HL 51: Functional Semiconductors for Renewable Energy Solutions II

Time: Friday 9:30–11:00 Location: ER 325

HL 51.1 Fri 9:30 ER 325

Investigation of a LID defect energy barrier using a P-line appearing in indium-doped silicon PL spectra — •Katharina Peh[1], Dominik Bratek[1], Kevin Lauer[1,2], Robin Lars Benedikt Müller[1], Dirk Schulze[1], Aaron Flöttotto[1] und Stefan Krischok[1] — [1]TU Ilmenau, Institut für Physik und Institut für Mikro- und Nanotechnologien, 98693 Ilmenau, Germany — [2]CiS Forschungsinstitut für Mikrosensorik GmbH, Konrad-Zuse-Str. 14, 99099 Erfurt, Germany

With the help of low-temperature photoluminescence (LTPL) it is possible to find photoluminescence (PL) lines that originate from defects. These PL lines can indicate not only the species, but also the density of one specific defect configuration. In indium-doped silicon, the P-line at 1.118 eV is used to investigate light-induced degradation (LID). [1,2] With illumination and annealing treatments, we are now able to reproducibly influence the intensity of the P-line, and thus identify the P-line as an intermediate state. It will be discussed within the A_{Si}-Si_i defect model. [3] Both Czochralski (CZ) and float zone (FZ) silicon wafers were examined and their behaviour compared. For the first energy barrier in annealing treatments of the LID defect, we obtain values between E_{FZ}=0.5±0.09 to E_{CZ}=0.84±0.22 eV. [4] [1] K. Lauer, C. Möller, D. Schulze, and C. Ahrens, AIP Advances 5(1), 017101 (2015). [2]C. Möller, and K. Lauer, Physica Status Solidi (RRL) - Rapid Research Letters 7(7), 461-464 (2013). [3]K. Lauer, K. Peh, D. Schulze, T. Ortlepp, E. Runge, and S. Krischok, Physica Status Solidi (a) 219(19), 2200099 (2022). [4]D. Bratek, Master thesis (2023).

HL 51.2 Fri 9:45 ER 325

The influence of structural dynamics on the macroscopic properties of the solar harvesting nitride CuTaN2 — •Franziska S. Hegner[1], Adi Cohen[2], Stefan S. Rudel[3], Silva Kronawitter[1], Manuel Grumet[1], Xiangzhou Zhu[1], Roman Korobko[2], Lothar Houben[2], Chang-Ming Jiang[1], Wolfgang Schnick[3], Gregor Kieslich[1], Omer Yaffe[2], Ian D. Sharp[1], and David A. Egger[1] — [1]TU Munich, Germany — [2]Weizmann Institute of Science, Israel — [3]LMU Munich, Germany

Ternary nitrides are an emerging class of materials that show large potential for solar energy conversion because of their favourable light absorption and carrier transport properties. Yet, they are relatively unexplored due to their metastability and the comparative difficulty of their synthesis. Here, we studied the representative copper tantalum nitride, CuTaN2, a particularly promising visible light absorbing semiconductor, using a combination of theoretical and experimental methods. Harmonic phonon calculations and finite-temperature Raman scattering experiments show that its structural dynamics display highly anharmonic character. We first elucidated the microscopic aspects of the atomic motions with ab initio Molecular Dynamics and then investigated their impact on their macroscopic characteristics. The latter are strongly influenced by the anharmonic nuclear motions, leading to negative thermal expansion and, especially important, a significant increase of the fundamental bandgap. This highlights that structural dynamics play a crucial role for the functional properties of energy materials.

HL 51.3 Fri 10:00 ER 325

Luminescence study of light induced degradation in thallium implanted silicon — •Robin Lars Benedikt Müller[1], Kevin Lauer[1,2], Katharina Peh[1], Zia Ul-Islam[1], Dirk Schulze[1], and Stefan Krischok[1] — [1]Technische Universität Ilmenau, Institut für Physik und Institut für Mikro- und Nanotechnologien, 98693 Ilmenau, Germany — [2]CiS Forschungsinstitut für Mikrosensorik GmbH, Konrad-Zuse-Str. 14, 99099 Erfurt, Germany

Light-induced degradation (LID) designates the loss of efficiency of doped silicon-based devices such as solar cells and detectors. Despite extensive research into this phenomenon in recent decades, the recombination-active defect responsible for degradation remains unidentified until today. Thereby a variety of dopants were examined, besides boron and copper, indium doped silicon was investigated. A potential explanation for LID in Si:In is the so-called ASi-Sii defect, whose possible defect configurations manifests itself by the appearance of the P-line in the spectrum of low-temperature photoluminescence (LTPL)[1]. Besides this P-line, the spectra of thallium-doped silicon reveal a so-called A-line, whereby this unusual luminescence system is based on a defect which is present in two different configurations[2]. After the first demonstration of LID in Si:Tl, we investigated differently doped samples with regard to the behaviour of these spectral elements under the influence of the LID cycle.[1] K.Lauer, C.Moeller, D.Schulze, and C. Ahrens. AIP Advances, 5(1):017101, 01 2015; [2] H. Conzelmann, A. Hangleiter, and J. Weber. physica status solidi (b), 133(2):655*668, 1986.

HL 51.4 Fri 10:15 ER 325

Water interaction in dependence of AlInP(100) surface reconstruction studied by in-situ RAS and XPS — •Mohammad Amin Zare Pour, Sahar Shekarabi, Agnieszka Paszuk, and Thomas Hannappel — Grundlagen von Energiematerialien, Institut für Physik, Technische Universität Ilmenau

n-AlInP(100) is commonly used for a selective transport of electrons in so-called window layers in high-efficiency III-V multijunction solar or photoelectrochemical (PEC) cells. A fundamental understanding of water interaction with the window layer is crucial for PEC applications as well as for atomic layer deposition of passivation layers such as TiO2. In this study, we investigate reaction mechanisms of water with well-defined surfaces using X-ray photoelectron spectroscopy (XPS) and in-situ reflection anisotropy spectroscopy (RAS). As prepared phosphorous rich and indium rich terminated n-AlInP(100) prepared by metalorganic chemical vapour deposition were exposed to water at room temperature and 10-5 mbar in an ultra-high vacuum chamber. In this work, exposure dosage was measured in langmuir (L) units, where 1 L = 1 Torr x 1s. Even after 75 kL of water exposure, the core-levels of P-rich AlInP do not exhibit any shift or significant changes in the line shape of the spectra. In contrast, In-rich AlInP is more likely to react with water molecules, and the RAS signal clearly changes after only 20 kL. The XPS results indicate that In-In bonds on In-rich surfaces are active sites, while neither P-P bonds nor III-P bonds on P-rich surfaces interact with water.

HL 51.5 Fri 10:30 ER 325

Emerging oxynitride photoelectrodes for stable and efficient energy conversion — •Tobias Haubold — Walter-Schottky-Institute, Technische Universität München, Germany

Photoelectrochemical solar water splitting represents a promising approach for the direct conversion of visible light into chemical fuels. To overcome the efficiency and stability limitations of pure oxide and nitride photosystems, respectively, high-throughput computational screening has identified oxynitrides as an interesting material space that offers narrower bandgaps and improved charge carrier mobility. While several studies have reported the synthesis of oxynitrides and demonstrated their application for photoelectrochemical energy conversion, controlled synthesis routes for high-quality materials and a fundamental understanding of semiconductor and defect-related properties are still lacking. Here, we leverage reactive magnetron sputtering and subsequent annealing as a controllable synthesis platform to deposit tantalum oxynitride thin films with controlled structure, chemical composition, and optoelectronic quality. By variation of the N2-O2 process gas mixture, we were able to systematically study the impact of anion non-stoichiometry on optical properties and photoelectrochemical performance. The gained insights will reveal the impact of electronically active oxygen- and nitrogen-related defect states within the bandgap on the semiconductor properties of oxynitrides.

HL 51.6 Fri 10:45 ER 325

Engineering interfaces for efficient and stable photoelectrochemical energy conversion — •Julian Müller[1,2], Matthias Kuhl[1,2], Ian D. Sharp[1,2], and Johanna Eichhorn[1,2] — [1]Walter Schottky Institute, Technische Universität München, Germany — [2]Physics Department, TUM School of Natural Sciences, Technische Universität München, Germany

For photoelectrochemical (PEC) energy conversion, transition metal nitrides emerged recently as a promising alternative to commonly studied metal oxides. Among others, tantalum nitride (Ta3N5) is highly interesting due to its bandgap of 2.1 eV, suitable band alignment for water splitting, and theoretical photocurrent density of 12.9 mA/cm2. However, Ta3N5 rapidly degrades under operation conditions due to self-oxidative decomposition in aqueous electrolytes. Here, we interfaced Ta3N5 photoanodes with cobalt oxide (CoOx) surface layers to overcome the current stability limitations. Specifically, we leveraged plasma-enhanced atomic layer deposition (PE-ALD) to deposit stable, conformal, and ultra-thin protection layers which are simultaneously robust and electrochemically active. To engineer efficient interfaces between photoelectrode and protection layer, we developed one- and two-step annealing processes in different gas atmospheres and correlated the change in interface properties to their PEC characteristics. Overall, this study highlights the beneficial role of the protection layer on the photoelectrode stability, but also emphasizes the dominating role of interface properties on the efficiency and the need for controlled interface engineering.