HL 42: Nitrides III – Emerging thin films and electrochemistry

Time: Thursday 11:15–12:45 Location: POT/0006

Invited Talk HL 42.1 Thu 11:15 POT/0006

Transition Metal Nitride Semiconductors for Photoelectrochemical Energy Conversion — •Verena Streibel[1,2], Laura I. Wagner[1,2], Elise Sirotti[1,2], David A. Egger[2], and Ian D. Sharp[1,2] — [1]Walter Schottky Institute, Technical University of Munich, Garching, Germany — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, Garching, Germany

Transition metal nitride thin films are emerging as promising materials for (photo)electrochemical applications. However, their synthesis and defect control remain challenging. Here, we use reactive co-sputtering to synthesize and engineer nitride thin films with precise control over composition and doping in the Ti-Ta-N,[1] Zr-Ta-N,[2,3] and Hf-Ta-N materials space. Starting from orthorhombic Ta_3N_5, we show that substitutional Ti doping improves photoconversion efficiency by modulating defects and recombination dynamics. While high Ti doping forms a secondary TiN phase, Zr and Hf yield tunable solid solutions in the Zr-Ta-N-(O) and Hf-Ta-N-(O) systems, exhibiting bandgap modulation and large refractive indices. Notably, a new bixbyite-type ternary compound, $ZrTaN_3$, forms at a 1:1 Zr:Ta ratio, showing strong visible light absorption and photoanodic activity. DFT calculations reveal a tunable direct bandgap driven by cation ordering.[3] Our findings establish composition engineering as a key strategy for tailoring band structure and charge transport in emerging nitride semiconductors.

[1] Wagner, L.I. et al., Adv. Funct. Mater. 2024, 34, 2306539.
[2] Wagner, L.I. et al., Adv. Mater. Interfaces 2025, 12, 2400745.
[3] Sirotti, E. et al., Adv. Energy Mater. 2024, 202402540.

HL 42.2 Thu 11:45 POT/0006

Analysis of the interface properties of cubic nitride thin films grown on 3C-SiC/Si templates using electrochemical impedance spectroscopy — •Hannes Hergert[1,2], Mario F. Zscherp[1,2], Silas A. Jentsch[1,2], Jörg Schörmann[1,2], Sangam Chatterjee[1,2], Peter J. Klar[1,2], and Matthias T. Elm[1,2] — [1]Center for Materials Research, Heinrich-Buff-Ring 16, 35392 Giessen — [2]Institute of Experimental Physics I, Heinrich-Buff-Ring 16, 35392 Giessen

Due to its lack of internal polarization fields cubic gallium nitride (c-GaN) is a promising semiconductor material for a variety of applications, such as high-power electronics or optoelectronic devices. High quality c-GaN can successfully be grown by molecular beam epiatxy on 3C-SiC/Si templates making use of a c-AlN buffer layer, which accommodates lattice mismatch between c-GaN and the 3C-SiC template. A reliable characterization of the interface properties as well as the electrical transport properties of c-GaN is crucial for optimizing the thin film growth as well as for designing advanced functional devices. In this work we employ electrochemical impedance spectroscopy (EIS) for characterizing the transport throught c-GaN/AlN/3C-SiC/Si sample structures with different c-GaN thicknesses and for analyzing the properties of the interface, such as the trap density.

HL 42.3 Thu 12:00 POT/0006

Investigating Charge Transport Limitations in $LaTiO_2N$ Thin Films for Photoelectrochemical Water Splitting — •Oliver Brune[1,2], Gabriel Grötzner[1,2], Katarina S. Flashar[1,2], Saswati Santra[1,2], Ian D. Sharp[1,2], and Verena Streibel[1,2] — [1]Walter Schottky Institute, Technical University of Munich, Garching, Germany — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, Garching, Germany

Photoelectrochemical water splitting offers a sustainable route to hydrogen production. On the photoanode side, $LaTiO_2N$ is a promising candidate due to its visible-light absorption, favorable band alignment and n-type semiconducting properties. However, its performance is limited by inefficient charge transport, the origin of which remains unclear. In this work, we synthesize $LaTiO_2N$ thin films by spin coating and reactive sputter deposition, both followed by ammonia annealing, yielding films with controlled structure and composition as confirmed by XRD and ERDA/RBS. Synchrotron-based XAS, XPS, UV-Vis spectroscopy, and PEC measurements reveal that a larger degree of nitridation in $LaTiO_2N$ correlates with higher short-range order and crystallinity, a decreasing bandgap, and an increase in photocurrent density. To elucidate charge transport mechanisms and carrier dynamics, we use Hall effect and temperature-dependent photocurrent measurements. Our findings establish a direct link between synthesis parameters, defect chemistry, and charge-carrier dynamics in $LaTiO_2N$, providing a foundation for overcoming transport limitations in oxynitride-based photoanodes for solar hydrogen production.

HL 42.4 Thu 12:15 POT/0006

Epitaxial YbN thin films grown by nitrogen plasma-assisted molecular beam epitaxy — Yitong Chen[1,2], •Anna Meléndez Sans[1,3], Shin-ichi Kimura[2,4,5], Liu Hao Tjeng[1], and Simone Altendorf[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Department of Physics, Graduate School of Science, The University of Osaka, Toyonaka, Japan — [3]Institut de Ciència de Materials de Barcelona, Bellaterra, Spain — [4]Graduate School of Frontier Biosciences, The University of Osaka, Suita, Japan — [5]Institute for Molecular Science, Okazaki, Japan

Rare-earth mononitrides display interesting magnetic and semiconducting properties due to the strongly correlated and localized $4f$ electrons. However, extreme air sensitivity and poor stoichiometry hindered research on bulk samples when they were first discovered. Modern advancements in UHV-based thin film growth techniques have opened the possibility to synthesize and study high quality samples.

Unlike most of the rare-earths, which can break the molecular nitrogen bond, Yb does not react with nitrogen gas and therefore requires an activated nitrogen source for the synthesis of YbN.

Here we present our growth study on YbN thin films grown by nitrogen plasma-assisted molecular beam epitaxy, using different substrates (MgO and $LaAlO_3$) and growth conditions. The films were characterized *in situ* with photoelectron spectroscopy, confirming their semiconducting character and the Yb valence as 3+. Photon-energy dependence of the valence band spectra revealed a significant hybridization of the Yb $4f$ and N $2p$ states.

HL 42.5 Thu 12:30 POT/0006

Novel $TbTa(O,N)_3$ perovskite oxynitride for photoelectrochemical energy conversion — •Aleksandr Kochergov[1,2], Gabriel Grötzner[1,2], Oliver Brune[1,2], Frans Munnik[3], Saswati Santra[1,2], Verena Streibel[1,2], and Ian D. Sharp[1,2] — [1]Walter Schottky Institute, Technical University of Munich, Germany — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Perovskite oxynitride semiconductors have emerged as promising candidates for photoelectrochemical (PEC) water splitting, given their smaller band gaps ($\sim$ 2 eV) compared to more extensively studied metal oxides. Previous studies show that in rare-earth lanthanide tantalum perovskite oxynitrides, PEC photocurrent density increases with the increment of the A-site cation atomic number [1]. However, no studies have investigated A-site cations heavier than gadolinium (Gd). This work presents a method for synthesizing the novel perovskite oxynitride $TbTa(O,N)_3$ as thin film via spin coating followed by a sequential two-step annealing procedure in air and ammonia. X-ray diffraction shows that proper NH_3 annealing conditions are crucial for obtaining the $TbTa(O,N)_3$ perovskite structure. The resulting films are investigated for their structural, compositional, and optoelectronic properties. The results suggest a 2.3 eV band gap and n-type conductivity. Given these favorable properties, the viability of $TbTa(O,N)_3$ as photoanode is evaluated.

[1] Zou, Qi, et al., J. Am. Chem. Soc. 2024, 146, 28182-28189