O 48: Poster Session IV: Surface dynamics II: Phase transitions and elementary processes

Time: Tuesday 13:30–15:30 Location: P

O 48.1 Tue 13:30 P

Ultrafast microscopy of charge density wave phase transitions using pump-probe imaging ellipsometry — •Sebastian Rohrmoser, Tobias Heinrich, Julius B. Peters, Murat Sivis, and Claus Ropers — IV. Physical Institute, Georg-August-University Göttingen, Germany

Null Ellipsometry has a long history of being a powerful, surface sensitive tool for measuring small changes in the refractive index of a sample with a high lateral resolution. These changes may stem from molecular adsorption [1], thin film growth [2] or phase transitions [3]. However, electronic phase transitions between charge density wave (CDW) phases occur on a much shorter timescale and are therefore inaccessible by conventional ellipsometry. Here, we present an all-optical, ultrafast approach to analyzing the phase transition between the nearly commensurate and incommensurate CDW phase in the transition-metal dichalcogenide (TMDC) 1T-TaS2. By combining a null ellipsometer with a pump probe setup, we are able to study the optically driven phase transition with a femtosecond temporal and micrometer lateral resolution. Using heat transfer simulations, we can disentangle the phase transition from the temperature contributions to give better insight in the surface-near dynamics. These results open the pathway for analyzing phase transitions on microstructured surfaces to investigate possible applications of TMDC's as optoelectronic components.

[1] H. Elwing, Elsevier 19, Issues 4-5, 397-406 (1998)
[2] J. Lee et al., Rev. of Scientific Instr. 69, 1800-1810 (1998)
[3] S. Faiss et at., J. Phys. Chem. B, 111, 50, 13979-13986 (2007)

O 48.2 Tue 13:30 P

Local impedance of Li-ion dynamics through complex interfaces in solid-state electrolytes — •Sina Stegmaier[1], Roland Schierholz[2], Ivan Povstugar[3], Juri Barthel[4], Christoph Scheurer[5], and Karsten Reuter[5] — [1]Theoretische Chemie, TU München — [2]IEK-9, Forschungszentrum Jülich — [3]ZEA-3, Forschungszentrum Jülich — [4]ERC, Forschungszentrum Jülich — [5]Theory Department, Fritz-Haber-Institut der Max-Planck-Gesellschaft

All-solid-state batteries (ASSB) present a next-generation technology, promising increased operation safety and lifetime as compared to state-of-the-art Li-ion cells. The practical performance of solid-state electrolytes (SSE) in ASSBs, though, is severely limited by poorly understood interfacial processes. Atomistic insight into the structure and transport processes at working SSE grain boundaries [1] is required to enable insight-driven progress.

Molecular Dynamics simulations employing a first-principles derived force field allow for a precise localization of Li ion impedance in the grain boundaries of the LATP SSE material. An explicit, experimentally guided atomistic model of such buried interfaces is established to capture nanoscale complexions and investigate their role in the observed Li ion impedance. Following this novel approach, we leverage experimental insights from transmission electron microscopy and atom probe tomography for computational modeling of detailed ion dynamics across realistic functional solid-solid interfaces.

[1] A. Mertens *et al.*, Solid State Ionics **309**, 180 (2017).

O 48.3 Tue 13:30 P

Solid state dewetting of thin bismuth films: a quantitative analysis of crystal truncation rods — •Constantin Wansorra and Wolfgang Donner — TU Darmstadt, Materials Science, Structure Research, Darmstadt, Germany

The dewetting of a thin film in the solid state represents a prominent destruction mechanism of thin films at elevated temperatures and is therefore researched with increasing importance. The activation of surface diffusion by temperature results in the transition of a flat thin film into separated islands, caused by a reduction of surface and interface energies [1].

While the major part of research about this topic is covered by microscopy methods, we apply x-ray diffraction and analyze crystal truncation rods quantitatively. With additional support from electron backscatter diffraction (EBSD) experiments, we determine unit cell coverage, lattice spacings and gradients thereof to reveal the impeding influence of a strain gradient present in thin bismuth films on solid state dewetting [2]. Furthermore, models of the step edge diffusion of bismuth were developed and the possible influence of a strain gradient on this model is discussed.

[1] Thompson, *Rev. Mater. Res.* 42 (2012): 399-434.
[2] Wansorra, et al., *Acta Mater.* 200 (2020): 455-462.

O 48.4 Tue 13:30 P

Computational insights into the buried interface of silica-coated Pt electrocatalysts — •Alexander Urban — Department of Chemical Engineering, Columbia University, New York, NY 10027, USA

Semipermeable membranes are attractive as protective coatings for metal electrocatalysts in harsh environments, but their impact on the catalytic properties has not been fully understood. Experimentally probing buried membrane-catalyst interfaces *in situ* is challenging because standard surface-science techniques cannot be directly used.

Here, we discuss insights from first-principles modeling of silica-coated platinum electrocatalysts. We introduce the concept of *interface Pourbaix diagrams* to investigate the interaction of silica membranes with the surface of platinum metal electrocatalysts under different electrochemical conditions. The structure, composition, and adhesion energy of the buried SiO_2/Pt interface depend on the pH value of the aqueous electrolyte and the electrode potential. Membrane-coating also affects the electronic structure of the catalyst surface, which has direct implications for the catalytic reactivity

Our analysis indicates that semipermeable membrane coatings are not passive bystanders but affect the properties of electrocatalysts, thereby offering as yet unexplored tuning knobs for the design of corrosion-stable electrocatalysts.

O 48.5 Tue 13:30 P

Interfacial phase transition in multiphase systems of environmental relevance — •Thorsten Bartels-Rausch, Xiangrui Kong, Fabrizio Orlando, Luca Artiglia, Astrid Waldner, Thomas Huthwelker, and Markus Ammann — Paul Scherrer Institut, Villigen PSI, Switzerland

Laboratory experiments are presented on the phase change at the surface of sodium chloride - water mixtures at temperatures between 259 K and 240 K. A high selectivity to the upper few nanometres of the frozen solution - air interface is achieved by using electron yield near-edge X-ray absorption fine structure (NEXAFS) spectroscopy. We find that sodium chloride at the interface of frozen solutions, which mimic sea-salt deposits in snow, remain as supercooled liquid down to 240 K. Below this temperature, hydrohalite exclusively precipitates, anhydrous sodium chloride is not detected. In this work, we present the first NEXAFS spectrum of hydrohalite.

Experiments were performed at the PHOENIX beam line of the Swiss Light Source (SLS) at the Paul Scherrer Institute using the Near Ambient Pressure Photoemission (NAPP) set-up. In this work, we focus on the sample environment an in particular the ability to accurately monitor and set temperature and partial pressure of water. The importance of precise knowledge the trajectories, or history of, relative humidity and temperature that the sample have been exposed to are discussed.