrt{3}\times 6\sqrt{3})R30^\circ$  buffer layer a gap opening is observed. The size of this gap, however, is varying with the periodicity of the interface structure, possibly due to a spatially dependent potential induced into the graphene layer. For the second layer we also observe the Dirac gap but no local spatial variation, i.e. the interface potential is too weak to modulate the electronic structure of the bilayer.

O 10.14 Mon 16:30 MA 042

**Graphene band structure near the Dirac point - lifting of the**

**degeneracy ?** — ELI ROTENBERG<sup>1</sup>, AARON BOSTWICK<sup>1</sup>, TAISUKE OHTA<sup>1,2</sup>, JESSICA MCCHESENEY<sup>1,2</sup>, THOMAS SEYLLER<sup>3</sup>, and ●KARSTEN HORN<sup>2</sup> — <sup>1</sup>Advanced Light Source, Lawrence Berkeley Lab, California USA — <sup>2</sup>Fritz-Haber-Institut der MPG, Berlin — <sup>3</sup>Institut für Physik der Kondensierten Materie, Universität Erlangen

The band structure of graphene exhibits a degeneracy of the valence and conduction bands where the linearly dispersing bands cross at the Brillouin zone boundary [1]. In contrast to previous experimental evidence which strongly supports this band crossing, recent photoemission data by Zhou et al. [2] suggest that this degeneracy is lifted in graphene layers on SiC(0001), through the influence of the substrate, and that a band gap opens at the crossing point. We discuss these results in the light of additional results and present a straightforward and rather intuitive explanation for the conflicting results in terms of the quality of the graphene films prepared on silicon carbide.

[1] J.C.Slonczewski and P.R.Weiss, Phys. Rev. 109, 272(1958). [2] A.Boswick et al., Nature Physics 3, 36(2007). [3] S.Y.Zhou et al., Nature Materials 6, 774(2007).