O 18: Semiconductor Substrates: Structure, Epitaxy and Growth

Time: Monday 16:00–17:30 Location: WIL C307

O 18.1 Mon 16:00 WIL C307

Deconstructing silicon: can surface reconstructions emerge from global geometry screening? — •Chiara Panosetti[1], Maximilian Bauer[1], Matt Probert[2], and Karsten Reuter[1] — [1]Technische Universität München, Germany — [2]University of York, GB

The Si(111) − (7 × 7) reconstruction is arguably the most complicated surface superstructure known to date. The details of its currently accepted geometry, described by the so-called Dimer-Adatom-Stacking fault (DAS) model, are the result of a 25-year long joint effort of experiments and theory. Attempting to solve such a complicated problem—with a known solution—by means of unbiased global structure optimization is therefore a suitable testbed for the performance of corresponding computational algorithms. We here specifically assess the performance of Genetic Algorithms (GA) and the Basin Hopping (BH) approach, where the generation of trial structures for canonical and grand canonical screening is applied to the surface layer in periodic boundary conditions and where different strategies are pursued to enhance the production of chemically sensible candidate geometries. Results suggests that robustness, success and speed of convergence of the employed approaches are strongly influenced by how much the trial moves tend to preserve favourable bonding patterns once they appear.

O 18.2 Mon 16:15 WIL C307

Patterning of ultra sharp dopant profiles in silicon — Simon Cooil[1,2], Federico Mazzola[1], Hagen Klemm[3], Gina Peschel[3], Yuran Niu[4], Alex Zhakarov[4], Andrew Evans[2], Thomas Schmidt[3], Michelle Simmons[5], •Jill Miwa[6], and Justin Wells[1] — [1]NTNU, Trondheim, Norway — [2]Aberystwyth University, Aberystwyth, UK — [3]Fritz Haber Institute, Berlin, Germany — [4]MAX IV Laboratory, Lund, Sweden — [5]UNSW, Sydney, Australia — [6]Aarhus University, Aarhus, Denmark

We present a method for patterning a buried two-dimensional electron gas (2DEG) in silicon. The buried 2DEG forms from placing an ultra sharp and dense profile of phosphorus dopants beneath the silicon surface; a so-called Si:P δ-layer. The composition and structure of these Si:P δ-layers have been studied down to the atomic limit by secondary ion mass spectrometry and scanning tunnelling microscopy. Both angle resolved photoemission spectroscopy and theoretical calculations have shown that these Si:P δ-layers host a 2DEG with properties desirable for atomic scale quantum electronic devices. Here, we provide a new method for patterning such buried 2DEGs using low kinetic energy electron beam lithography. Using a combination of microscopic and spectroscopic techniques, we demonstrate the formation of patterned features with dopant concentrations sufficient to create 2DEG states.

O 18.3 Mon 16:30 WIL C307

Surface Structure of MOVPE-prepared GaP(111)B — •Peter Kleinschmidt[1], Pingo Mutombo[2], Oleksandr Romanyuk[2], Marcel Himmerlich[3], Theresa Berthold[3], Xin Wen[1], Andreas Nägelein[1], Matthias Steidl[1], Agnieszka Paszuk[1], Oliver Supplie[1], Stefan Krischok[3], and Thomas Hannappel[1] — [1]Photovoltaics Group, Institute of Physics, Technische Universität Ilmenau, 98684 Ilmenau, Germany — [2]Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnicka 10, 162 00 Prague 6, Czech Republic — [3]Technical Physics I, Institute of Physics and IMN MacroNano, Technische Universität Ilmenau, 98684 Ilmenau, Germany

We have characterized the structure of MOVPE-prepared GaP(111)B surfaces by STM, XPS and ab intio DFT. After deoxidation under tertiarybutylphosphine and subsequent annealing in H_2, STM images show flat terraces with an atomic surface structure which is congruent with the underlying lattice, but only locally exhibits ordered regions of (2×2), $c(4 \times 2)$ and $(\sqrt{3} \times \sqrt{3})$ reconstruction. We identify the protrusions in the images as dangling bonds of an otherwise H-terminated phosphorus face. The DFT calculations predict a (2×2)-3H and $c(4 \times 2)$-3H reconstruction under H-rich conditions, while the $(\sqrt{3} \times \sqrt{3})$-2H reconstruction is less favorable. Preparation without annealing in H leads to a P-rich surface with an additional adlayer of trimers.

O 18.4 Mon 16:45 WIL C307

In situ surface control of AlP on GaP(100) substrate during processing in MOCVD ambient — •Manali Nandy, Agnieszka Paszuk, Anja Dobrich, Oliver Supplie, Peter Kleinschmidt, and Thomas Hannappel — TU Ilmenau, Gustav-Kirchhoff-Straße 5 (Meitnerbau) 98693 Ilmenau

Epitaxial growth of III-V materials on Si substrate can be beneficial for cost-effective devices in optoelectronic applications. However the nucleation of III-V materials like AlxGa1-xP material grown on Si(100) substrate could serve as a buffer layer for other III-V materials, due to small lattice mismatch between the Si and AlxGa1-xP(from 0.36%-0.37% for x=0 to 1)[2]. Here,first we focus on the growth of AlP buffers on GaP(100) substrate. After deoxidation of GaP(100) substrates at 630°C under H2 ambient, we have grown GaP buffer layer prior to growth of AlP epilayer. The growth temperature was kept at 600°C and the reactor pressure was constant at 100 mbar throughout the process. The whole process was monitored in-situ by reflection anisotropy spectroscopy (RAS). The RAS signal taken at 300°C from the AlP surface shows a clear, distinguishable intense peak at 3.62 eV; probably corresponds to a Phosphorus-rich AlP(100) surface and in addition, we observe a continuous change in the RAS line shape with increasing temperature without phosphorus stabilization. Above 720°C we observe a second clear distinguishable RA-signal which may be corresponds to a Al-rich surface. [1] H. Kawanami, Solar Energy Materials & Solar Cells 66, 479 (2001) [2] H. Kroemer, J. Cryst. Growth, 81,193 (1987)

O 18.5 Mon 17:00 WIL C307

The structure of single-crystalline ZnO surfaces — •Jens Niederhausen[1,2], Antoni Franco-Cañellas[3], Simon Erker[4], Martin Oehzelt[2], Thorsten Schultz[1], Patrick Amsalem[1], Pardeep K. Thakur[5], Katharina Broch[6], David Duncan[5], Anton Zykov[1], Stefan Kowarik[1], Tien-Lin Lee[5], Alexander Gerlach[3], Oliver T. Hofmann[4], Frank Schreiber[3], and Norbert Koch[1,2] — [1]Institut für Physik, Humboldt-Universität, Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [3]Institut für Angewandte Physik, Universität Tübingen, Tübingen, Germany — [4]Institut für Festkörperphysik, TU Graz, Graz, Austria — [5]Diamond Light Source, Oxfordshire, UK — [6]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

The electronic and catalytic properties of metal oxide surfaces are controlled by their atomistic details. For ZnO, ab-initio calculations predict rich phase diagrams, with the resulting structures varying significantly in terms of surface reconstruction, adsorbate species, and surface relaxation. A clear experimental identification of a predicted surface structure as well as the identification of thus far disregarded chemical species and structural effects arising from the surface preparation procedure are significantly assisted by the X-ray standing waves (XSW) technique that yields structural information with chemical sensitivity. We employed XSW to monitor how Ar^+ sputtering deteriorates the surface crystallinity and show that this effect can be largely reversed by annealing. By variation of temperature and H_2O partial pressure we determined surface structures for selected phase diagram points.

O 18.6 Mon 17:15 WIL C307

Atomic scale STM and nc-AFM study of the Hematite (012) surface — •Zdenek Jakub[1], Florian Kraushofer[1], Magdalena Bichler[2], Jan Hulva[1], Martin Setvin[1], Michael Schmid[1], Ulrike Diebold[1], Peter Blaha[2], and Gareth. S. Parkinson[1] — [1]Institute of Applied Physics, TU Wien, Austria — [2]Institute of Materials Chemistry, TU Wien, Austria

For its abundance, low cost, stability and environmental benignity, hematite (α-Fe2O3) is a promising material for utilization in a wide range of fields, including as a photoanode for photoelectrochemical water splitting [1]. Although (012) is known to be one of the most stable surfaces of hematite, the atomic-scale structure remains unknown. Here we present the first-ever atomic-scale scanning tunneling microscopy (STM) and non-contact atomic force microscopy (nc-AFM) study of the surface. Our data suggests that a bulk termination model for the oxidized (1x1) surface is plausible, but images of the reduced (2x1) surface are inconsistent with any of the previously proposed structural models. Based on the experimental data we propose a new model for the (2x1), whose plausibility is supported by our DFT

calculations. We also present the results of H2O adsorption studies on the (2x1) surface and discuss the data in the context of previously published results [2].

[1] Parkinson, G.S., Surface Science Reports, 71, 272-365 (2016).

[2] Henderson, M.A. et al.. Surface Science, 417, 66-81 (1998).