MM 35: Topical Session: Hydrogen in Materials: from Storage to Embrittlement VI

Time: Wednesday 11:45–13:00 Location: C 130

Topical Talk MM 35.1 Wed 11:45 C 130

Palladium nanoparticles as hydrogenation catalysts — •Petra de Jongh, Jessi van der Hoeven, and Oscar Brandt Corstius — Debye Institute for Nanomaterials Science, Utrecht University, Utrecht The Netherlands

Regarding metal hydrogen interaction, palladium is one of the most investigated systems. An interesting application of this interaction is the use of palladium as hydrogenation catalyst. Due to its electronic properties and hence strong interaction with the dihydrogen molecule, palladium is one of the fastest hydrogenation catalysts (about six orders of magnitude faster than for instance copper), but a challenge is to control the surface properties of palladium to such an extent that it is also selective.

In this contribution I will introduce supported Pd nanoparticles as hydrogenation catalysts, and share some recent results of our group on the effect of Pd nanoparticles size, and the influence of alloying these nanoparticles with a second metal such as copper or gold.

MM 35.2 Wed 12:15 C 130

In-situ TEM reduction of a solid oxide cell with NiO/YSZ and NiO/BZCY materials for fuel electrode — •Svetlana Korneychuk[1,2], Cedric Grosselindemann[1], Norbert H Menzler[3], André Weber[1], and Astrid Pundt[1] — [1]Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]KNMFi, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]Forschungszentrum Jülich GmbH, Jülich, Germany

Solid oxide fuel cells play a key role in the transition to the green economy. The quality of the electrode plays a major role in the performance and durability of a fuel cell. Ni/YSZ or Ni/BZCY fuel cell electrodes of solid oxide cells are commonly reduced from NiO/YSZ or NiO/BZCY under hydrogen atmosphere at high temperatures, prior to operation. The reduction results in a significant change in microstructure. As specific microstructural properties are crucial to achieve high performance and durability of the cell, a comprehensive understanding of the reduction process is required. Using in-situ TEM atmosphere system from Protochips we studied the electrode reduction at the H2 pressures up to 1 atmosphere and temperatures up to 850 °C [1] which fit the real working condition of a solid oxide cell. Grain boundaries and triple junctions between NiO and YSZ or BZCY are determined as the starting points of the reduction process at lower temperatures. The initial temperature of the reduction is crucial to achieve a high number of electrochemically active triple phase boundaries between Ni/YSZ and gas. [1] Korneychuk, S. et al., Rochester, NY October 17, 2023. https://doi.org/10.2139/ssrn.4604921

MM 35.3 Wed 12:30 C 130

Computational optimization of nanoalloy hydrogen sensors via composition and geometry — •Pernilla Ekborg-Tanner[1], Magnus Rahm[1], Victor Rosendal[1], Tuomas Rossi[2,1], Tomasz Antosiewicz[3,1], and Paul Erhart[1] — [1]Department of Physics, Chalmers University of Technology, Gothenburg, Sweden — [2]Department of Applied Physics, Aalto University, Aalto, Finland — [3]Faculty of Physics, University of Warsaw, Warsaw, Poland

Plasmonic hydrogen sensing based on nanoalloys could be a solution to the safety issues related to operating hydrogen gas under ambient conditions, which are currently hindering the hydrogen economy. In particular, random arrays of Pd-Au nanodisks have shown great potential as hysteresis-free, reliable hydrogen sensors. While several experimental studies have been conducted, computational studies necessary to efficiently span the rich parameter space in terms of nanodisk geometry and alloy composition are rare. Here, we therefore present a multi-scale modeling approach to hydrogen sensing from atomic scale ab-initio calculations (DFT, TD-DFT) to continuum scale electrodynamic simulations (FDTD) with the purpose of optimizing the sensitivity. In this work, the sensitivity is defined as the shift in peak position with respect to the absorbed hydrogen concentration. The sensitivity is highly tunable via the disk diameter. In addition, it displays a distinct two-regime behavior governed by peak splitting, in contrast to experimental studies. The peak splitting is, in turn, caused by an avoided crossing between the plasmon peak and an interband transition which comes into play at high H content.

MM 35.4 Wed 12:45 C 130

Probing hydrogen with high spatial resolution: a new correlative deformation/hydrogen sensing technique for hydrogen embrittlement study — •Maria Vrellou[1], Xufei Fang[1], Hans-Christian Schneider[1], Alexander Welle[2], Astrid Pundt[1], and Christoph Kirchlechner[1] — [1]Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institute of Functional Interfaces, Karlsruhe Institute of Technology, Karlsruhe, Germany

Hydrogen is one of the most promising alternatives to fossil fuels. The green hydrogen produced using energy from processes with low gas emissions or from renewable sources is considered as a potential game changer. However, hydrogen embrittlement (HE) is a major concern in hydrogen storage and transportation, and the underlying mechanisms need to be better addressed. Here, we present a novel approach aiming to isolate, observe and quantify the debated mechanisms responsible for HE. Our project, TRITIum based microMEchanics (TRITIME), aims to use techniques capable of achieving hydrogen imaging at quasi-atomistic resolution. APT and ToF-SIMS will be used to study the local and global tritium content in different microstructures in Ti and Zr samples that are susceptible to hydride formation, which is expected to provide better localization of the "hydrogen reservoir" facilitating hydrogen detection and quantification when employing the high-spatial-resolution techniques. To decipher the contribution of each one of the HE mechanisms, mechanical testing such as micro-pillar compression will be applied and studied.