MM 4: Materials for the Storage and Conversion of Energy I

Time: Monday 10:15–13:00 Location: SCH/A216

Topical Talk MM 4.1 Mon 10:15 SCH/A216

Photoelectric properties of dislocations in SrTiO3 single crystals — •Marin Alexe — University of Warwick

Dislocations are one-dimensional crystallographic line defects traditionally regarded as detrimental to the functional properties of conventional semiconductors. However, it has been recently shown on Fe-doped SrTiO3 single crystals containing well-ordered, high-density dislocation structures that dislocations can significantly enhance photoconductivity. Local photoconductivity measurements using atomic force microscopy (AFM) revealed that regions surrounding dislocation cores exhibit up to a fourfold increase in photoconductivity compared with dislocation-free areas of the crystal. Furthermore, macroscopic in-plane surface measurements using microcontacts aligned along dislocation slip bands showed orders-of-magnitude enhancement in photoconductivity. This might be due a significant increase of the carrier density at the core of dislocation due to a to a non-chemical local doping induced by the strain or strain gradient.

These results provide unambiguous evidence that dislocations in oxide semiconductors can be beneficial for specific functional properties. The anisotropic enhancement of photoconductivity along dislocation cores highlights their potential as active elements in future one-dimensional oxide electronic and optoelectronic devices.

MM 4.2 Mon 10:45 SCH/A216

Defect-driven carrier dynamics in tantalum nitride photoelectrodes — •Lukas M. Wolz[1], Johannes Dittloff[1,2], Laura I. Wagner[1,2], Julius Kühne[1,2], Luc-Fabrice Tremel[1], Lina M. Todenhagen[1,2], Lissa Eyre[1,2], Felix Deschler[1,2,3], Ian D. Sharp[1,2], and Johanna Eichhorn[1] — [1]Physics Department, TUM School of Natural Sciences, Technische Universität München, Germany — [2]Walter Schottky Institute, Technische Universität München, Germany — [3]Institute for Physical Chemistry, Heidelberg University, Germany

Tantalum nitride (Ta_3N_5) is a widely studied semiconductor for solar-driven water splitting. Yet, experimentally realized efficiencies often remain below theoretical limits largely because native and impurity-related defect states alter charge carrier dynamics by promoting trapping and recombination. Here, we investigate how distinct defect properties in Ta_3N_5 thin films govern ultrafast photocarrier behavior using femtosecond transient absorption spectroscopy, complemented by photoluminescence (PL) and PL excitation measurements. Ta_3N_5 photoelectrodes were synthesized by annealing TaO_x, TaN_x, and Ta precursor films in NH_3, enabling systematic control over shallow and deep defect state concentrations. The controlled defect properties allow us to disentangle the roles of nitrogen vacancies and oxygen-related defects in shaping carrier dynamics. Our results reveal that deep defects function as efficient trapping and recombination centers for free carriers. Here, we correlate ultrafast spectroscopy with complementary optical and photoelectrochemical data.

MM 4.3 Mon 11:00 SCH/A216

Probing Defect-State Photoionization in Ta_3N_5 Thin Films via Photocurrent Excitation Spectroscopy — •Luc-Fabrice Tremel[1], Lukas M. Wolz[1], Johannes Dittloff[1,2], Ian D. Sharp[1,2], and Johanna Eichhorn[1] — [1]Physics Department, TUM School of Natural Sciences, Technische Universität München, Germany — [2]Walter Schottky Institute, Technische Universität München, Germany

Transition-metal nitrides are a highly interesting material space for solar-energy conversion due to their suitable bandgap for visible light absorption and high theoretical solar-to-hydrogen efficiencies. A prominent example is Ta_3N_5, which combines a bandgap of 2.2 eV with favorable band alignment for solar water splitting. In practice, however, its photoelectrochemical performance is strongly constrained by shallow and deep defects. Here, we use photocurrent excitation spectroscopy, complemented by power-dependent photocurrent measurements, to determine how these defect states shape the spectral photocurrent response of Ta_3N_5. By tracking photocurrent as a function of photon energy, light intensity, and applied potential, we distinguish the sharp band-edge transition from a broadened onset dominated by defect-assisted photoionization into the conduction band. These insights into the defect-controlled photoresponse of Ta_3N_5 provide guidance for improved fabrication strategies and the development of higher-performing nitride-based solar-fuel devices.

MM 4.4 Mon 11:15 SCH/A216

Piezoresponse force microscopy on substituted BaTiO3-relaxors — •Markus Kratzer[1], Philipp Fahler-Muenzer[2], Christian Maier[4], Klaus Reichmann[3], Marco Deluca[5], and Christian Teichert[1] — [1]Chair of Physics, Department of Physics, Mechanics and Electrical Engineering, TU Leoben, Leoben, Austria — [2]University of Warwick - Department of Physics, Coventry, United Kingdom — [3]Institute for Chemistry and Technology of Materials, Graz, Austria — [4]Materials Center Leoben GmbH, Leoben, Austria — [5]Silicon Austria Labs GmbH, Sandgasse 34, 8010 Graz, Austria

Relaxor ferroelectrics are key materials in electrostatic capacitors for energy storage but also for high-performance actuators and transducers. Classical relaxor ferroelectric systems often contain lead, which is environmentally unsound. Thus, lead free relaxors are highly desired. A promising route is via substituted barium titanate (BaTiO3). In this study we focus on B-site-substituted polycrystalline BaTiO3, where the central Ti ion in the perovskite lattice is partially substituted by Zr or Nb. In such systems, information on the microscopic ferroelectric domain structure is still lacking, even though detailed macroscopic characterization using a variety of techniques has been undertaken. We use piezoresponse force microscopy to investigate domain structure and local polarization switching at different temperatures and compositions. We find that temporal stabilization of domains with limited volume is still possible, even though long-range ferroelectric order is strongly supressed with increasing levels of substitution. This suggests the presence of residual highly unstable polar nanoregions.

15 min. break

MM 4.5 Mon 11:45 SCH/A216

Tunable TiO_xN_y Photoelectrodes for Efficient Solar Energy Conversion — •Sebastian Trautschold and Johanna Eichhorn — TUM School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany

Oxynitrides have recently emerged as a versatile material class for photoelectrochemical energy conversion, offering a pathway to combine the stability of oxides with the visible-light absorption and favorable charge transport of nitrides. Their key advantage lies in the continuous tunability of optical and electronic properties via adjusting the O/N ratio. TiO_xN_y provides a particularly illustrative platform: while TiO_2 is limited by a wide bandgap and TiN is metallic, TiO_xN_y can be tuned into an intermediate semiconducting regime, enabling improved utilization of the solar spectrum without sacrificing transport.

Here, we deposit TiO_xN_y thin films by pulsed gas reactive sputtering, enabling precise stoichiometric control over a broad composition range. Post-annealing in ammonia and nitrogen is then used as an additional handle to tailor crystallinity, phase evolution, and defect chemistry. By correlating deposition and annealing parameters with structural, chemical, and optoelectronic characteristics - particularly bandgap and defect properties - we identify processing windows that optimize qualities relevant for solar harvesting. Our results demonstrate the strong sensitivity of TiO_xN_y to both growth kinetics and thermal treatment, and establish practical guidelines for engineering oxynitride photoelectrodes toward efficient and durable solar energy conversion systems.

MM 4.6 Mon 12:00 SCH/A216

In Situ Scanning Transmission Electron Microscopy Investigation of Solid-State Batteries Under Realistic Processing Conditions — •Thomas Demuth, Shamail Ahmed, and Kerstin Volz — Philipps Universität Marburg, Department of Physics and mar.quest, Marburg, Germany

Solid-state batteries promise safer energy storage with higher energy density compared to conventional lithium-ion batteries with liquid electrolytes. To ensure good ionic conductivity between the cathode active material (CAM) and solid electrolyte (SE), the interface area must be maximized. This can be achieved by co-sintering the materials at elevated temperatures. However, high-temperature treatment can induce secondary phase formation at the SE - CAM interface. To optimize material stability, a fundamental understanding of the materials' structure and the processes occurring at the interface are required. Here, in situ (scanning) transmission electron microscopy ((S)TEM) offers insights into nanoscale reaction processes. In our study, we have heated the CAM LiNiO2 (LNO) as a model system in an oxygen atmosphere, utilizing a closed gas cell heating holder, which enables heating the sample in a gaseous atmosphere of 1 bar to temperatures of up to 1000 °C. Using a scanning nanobeam mode allows rapid switching between live imaging for the observation of morphological changes and recording of 4D diffraction pattern datasets for structural analysis. Our findings indicate that the onset temperature for phase degradation is significantly higher in an oxygen atmosphere compared to vacuum, highlighting the importance of replicating realistic processing conditions.

MM 4.7 Mon 12:15 SCH/A216

Voltage-Dependent CEI Development on LMO Cathodes in-situ monitored via Langasite Microgravimetry — •Robert Löser and Guido Schmitz — University of Stuttgart, Stuttgart, Germany

Understanding the formation and evolution of the cathode-electrolyte interphase (CEI) is essential for improving the stability of high-voltage lithium-ion battery materials such as LiMn2O4 (LMO). In this work, we investigate the CEI formation and composition in-situ on sputtered LMO thin films using an electrochemical microbalance based on a Langasite (La3Ga5SiO14) resonator. Unlike conventional quartz crystal microbalances, Langasite substrates enable high-temperature annealing of sputtered oxide films while keeping their piezoelectric properties, making them uniquely suited for preparing crystalline cathode layers directly on the resonator surface. LMO films were cycled to different upper voltage cutoffs to investigate how oxidative potentials influence CEI formation. The coupled electrochemical-gravimetric data reveal clear voltage-dependent mass changes associated with electrolyte decomposition, surface reconstruction, and dissolution processes. By correlating frequency shifts with electrochemical signatures, we quantify the onset, magnitude, and reversibility of CEI species formation dependent of the upper voltage boundary. This study demonstrates that Langasite-based microgravimetry enables powerful, in-situ investigation of CEI evolution and interphase dynamics on annealed cathode films such as LMO, opening the way for systematic studies across a broader range of high-temperature processed electrodes.

MM 4.8 Mon 12:30 SCH/A216

Tuning electronic structure of CoNi LDHs via surface Fe doping for achieving effective oxygen evolution reaction — •Yunli Shi[1,2], Huaping Zhao[1], Junqi Li[2], and Yong Lei[1] — [1]Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]School of Materials Science and Engineering, Shaanxi University of Science and Technology, Xian 710021, China

Cobalt and nickel based layered double hydroxides (LDHs) are promising oxygen evolution reaction (OER) catalysts, but their performance is limited by poor conductivity and low intrinsic catalytic activity. In this study, CoNi LDHs were used as a matrix, with iron sites introduced onto the surface via cation replacement (Fe-CoNi LDHs). Unlike ternary Fe-CoNi LDHs synthesized through conventional one-step methods, the iron sites in Fe-CoNi LDHs are primarily located on the surface and edges of nanosheets, ensuring abundant exposure of reactive sites. Surface doping was found to optimize the coordination environment and electronic structure, reducing the binding energy between reactants and active sites. As a result, Fe-CoNi LDHs exhibit an overpotential of only 260 mV at 10 mA cm**, demonstrating superior OER performance. This study elucidates the electronic structure and mechanism of enhanced activity, highlighting the potential of surface doping to advance electrocatalytic applications.

MM 4.9 Mon 12:45 SCH/A216

NiCo2O4/Fe3O4 Nanocomposite with a Sea Urchin-like Morphology as a High-Performance Dual-Functional Material for Advanced Lithium-Ion Batteries and Supercapacitors — •Amina Zafar, Amjad Nisar, and Mashkoor Ahmad — Pakistan Institute of Nuclear Science and Technology (PINSTECH), Islamabad, Pakistan

The development of advanced electrode materials with multifunctional electrochemical properties is critical for next-generation energy storage systems. In this study, mesoporous sea urchin-like nickel cobaltite/magnetite (NiCo2O4/Fe3O4) composite was synthesized and systematically investigated for lithium-ion batteries and supercapacitors. The resulting composite offers high specific surface area, improved conductivity, abundant active sites and favorable structural characteristics. DFT calculations reveal that the composite exhibits enhanced redox kinetics and improved charge transfer compared to pristine NiCo2O4, leading to superior electrochemical performance. As an anode for lithium-ion batteries, the NiCo2O4/Fe3O4 electrode delivers a high reversible capacity of around 730 mAh/g at 0.3 A/g with excellent cycling stability, retaining 87.1 % of its capacity after 1000 cycles. For supercapacitor, the electrode exhibits an enhanced specific capacitance of 1330 F/g at 1 A/g, outperforming both NiCo2O4 and Fe3O4. The assembled (NiCo2O4/Fe3O4//activated carbon) device achieved a specific capacitance of 221 F/g and an energy density of 69.6 Wh/kg, along with excellent cycling stability, retaining around 94 % capacitance after 8000 cycles.