O 91: Poster Session - Semiconductor Substrates: Structure, Epitaxy and Growth

Time: Wednesday 18:15–20:00 Location: P2/1OG

O 91.1 Wed 18:15 P2/1OG

A First-Principles Study of the Structure and Stability of Oxygen-Terminated Diamond(110) Surfaces — •Shayantan Chaudhuri[1,2] and Reinhard J. Maurer[2] — [1]EPSRC Centre for Doctoral Training in Diamond Science and Technology, University of Warwick, Coventry, CV4 7AL, United Kingdom — [2]Department of Chemistry, University of Warwick, Coventry, CV4 7AL, United Kingdom

Diamond is a material that possesses numerous properties and applications in a variety of fields, such as photonics and electrochemistry. Boron-doped diamond (BDD) is electrically-conducting and can be used as a working electrode for electrodeposition and electrochemical sensor applications. BDD crystals can be grown by chemical vapour deposition (CVD), which appears to favour the growth of the (110) facet amongst others. Under such reaction conditions, diamond surfaces will be partially oxidised and oxygen-terminated. Infrared (IR) and X-ray photoelectron spectroscopy (XPS) measurements in literature provide indications of the co-existence of different oxygen species. We have conducted density functional theory (DFT) calculations to understand the surface structure and chemical composition of the oxidised diamond(110) surface. By constructing a large set of possible terminations and coverages, we construct a phase diagram of surface terminations, which is dominated by an unexpectedly stable co-existence phase of keto and ether groups. By explicit simulation of IR and XPS signals, we establish the most likely dominant oxygenation state of the surface.

O 91.2 Wed 18:15 P2/1OG

Surface structure of MOVPE-prepared GaP(111)B — •Peter Kleinschmidt[1], Pingo Mutombo[2], Theresa Berthold[1,3], Agnieszka Paszuk[1], Matthias Steidl[1], Gernot Ecke[4], Andreas Nägelein[1], Christian Koppka[1,3], Oliver Supplie[1], Stefan Krischok[1,3], Oleksandr Romanyuk[2], Marcel Himmerlich[1,3,5], and Thomas Hannappel[1] — [1]Institut für Physik, Technische Universität Ilmenau PF 100565, 98684 Ilmenau — [2]Institute of Physics of the Czech Academy of Sciences, Cukrovarnická 10, 16200 Prague, Czech Republic — [3]Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, PF 100565, 98684 Ilmenau, Germany — [4]Institut für Mikro- und Nanoelektronik, Technische Universität Ilmenau, PF 100565, 98684 Ilmenau, Germany — [5]European Organization for Nuclear Research - CERN, 1211 Meyrin, Switzerland

The MOVPE-prepared GaP(111)B surface was studied by XPS, STM, LEED, AES and AFM as well as ab initio DFT. Deoxidation under TBP, followed by high-temperature annealing under pure hydrogen results in the formation of Ga-rich islands, whereas the regions in between are atomically flat. Atomically resolved STM of these regions shows a largely disordered surface, but small units of (2×2), $c(4 \times 2)$, and $(\sqrt{3} \times \sqrt{3})R30°$ ordering can be identified. According to DFT calculations, these are the most favorable reconstructions under hydrogen-rich conditions. We conclude that STM images the dangling bonds of an otherwise hydrogen-terminated phosphorus face.

O 91.3 Wed 18:15 P2/1OG

Impact of Al on defect formation in GaP buffer layers grown on Si(100) substrates in CVD ambience — •Manali Nandy[1], Agnieszka Paszuk[1], Christian Koppka[1], Markus Feifel[2], Peter Kleinschmidt[1], Frank Dimroth[2], and Thomas Hannappel[1] — [1]Institute of Physics, TU Ilmenau, Ilmenau, Germany — [2]Fraunhofer Institute for Solar Energy Systems ISE, Freiburg, Germany

The performance of III-V-on-Si multi-junction solar cells is still limited by a high density of defects at the GaP/Si heterointerface and in the III-V buffer layer. Here, in order to improve the crystal quality of the GaP buffer layer grown on Si(100) substrates by MOCVD, we modify the GaP nucleation, which consists of 10 alternating pulses of TBP and TEGa, by substituting the first few selected TEGa pulses with TMAl. Crystal defects in the GaP(100) buffer layers are investigated by electron channeling contrast imaging. GaP buffer layers grown on the GaP nucleation exhibit short misfit dislocations (MDs), and therefore, a high density of threading dislocations (TDs), which are located at the ends of each MD. In contrast, in the GaP buffer layer grown on the AlGaP nucleation the MDs are significantly longer, which results in lower density of TDs. In addition, we find lower density of stacking faults and stacking fault pyramids compared to the GaP buffer layer grown on the GaP nucleation. We conclude that the Al induced in the GaP nucleation layer suppresses defect formation and improves crystal quality of the epilayer. Further studies of reciprocal space map by x-ray diffraction aim to investigate strain in both GaP buffer layers and its correlation to the defect density.