

O 33: Semiconductor substrates: Structure, epitaxy and growth

Time: Tuesday 14:00–15:15

Location: MA 005

O 33.1 Tue 14:00 MA 005

Growth, structure and morphology of tin deposited on Silicon and germanium surfaces — ●NICOLAS BRAUD, THOMAS SCHMIDT, and JENS FALTA — Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany

SnGe is expected to play an important role in optoelectronic and in future Ge device modules integrated into CMOS technologies due to its potentially indirect to direct band gap transition and its higher carrier mobility compared to Ge.

Here we present the investigation of the initial growth and adsorption of Sn on Si(001), Ge(001) and on a compressively strained Ge wetting layer grown on Si(001) by means of low energy electron diffraction and microscopy.

After the deposition of Sn on Si(001) at elevated temperature, a (2×N)-reconstruction was observed. The N-fold periodicity evolved immediately after the beginning of the deposition and decreased from N≈50 to N=4.6 with increasing Sn coverage. For Sn on a strained Ge wetting layer a similar behavior was observed. Also for growth of Sn on bulk Ge(001), an N-fold superstructure was observed. However, the minimum value of N=6.4 was higher than on bulk Si and than on strained Ge/Si.

This leads to the conclusion that strain is the driving force for these reconstructions.

O 33.2 Tue 14:15 MA 005

Study of As-modified Si(100) surfaces for III-V-on-Si heteroepitaxy in CVD ambient — ●AGNIESZKA PASZUK, OLIVER SUPPLIE, MANALI NANDY, ANJA DOBRICH, PETER KLEINSCHMIDT, and THOMAS HANNAPPEL — Institute of Physics, Technische Universität Ilmenau, Germany

III-V heteroepitaxy on Si(100) holds promise for low cost, high-efficiency optoelectronic devices. In polar-on-nonpolar epitaxy, it is crucial to prepare Si(100) surfaces with double-layer (DL) steps in order to avoid antiphase domains, which can significantly reduce the efficiency of the device. Here, we employ vicinal and almost exactly oriented Si(100) substrates relevant for photovoltaic and CMOS applications, respectively. We study the interaction of Si(100) surfaces with Arsenic, which is present in most application-relevant III-V MOCVD reactors, supplied either directly via the TBAs precursor or indirectly as background As_x. The entire process is controlled *in situ* by reflectance anisotropy spectroscopy (RAS) and the obtained spectra are benchmarked by UHV surface analytic techniques. We show that specific processing routes enable control of the dimer orientation on Si(100):As surfaces and we demonstrate low-offcut *single-domain* Si(100):As surfaces with regular, true DL steps. The process conditions to obtain a DL stepped surface depend on the offcut magnitude. We found that both As coverage and dimer orientation on the Si surface contribute to the RAS spectral line-shape, which opens perspectives to fine-tune the surface structure as desired for further III-V growth.

O 33.3 Tue 14:30 MA 005

Molecular dynamics simulations of vapor-deposited amorphous selenium — ●JULIAN SCHNEIDER¹, AMIRHOSSEIN GOLDAN², and ANDERS BLOM¹ — ¹Synopsys QuantumWise, Copenhagen, Denmark — ²Department of Radiology, Stony Brook University, Stony Brook, USA

The structure of amorphous selenium is clouded with much uncertainty and contradictory results regarding the dominance of polymeric chains versus monomer rings. Here, we present Molecular Dynamics simulations using the VirtualNanoLab (VNL) and Atomistix ToolKit (ATK) with the ATK-ForceField module [1] to elucidate atomistic details of the structure of vapor-deposited amorphous selenium and compare these to melt-quenched amorphous selenium. We find pronounced differences depending on the preparation procedure, suggesting that the as-deposited structures predominantly consist of a ring-like topology,

whereas melt-quenched samples reveal a more chain-like structure [2]. Although the exact topological details of the atomic structure of amorphous selenium is difficult to access via experimental techniques, these findings are indirectly corroborated by analyzing the conversion of vapor-deposited samples between various metastable structures.

[1] J. Schneider et al. "ATK-ForceField: A new generation molecular dynamics software package" Modelling Simul. Mater. Sci. Eng. 25, 085007 (2017)

[2] A.H. Goldan, C. Li, S.J. Pennycook, J. Schneider, A. Blom, and W. Zhao, "Molecular structure of vapor-deposited amorphous selenium" J. Appl. Phys. 120, 135101 (2016)

O 33.4 Tue 14:45 MA 005

Delta-doped phosphorus layers in silicon — ●ANN-JULIE UTNE HOLT¹, SANJOY MAHATHA¹, RALUCA-MARIA STAN¹, FRODE SN-EVE STRAND², THOMAS NYBORG², ALEX SCHENK², SIMON PHILLIP COOIL³, MARCO BIANCHI¹, PHILIP HOFMANN¹, JUSTIN WELLS², and JILL MIWA¹ — ¹Department of Physics and Astronomy, Interdisciplinary Nanoscience Center (iNANO), University of Aarhus, 8000 Aarhus C, Denmark — ²Department of Physics, Norwegian University of Science and Technology (NTNU), N-7491 Trondheim, Norway — ³Institute of Mathematics and Physics, Aberystwyth University, Aberystwyth SY23 3BZ, UK

A δ -layer is a buried, high-density, doping profile in a semiconductor host. Such a doping profile may give rise to the formation of a two-dimensional electron gas (2DEG) in the dopant layer [1]. Phosphorus δ -layers in silicon combined with scanning tunneling microscope lithography have led to the fabrication of functional atomic scale devices [2]. By creating such δ -layers, varying in thickness from an atomically sharp doping profile to a 4.0 nm thick dopant layer, the effect of quantum confinement on the electronic structure of a induced 2DEG was studied using angle-resolved photoemission spectroscopy. The location of theoretically predicted, but experimentally undiscovered, quantum well states known as the Δ -manifold was revealed, validating density functional theory calculations developed for describing these δ -layer systems. Verification of these states contributes to the development of accurate models describing the electronic behavior of δ -layer derived devices.

O 33.5 Tue 15:00 MA 005

In situ study of Al_xGa_{1-x}P nucleation on As-modified Si(100) 2° surfaces — ●MANALI NANDY, AGNIESZKA PASZUK, ANJA DOBRICH, OLIVER SUPPLIE, PETER KLEINSCHMIDT, and THOMAS HANNAPPEL — TU Ilmenau, Gustav-Kirchhoff-Straße 5, 98693 Ilmenau

Epitaxial growth of III-V materials on Si substrates is promising for cost-effective, tandem solar cells with high photovoltaic conversion efficiency. In order to avoid antiphase domains during polar-on-non polar heteroepitaxy, an atomically ordered, As-modified double layer (DL) stepped Si(100)2° surface is employed here for further low-defect III-V growth. After the Si surface preparation, a common approach is to subsequently grow a thin GaP nucleation layer, since this material is almost lattice matched to Si[1]. Here we apply Al_xGa_{1-x}P nucleation layer instead of established GaP-on-Si nucleation in order to further modify the atomic and electronic structure of the heterointerface as well as to yield adequate nucleation conditions. Prior to the nucleation, the Si(100)2° surface is exposed to TBAs in an Al-containing III-V MOVPE reactor. We observe that the oxide removal of the Si substrate by HF pre-treatment lowers the maximum process temperature below 820°C[2]. Subsequently the pulsed Al_xGa_{1-x}P nucleation layer consisting of Al, Ga, and P pulses is grown at 420°C, followed by a GaP epilayer growth at 600°C. The RAS signal of the grown GaP is benchmarked by low energy electron diffraction (LEED) and the surface morphology is studied by atomic force microscopy (AFM).[1]O. Supplie et al., APL Mater.3(2015)126110.[2]A. Paszuk,...M. Nandy et al., Sol. Energ. Mat. Sol. Cells, in press(2017), doi:10.1016/j.solmat.2017.07.032.