

O 17: Semiconductor Substrates II: Structure, Epitaxy, Growth

Time: Monday 15:00–17:00

Location: MA 144

O 17.1 Mon 15:00 MA 144

Bimodal Growth of Fe islands on graphene — •YISHENG GU — Shanghai Jiao Tong University, Shanghai, China

Nucleation of different materials on graphene may improve our cognizing of further application of graphene related systems, among which the combinations of graphene and magnetic materials are promising in spin related technics. We have prepared Fe islands on epitaxial graphene on SiC by molecular beam epitaxy, and then directly examine the topography by scanning tunneling microscope. At room temperature, Fe forms cluster. However, by annealing at relatively high temperature, Fe flat islands and Fe polyhedrons arise. The electronic states with certain patterns that differs from normal lattice are detected on top of the flat islands. This difference of Fe topography between room temperature growth and relatively high temperature annealing may be generalized to deposition of other metals on graphene.

O 17.2 Mon 15:15 MA 144

Local GaAs growth on patterned Si(001) surfaces by Laser-assisted MOVPE — •CHRISTIAN BRUCKMANN, JÜRGEN BLÄSING, ARMIN DADGAR, and ANDRÉ STRITTMATTER — Institut für Physik, Otto-von-Guericke-Universität Magdeburg, PF4120 Magdeburg, Germany

Monolithic integration of group III-V compound semiconductors on a silicon-based platform is the ultimate solution for combining optoelectronics based on compound semiconductors with Si-based integrated circuit technology. Heteroepitaxy of group III-V semiconductors on Si wafers is a common approach as it facilitates large-scale production. However, for the realization of complex networks by implementing different high performance devices on the same chip a local growth approach of III-V-compound semiconductors can be a viable path to achieve cost-effective monolithic integration. The newly developed Laser-assisted Metal Organic Vapor Phase Epitaxy features local heating via high-power laser radiation enabling controllable local epitaxial growth¹. In order to improve the crystalline quality of GaAs islands, the local growth is now performed on patterned Si(001)-wafers. In addition n-/p-type doping of GaAs-based structures is also presented.

¹M. Trippel et al., "Laser-assisted local metal-organic vapor phase epitaxy", Rev. Sci. Instrum. 93, 113904 (2022)

O 17.3 Mon 15:30 MA 144

Growth of vanadium on Si(111) — •DANG LIU — School of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai, China

Vanadium is a type-II superconductor with a $T_c=5.3$ K. Due to its high melting temperature, it is difficult to grow Vanadium material by thermal evaporation. We use molecular beam epitaxy method to deposit Vanadium on silicon substrate, and then characterized by low temperature scanning tunnelling microscope. Vanadium islands with many facets are successfully grown on Si(111) with ultra-high substrate temperature. The lateral dimensions of Vanadium islands are from dozens to several hundred nanometers, and their heights are around several tens of nanometers. Atomic images of different facets are obtained by constant current mode of STM. We also get scanning tunneling spectroscopy on the surface of vanadium island, and a small gap shows around zero bias, which is a signal of superconductivity.

O 17.4 Mon 15:45 MA 144

In-situ analysis of phase transitions in ultrathin nickel silicides by time-of-flight medium energy ion scattering — •CAROLIN FRANK¹, KEVIN VOMSCHEE¹, RADEK HOLEŇÁK², ELENI NTEMOU², and DANIEL PRIMETZHOFFER² — ¹Faculty of Physics and CENIDE, University of Duisburg-Essen, Duisburg, Germany — ²Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

We present first results obtained during the commissioning phase of recent upgrades to the Time-of-Flight Medium Energy Ion Scattering (ToF-MEIS) set-up at Uppsala University: A new UHV sample preparation chamber enables growth of thin films with a high precision in thickness by deposition from electron beam evaporators. We focus on calibration of the growth rate, in-situ deposition of thin nickel films on silicon and subsequent ToF-MEIS analysis of these films regarding

phase transitions. Prior to deposition of nickel, the silicon substrates were treated ex-situ with hydrofluoric acid and annealed. To study the phase transition from the nickel layer deposited on silicon to epitaxial nickel silicide step-by-step, the samples were subsequently annealed up to 1500 K by an electron impact heater. During the stepwise annealing process, the transition to a well-ordered cubic nickel disilicide phase was found at 648 K. 2D scattering maps enable the analysis of intensity distributions of backscattered ions for selected energies. Since each of these energies corresponds to different chemical elements and - for a specific element signal - to specific depths within the sample, the epitaxy of the nickel silicide films due to blocking effects is verified.

O 17.5 Mon 16:00 MA 144

XPS study on composition and band structure of aluminum alloyed β -gallium oxide bulk crystals and thin films — •LUKAS SCHEWE¹, JANA REHM², MING CHAO KAO³, VEDRAN VONK³, ZBIGNIEW GALAZKA², SAUD BIN ANOOZ², ANDREAS POPP², and JAN INGO FLEGE¹ — ¹Fachgebiet Angewandte Physik und Halbleiterspektroskopie, BTU Cottbus-Senftenberg — ²Leibnitz-Institut für Kristallzüchtung, Berlin — ³CXNS-Center for X-ray and Nano Science, DESY Hamburg

Beta-phase gallium oxide is a wide gap semiconductor with promising applications in high-power devices. To further increase the high-power capabilities of a material with dielectric constant ϵ , as suggested by the Baliga figure of merit $BFOM = \epsilon\mu E_b^3$, it is desirable to increase the electric breakdown field E_b , e.g., by alloying with aluminum.

The present work discusses structural and electronic properties of $\beta - (Al_xGa_{1-x})_2O_3$ thin films grown by metal organic vapour-phase epitaxy and bulk crystals grown by the czochralski method. The predicted Al content ranges up to 30%. The Al concentration has been measured by X-ray photoelectron spectroscopy (XPS) and will be compared to the Al content calculated from the lattice parameter measured by X-ray diffraction for thin films and inductively coupled plasma-optical emission spectrometry for bulk samples. Additionally the thin films have been investigated for homogeneity through XPS depth profiling obtained by sequential Ar ion sputtering. Furthermore the band gap has been determined by electron loss spectra from XPS depending on Al content and compared to optical absorbance measurements.

O 17.6 Mon 16:15 MA 144

Atomic structure of As-modified Si(100) surfaces prepared in MOCVD ambience utilizing background arsenic — CHRIS YANNICK BOHLEMANN¹, AGNIESZKA PASZUK¹, MANALI NANDY¹, AARON FLÖTTOTTO^{2,3}, MAX GROSSMANN^{2,3}, OLEKSANDR ROMANYUK⁴, •KAI DANIEL HANKE¹, PETER KLEINSCHMIDT¹, ERICH RUNGE^{2,3}, and THOMAS HANNAPPEL¹ — ¹TU Ilmenau, Institute of Physics, Fundamentals of Energy Materials — ²TU Ilmenau, Institute of Physics, Theoretical Physics I — ³TU Ilmenau, Centre of Micro- and Nanotechnologies — ⁴Institute of Physics, Academy of Sciences of the Czech Republic, 182 00 Prague 8

A low-defect III-V nucleation layer and a well-defined atomically abrupt interface between the Si(100) substrate and the III-V nucleation layer are essential prerequisites for subsequent low-defect III-V layer growth. Preparation of a well-ordered Si(100) surface in industrially-relevant MOCVD ambience with arsenic benefits in a significant temperature reduction during the deoxidation step. In this study, we investigate the atomic structure of Si(100) surfaces prepared in As-rich MOCVD reactor, employing background arsenic as the arsenic source. The preparation of the samples in the MOCVD reactor was monitored in situ by surface sensitive optical spectroscopy and the surfaces were characterized in UHV by FTIR and STM. The measurements are supported by complementary DFT calculations. We confirm presence of hydrogen on the surface and mixed As-Si-H dimers, which was previously unrecognized.

O 17.7 Mon 16:30 MA 144

Towards an ab initio kinetic Monte Carlo model for the growth of β -Ga₂O₃ (100) — •QAEM HASSANZADA¹, KONSTANTIN LION^{1,2}, CLAUDIA DRAXL², and MATTHIAS SCHEFFLER¹ — ¹The NOMAD Laboratory at the FHI of the Max-Planck-Gesellschaft and IRIS-Adlershof of the Humboldt-Universität zu Berlin — ²Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

Ga₂O₃ is gaining attention in diverse applications [1]. Insights from molecular beam epitaxy (MBE) indicate that varying Ga-to-O ratios influence its growth modes [2], and volatile suboxide (Ga₂O) desorption limits growth rate under Ga-rich conditions [3]. However, the atomic-level mechanisms underlying these observations remain elusive. This project focuses on studying β -Ga₂O₃(100) growth using density functional theory (DFT) calculations. The study uncovers distinct stable sites for single adatoms and clusters. Ga adatoms diffuse more favorably than O adatoms at both stoichiometric terminations. Both adatoms and Ga-O pairs preferentially diffuse along the b crystallographic direction. This directional mobility aligns with experimental observations of elongated islands along the b direction in MBE growth [4]. The results lay the groundwork for developing a comprehensive ab initio kinetic Monte Carlo model for Ga₂O₃ growth.

[1] D. Guo et al. *Materials Today Physics* 11, 100157 (2019) [2] P. Mazzolini et al., *J. Phys. D: Appl. Phys.* 53, 354003 (2020). [3] P. Vogt et al., *Appl. Phys. Lett.* 106, 081910 (2015). [4] Z. Cheng et al., *Nanotechnology* 29, 395705 (2018).

O 17.8 Mon 16:45 MA 144

Exploring surface properties of hexagonal Si and Ge
— •MARTIN KELLER¹, JÜRGEN FURTHMÜLLER¹, FRIEDHELM BECHSTEDT¹, and SILVANA BOTTI^{1,2} — ¹Friedrich-Schiller-Universität Jena, Germany — ²Ruhr-Universität Bochum, Germany

The determination of surface energy is essential to provide guidelines for choosing proper substrates for high-quality epitaxial growth. At the same time interface electronic states are crucial to determine the functionality of a heterostructure. We present ab initio calculations, using density functional theory in a slab geometry, that explore structural and electronic properties of the surfaces of hexagonal silicon and germanium, which are novel materials for active optoelectronic applications. We study the a, m, c and r-plane orientations, which are being considered as preferential facets for the growth of hexagonal SiGe nanowires. Our focus lies on understanding surface and interface stability and its implications on material and device design. Our calculations and the comparison with experimental findings offer practical insights for substrate selection for thin film growth and the construction of heterostructures.