O 40: Poster: Semiconductor Substrates

Time: Tuesday 18:00–20:00 Location: P2/EG

O 40.1 Tue 18:00 P2/EG

Si(553)-Au and Si(775)-Au surface reconstructions with a genetic algorithm approach — •Leonard M. Verhoff and Simone Sanna — Instutute for theoretical physics, Giessen, Germany

It was found by simulations and experiments, that Au atoms on a Si(553)- and Si(755)-surface form metallic nanowires. However, their precise atomic structure is still under discussion.

In this work, the respective surface reconstructions with N adatoms are searched, using a genetic algorithm implemented in the program *CALYPSO*. Genetic algorithms are reported to be efficient methods for structure predictions.

In the first generation, all Au atoms are distributed randomly on the surface, meaning every adatom introduces 3 degrees of freedom. For each generated structure, the fitness, i.e. the configuration's free energy, is then calculated from first principles with density functional theory implemented in *VASP*.

The next generation's individuals are created by moving every structure in the $3N$-dimensional space towards the structure that minimizes the fitness so far. To avoid getting stuck in a local energy minimum, 20% of the structured are created randomly in each generation.

The last step is repeated, until a certain convergence criterion is reached.

O 40.2 Tue 18:00 P2/EG

Assessing and processing the surface quality of free-standing wurtzite GaN in ultra-high vacuum — •Mohammadreza Rostami[1], Biao Yang[1], Felix Haag[1], Francesco Allegretti[1], Lifeng Chi[2], Martin Stutzmann[3], and Johannes V. Barth[1] — [1]Physics Department E20, Technical University of Munich, Garching, 85748, Germany — [2]Institute of Functional Nano & Soft Materials, Collaborative Innovation Center of Suzhou Nano Science and Technology, Soochow University, Suzhou 215123, P. R. China — [3]Walter Schottky Institute and Physics Department, Technical University of Munich, 85748 Garching, Germany

Gallium nitride (GaN) is proposed as an alternative candidate to metallic substrates for assembling organic molecular structures 1. However, the formation of a persistent surface oxide layer in air considerably limits the use of GaN for well-defined interfaces 1. We have investigated n-type free-standing c-plane wurtzite GaN crystals. The effect of electron bombardment on the surface quality of free-standing GaN during ammonia annealing was studied. Surface cleaning and full removal of the oxide layer on GaN surfaces could be reproducibly achieved via sputtering and annealing cycles, leading to substantial roughening of the GaN surface. Although ammonia annealing with electron bombardment increased the N/Ga atoms ratio, the surface morphology remained rough. In addition, the on-surface chemistry of 1,3,5-Tris(4-bromophenyl) benzene (TBB) 2 was studied on the cleaned GaN surface. [1] V. Bermudez, Surf. Sci. Rep. 72 (4), 147-315 (2017) [2] M. Fritton et al. J. Am. Chem. Soc 141 (12), 4824-4832 (2019)

O 40.3 Tue 18:00 P2/EG

A super-cycle approach to atomic layer deposition of indium-gallium-zinc oxide at low temperature — Ali Mahmoodinezhad[1], Carlos Morales[1], Małgorzata Kot[1], Franziska Naumann[2], Paul Plate[2], •Karsten Henkel[1], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Germany — [2]SENTECH Instruments GmbH, Berlin, Germany

The continuing development of multifunctional devices needs novel multicomponent oxide layers, demanding a high control of both composition and thickness during their preparation. To this end, single metal oxides exhibiting high structural quality and conformity have successfully been grown by atomic layer deposition (ALD). However, the deposition of more complex compounds with specific optical and electrical properties is still challenging. In this work, we follow a bottom-up approach to design an ALD super-cycle to grow mixed indium-gallium-zinc oxide (IGZO) films with a controllable composition. For the formation of the individual indium, gallium, and zinc oxides, we found the use of plasma-enhanced ALD (PEALD) at 150 °C to be favorable when using the organometallic precursors trimethylindium, trimethylgallium, and diethylzinc together with oxygen plasma. The PEALD approach of IGZO films can particularly overcome a nucleation delay within the ZnO sub-cycle known from thermal ALD, achieving a higher growth per cycle and improving the quality and composition homogeneity of the films as shown by in-situ spectroscopic ellipsometry and ex-situ X-ray photoelectron spectroscopy.

O 40.4 Tue 18:00 P2/EG

Adsorption of spike amino acids, asparagine and cysteine, on the surface of model catalyst TiO2 — •Miguel Blanco Garcia[1], Mona Kohantorabi[1], Michael Wagstaffe[1], Mohammad Tehrani[1], Silvan Dolling[1], Andreas Stierle[1,2], and Heshmat Noei[1] — [1]Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany — [2]Mathematics, Informatics, and Natural Sciences (MIN) Faculty, University of Hamburg, 20354 Hamburg, Germany

Titanium oxides are excellent candidates for the inactivation of viruses using light due to their photocatalytic properties [1]. In this study we are aiming to determine the mechanism of inactivation of SARS-CoV-2 on TiO2 under ultraviolet treatment [2]. The two most abundant amino acids in the spike protein of the SARS-CoV-2 virus (cysteine and asparagine) [3] are adsorb under UHV and aqueous solution on TiO2 surfaces. Surface sensitive techniques such as X-ray photoelectron spectroscopy shows changes in the amino acids upon UV treatment. Furthermore, scanning tunneling microscopy demonstrates the disposition of the amino acid molecules on the surface and the changes upon UV irradiation. GISAXS data was obtain at DESY P03 for the adsorption in aqueous solution, to understand the adsorption geometry and self-assembly of the cysteine amino acids on the rutile and anatase TiO2 surfaces.

References: [1] Diebold, U. Surface science reports 48.5 (2003): 53-229. [2] Kohantorabi, et al., ACS Appl. Mater. Interface., Under Review. [3] Wang D, et al., Nano today 40 (2021): 101243.