O 46: Poster Session IV: Semiconductor substrates II

Time: Tuesday 13:30–15:30 Location: P

O 46.1 Tue 13:30 P

Atomistic Modeling for the Vapor-Phase Growth of GaAs Nanowires: from DFT to Growth Kinetics — •In Won Yeu[1], Gyuseung Han[1,2], Cheol Seong Hwang[2], and Jung-Hae Choi[2] — [1]Electronic Materials Research Center, Korea Institute of Science and Technology, Seoul 02792, Korea — [2]Department of Materials Science and Engineering, Seoul National University, Seoul 08826, Korea

Based on density functional theory (DFT), this study introduces an ab initio approach tackling the vapor-phase growth kinetics of III-V nanowire (NW) depending on temperature (T) and pressure (P) conditions. By evaluating the vibrational entropy contribution to the surface energy through surface phonon calculations, the T-P dependent variation in surface reconstructions was successfully predicted by the authors. Considering the surface transitions, the change in Gibbs free energy is calculated as a function of T and P at each growth process on surfaces: adsorption and nucleation. The comparison of the free energy among different surfaces enables us to predict the relative rate of growth depending on crystallographic directions and stacking sequences. As a result, we identify the mechanism of extreme anisotropic growth of GaAs (spontaneous NW formation) along a certain polar direction, <111>B; the preferential adsorption of vapor sources on (111)B surface, allowed at narrow T-P range, induces the unidirectional growth. In addition, the asymmetric formation of stacking sequence during the growth along the two opposite directions of a polar direction, <111>A and <111>B, is elucidated, showing a perfect agreement with experimental observations.

O 46.2 Tue 13:30 P

3D Active Sites of Te in Hyperdoped Si by Hard X-ray Photoelectron Kikuchi-Diffraction — •Moritz Hoesch[1], Mao Wang[2], Shengqiang Zhou[2], Christoph Schlüter[1], Olena Fedchenko[3], Katerina Medjanik[3], Sergej Babenkov[3], Aimo Winkelmann[4], Hans-Joachim Elmers[3], and Gerd Schönhense[3] — [1]DESY Photon Science, Notkestraße 85, Hamburg, Germany — [2]Helmholt-Zentrum Dresden-Rossendorf, — [3]JGU, Institut für Physik, Mainz, Germany — [4]Academic Centre for Materials and Nanotechnology, AGH University of Science and Technology, Krakow, Poland

n-type doping of Si by the deep chalcogen donor Te in excess of the solubility limit was recently demonstrated to lead to hyperdoped material [1]. These samples are made by ion im*plantation into an intrinsic Si substrate combined with pulsed laser melting. Our investigation by hard x-ray photoelectron spectroscopy (hXPS) reveals at least two different Te species with different binding energy and systematically varying concentrations as a function of increasing Te-content. At the highest doping concentration we study the photoelectron scattering patterns using hard x-ray photoelectron diffraction (hXPD) [2]. Substitutional site occupation of both Te monomers as well as dimers is identified with increasing binding energy leading to the main features in the XPS spectra. The sharp hXPD patterns allow the detailed analysis of the local surrounding of the dopant atoms [3]. — References: [1] M. Wang et al. Phys. Rev. Appl. 11 054039 (2019) and references therein. [2] O. Fedchenko et al NJP 21, 113031 (2019); [3] O. Fedchenko et al NJP 22, 103002 (2020).

O 46.3 Tue 13:30 P

GaInP(100) and InP(100) with different surface reconstructions for photoelectrochemical water splitting — •Olfa Dani[1], David Ostheimer[1], Mario Kurniawan[2], Agnieszka Paszuk[1], Andreas Bund[2], and Thomas Hannappel[1] — [1]Institute of Physics, Technische Universitaet Ilmenau, Germany — [2]Institute of Materials Science and Engineering, Technische Universitaet Ilmenau, Germany

To date, III-V semiconductor device structures enable the highest solar-to-hydrogen efficiencies, exceeding 19%. In this approach, a detailed understanding of the reactions at the semiconductor-electrolyte interface is essential to design the semiconductor surface for efficient charge transfer. In this present work, we study photoelectrochemical (PEC) performance of atomically well-ordered surfaces of GaInP(100)and InP(100) grown by MOVPE. p-type InP have been grown homoepitaxially on InP(100) substrates. GaInP buffer layers were grown lattice matched, on either GaAs or Ge (100) substrates. In order to avoid anti-phase boundaries in the III-V epilayers, the Ge(100) surface was prepared with double-atomic steps prior to growth. The surfaces involved were prepared with either P-rich (2x1) or III-rich (2x4) surface reconstructions via specific preparation routes controlled by optical in situ spectroscopy and identified in UHV by LEED. Selected samples were in system transferred in an inert nitrogen ambiance to a PEC cell, where they were exposed to an aqueous electrolyte. For comparison, the same measurements were performed on samples with a native oxide layer. We show that a precise surface preparation is crucial for efficient PEC processes.

O 46.4 Tue 13:30 P

Caesium deposition on GaN to obtain a photocathode for particle accelerators — •Jana Schaber[1,2], Rong Xiang[1], Jochen Teichert[1], and André Arnold[1] — [1]Department of Radiation Physics, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Department of Physical Chemistry, Technical University Dresden, Dresden, Germany

Negative electron affinity (NEA) GaAs- and GaN-based photocathodes are used in modern night vison detectors and light emitting diodes. GaAs semiconductors are already used as electron sources in particle accelerators and well- studied. Like GaAs, GaN belongs to the III-V semiconductor group with similar properties. It is assumed that GaN, like GaAs, shows enormous potential as a novel electron source for particle accelerators.

P-type GaN on different substrate material (sapphire, silicon, copper or SiC) is activated by a thin layer of caesium and illuminated by ultra-violet (UV) light at the same time. As a consequence of negative electron affinity (NEA) and photoeffect, the generated photoelectrons enter into vacuum and are collected by a copper ring anode. The resulting photocurrent is detected during the whole activation process and stopped when a maximum photocurrent is reached. By a comparison of differences in substrate material, chemical pre-cleaning, thermal heat treatment and activation parameters (e.g. caesium-flux), the photocurrent, quantum efficiency and the re-activation of the photocathode is studied. Additionally the GaN samples are examined by AFM, SEM and EDX.

O 46.5 Tue 13:30 P

Au silicide nanowires on Si(110) — •Stephan Appelfeller — MAX IV Laboratory, Lund University, Sweden

The Au-Si phase diagram is of simple eutectic nature without any stable bulk Au silicide. Nevertheless, metastable Au silicide structures have been observed at Au-Si interfaces and on surfaces. Especially, Au atomic chains on planar and vicinal Si(111) surfaces were investigated in recent years since they showed very enticing properties, e.g., self-doping by adatoms, 1D metallic behavior, or spin chain formation.

Here, Au induced nanostructures on the Si(110) surface are studied using LEED, STM and STS, and core-level and valence band PES. Due to the symmetry of the substrate, single-domain Au reconstructions form, e.g., a 2×5 superstructure known to show a 1D metallic band structure, which show interesting adatom structures. However, the focus of this study is on Au silicide nanowires. Their diffraction data are not characterized by well-defined spots, but by streaky features. While the dimensions of the nanowires are directly obtainable in STM, they only show a structurless appearance for widely varying tunneling conditions. Nevertheless, structural information is available by tuning the surface sensitivity in PES indicating silicide formation. Both PES and STS experiments show a finite density of states at the Fermi level for the nanowires suggesting (semi-)metallic behaviour.