

O 33: Poster Session III: Semiconductor substrates I

Time: Tuesday 10:30–12:30

Location: P

O 33.1 Tue 10:30 P

Engineering the surface of homoepitaxially MBE grown InAs(111)A — ●STEFFEN ZELZER^{1,2}, RAJIB BATABYAL^{1,2}, MOHANA RAJPALKE², and PETER KROGSTROP^{1,2} — ¹Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, 2100 Copenhagen, Denmark — ²Microsoft Quantum Materials Lab Copenhagen, 2800 Lyngby, Denmark

The surface morphology in the μm and (sub) nm range of homoepitaxially molecular beam epitaxy (MBE) grown planar InAs(111)A buffer layer has been studied by scanning tunneling microscopy (STM) and reflection high energy electron diffraction (RHEED). We show how an optimized cool-down procedure can lead to atomically clean surfaces and present an approach to map the growth parameter space for the two relevant stages of nucleation (step flow and 2D nucleation) on this surface which determines the macroscopical surface morphology. Transition state kinetics are used in combination with critical growth conditions extracted from RHEED intensity measurements to explain the transition from step flow to 2D nucleation.

O 33.2 Tue 10:30 P

Virtual III-V-on-Si substrates grown by MOVPE - reduction of stacking faults — ●MANALI NANDY¹, AGNIESZKA PASZUK¹, MARKUS FEIFEL², CHRISTIAN KOPPKA¹, PETER KLEINSCHMIDT¹, FRANK DIMROTH², and THOMAS HANNAPPEL¹ — ¹TU Ilmenau, Ilmenau, Germany — ²Fraunhofer Institute for Solar Energy Systems ISE, Freiburg, Germany

The performance of III-V-on-Si multijunction solar cells is still limited by their density of defects at the GaP/Si(100) heterointerface and in the GaP buffer layers. In order to improve the crystal quality of the GaP buffer layer, we modified the GaP pulse nucleation by substituting the first five TEGa pulses with TMAI. Influence of Al on the defect density in the GaP buffer layers are investigated by electron channeling contrast imaging. 60 nm thick GaP(100) buffer layers grown on GaP nucleation exhibit short misfit dislocations (MDs) and therefore, a high density of threading dislocations (TDs). In contrast, GaP(100) buffer layers grown on AlGaP nucleation exhibit less, but longer MDs, which result in a lower density of TDs. In addition, the density of stacking faults and stacking faults pyramids in the GaP layer grown on the AlGaP nucleation is significantly reduced. The surface morphology at the initial growth stage of GaP buffer layers grown on AlGaP nucleation, is smoother compared to the buffer layer grown on the GaP nucleation. The application of TMAI in the GaP nucleation process provides a two-dimensional, smooth layer, on which subsequent, high-quality GaP films could be grown, and therefore, shows a promising pathway for improving the performance of III-V-on-Si devices.

O 33.3 Tue 10:30 P

Atomic and electronic structure of the GaP/Si(001) heterointerface studied by HAXPES — ●AGNIESZKA PASZUK¹, OLEKSANDR ROMANYUK², IGOR BARTOŠ², REGAN G. WILKS³, MANALI NANDY¹, JAKOB BOMBSCH³, CLAUDIA HARTMANN³, RAÛL GARCIA-DIEZ³, SHIGENORI UEDA⁴, IVAN GORDEEV², JANA HOUDKOVA², PETER KLEINSCHMIDT¹, MARCUS BÄR³, PETER JIŘÍČEK², and THOMAS HANNAPPEL¹ — ¹Institute of Physics, University of Technology, Ilmenau, Germany — ²Institute of Physics, Prague, Czech Republic — ³Department Interface Design, Helmholtz-Zentrum Berlin, Germany — ⁴SPRING-8, National Institute for Materials Science, Japan

For highly efficient III-V-on-Si optoelectronic devices it is crucial to prepare defect-free heterointerfaces with defined electronic properties. Commonly a thin, pseudomorphic GaP epilayer is deposited on Si prior to further III-V buffer growth, due to its close lattice matching to Si. Here, the atomic and electronic structure of buried GaP/Si(001) heterointerfaces prepared by MOCVD were investigated by hard X-ray photoelectron spectroscopy combined with theoretical modelling. 4 - 50 nm thick GaP films with a different density of antiphase domain boundaries were grown on Si(001) H-terminated surfaces, as controlled by optical *in situ* spectroscopy. We found that the core-level positions and width changes with GaP film thickness and Si substrate type. These observations were related to charge displacements and band bending effects at the interface. In consequence, an inter-diffused layer interface structure model based on the formation of Si-P bonds at the heterointerface and P-doping of the Si substrate was suggested.

O 33.4 Tue 10:30 P

Structural LEED analysis of the reconstructed Si(001) surface — ●JASCHA BAHLMANN¹, KRIS HOLTGREWE², SIMONE SANNA², and JOACHIM WOLLSCHLÄGER¹ — ¹Fachbereich Physik, Universität Osnabrück, 49076 Osnabrück, Germany — ²Institut für Theoretische Physik and Center for Materials Research (LaMa), Justus-Liebig-Universität Gießen, 35392 Gießen, Germany

Previous attempts to solve the atomic geometry of the Si(001)-(2x1) reconstructed surface by means of LEED yielded so far only ambiguous results. We present a geometrical model with asymmetric and buckled dimers with an excellent agreement between the experimental and calculated spectra by dynamic LEED theory. Furthermore, we reveal which parts of the analysis were particularly crucial for obtaining this conclusive IV-LEED result.

Additionally, a comparison between our model, the models of DFT calculations and X-ray diffraction is presented. Moreover, we go a step further and examine also the transition to the higher order reconstruction c(4x2).

O 33.5 Tue 10:30 P

Temperature dependent adsorption of Trimethylamine (TMA) on water-functionalized Si(001)-(2x1) surfaces — ●NIKLAS FORNEFELD¹, LUCIA PÉREZ RAMÍREZ², FRANÇOIS ROCHET², STEFAN KUBSKY³, and ULRICH KÖHLER¹ — ¹Experimentalphysik IV, Ruhr-Universität Bochum, Bochum, Germany — ²Laboratoire de Chimie Physique matière et Rayonnement, Univ. P. et M. Curie, Paris, France — ³Synchrotron Soleil, St. Aubin (Paris), France

Concerning functionalization of Si(001)-(2x1) with organic molecules, an intermediate water layer enables better control of the adsorption processes due to the reduction of possible adsorption sites. To investigate the binding properties on surface silanols (SiOH) and to examine the chemical reactivity we studied the vibrational modes of TMA in the temperature range between 100 K and 300 K during adsorption on a H₂O/D₂O reacted Si(001)-(2x1) surface using HREELS in comparison to XPS results. Both complementary techniques indicate that TMA adsorbs non-dissociatively to surface silanols forming acceptor H-bonds at T < 120 K and at T < 135 K under constant TMA flux. Self-limited TMA adsorption was found to occur already for T < 175 K affecting 80 % of the SiOH without the appearance of the characteristic $\nu(\text{Si-O-H})$ redshift for H-bonding seen at lower temperature. Both adsorption reactions are reversible processes involving TMA N lone pair electrons thus ruling out TMA protonation by either SiH or SiOH. Analyzation of the $\nu(\text{CH}_3)$ Bohlmann band allows us to estimate the bond strength of adsorbed TMA to be in between dative and intermolecular bonding found in TMA mono-/multilayers on pristine Si(100).

O 33.6 Tue 10:30 P

Enhancing structural order by random Au adsorption on the Si(553)-Au system — ●CHRISTA FINK¹, KRIS HOLTGREWE¹, SIMONE SANNA¹, ZAMIN MAMIYEV², and HERBERT PFNÜR² — ¹Justus-Liebig-Universität, Gießen, Germany — ²Leibniz Universität, Hannover, Germany

Nanowires on semiconductor surfaces have drawn the attention from a broad research community as they are promising systems for realizing and studying quasi 1D physics. We investigate the adsorption of additional Au adatoms on the Au double chain system supported by the silicon (553) surface by means of density functional theory and slab models. One adatom per (5 × 2) unit cell strongly enhances the Au chain dimerization, although the favored adsorption site is at the Si step edge far away from the chains. This non-local structure manipulation is related to the two-dimensional coupling between the wire and the substrate. The electronic band structure proves that the hybridization between the Au adatom and the Si step edge transfers charge to the surface. Because of the strong electronic correlation, a band gap opens within the Au related states which is accompanied by an increased dimerization of the Au chains. The Au adsorption has a similar impact on the surface morphology as a pure electron injection. As the enhanced dimerization puts a penalty on the formation energy of defects, the not necessarily ordered adsorption of Au adatoms reduces the number of defects and leads to more order in the wires. This counter-intuitive order-by-disorder mechanism is confirmed by experimental results and transferable to other quasi 1D nanowire systems.