

MM 42: Functional materials III: Actuators, sensors and functional devices

Time: Wednesday 15:45–17:30

Location: H53

MM 42.1 Wed 15:45 H53

Potential impurity dopants in molybdenum oxide — ●JULIANA SCHELL^{1,2}, CARLOS DÍAZ-GUERRA³, KATHARINA LORENZ⁴, and JOÃO GUILHERME MARTINS CORREIA^{1,5} — ¹Isotope Mass Separator On-Line ISOLDE, CERN, Switzerland — ²Universität des Saarlandes, Saarbrücken, Germany — ³Dpto. Física de Materiales, Facultad de Ciencias Físicas, Universidad Complutense de Madrid, Spain — ⁴Instituto Superior Técnico, Universidade de Lisboa, Portugal — ⁵Centro de Ciências e Tecnologias Nucleares, Universidade de Lisboa, Portugal

Important technological applications, especially as a promising material for future electrochromic imaging devices have motivated the present work where we investigate at the atomic scale the introduction of potential dopants (Cd, Lu) in molybdenum oxide by ion implantation. Cd in MoO₃ is intended to be an electrical dopant and may improve the transport properties of these materials while rare earth doping is investigated for their light emission characteristics. At ISOLDE-CERN Perturbed Angular Correlation Spectroscopy (PAC), has been used to study recovery of defects and the local situation of implanted 111mCd and 172Lu on single crystals as a function of annealing and measuring temperatures. The electric field gradients (EFG) show evidence for Cd or Lu occupying two regular sites on MoO₃. In the case of the Lu/Yb, most of the probe atoms interact with lattice or electronic defects. This might be related to irregular lattices sites, damaged environment or dynamic electronic effects resulting from the electronic recombination after decay of 172Lu.

MM 42.2 Wed 16:00 H53

Energiespeicherung in Textilien mit faserbasierten Batterien — ●MARINA NORMANN¹, ANNE SCHWARZ-PFEIFFER¹ und ANDREA EHRMANN² — ¹Niederrhein University of Applied Sciences, Faculty of Textile and Clothing Technology, Mönchengladbach (Germany) — ²Bielefeld University of Applied Sciences, Faculty of Engineering Sciences and Mathematics, Bielefeld (Germany)

Im Bereich der "Smart Textiles", der intelligenten Textilien, werden herkömmliche textile Materialien mit neuen Funktionalitäten versehen. Die Integration elektronischer Bauteile in Textilien erlaubt es beispielsweise, neue Design-Effekte und Funktionen zu erzeugen oder Vitalfunktionen mit tragbaren Diagnosesystemen rund um die Uhr zu detektieren. Auch die Weiterentwicklung von Fasern zu Sensoren und Aktuatoren wird durch neue Materialien, wie leitfähige Polymere, möglich. Solche elektronischen Zusatzfunktionen erfordern jedoch eine adäquate Energieversorgung.

Hierzu wird in einem aktuellen Projekt eine textile Batterie entwickelt, in der verschiedene metallische und metallbeschichtete textile Strukturen als Elektroden dienen, die durch eine elektrolytgetränkte Vliesstruktur separiert werden. Auf diese Weise kann eine rein textile Lösung zur Energiespeicherung erzeugt werden, um vollständig faserbasierte "Smart Textiles" zu entwickeln. Die Kombination traditioneller textiler Prozesse mit leicht hochskalierbaren Technologien erlaubt es zudem, die Produktionskosten niedrig zu halten.

Der Vortrag zeigt aktuelle Forschungsergebnisse und gibt einen Ausblick auf die geplanten weiteren Forschungsansätze in dem Projekt.

MM 42.3 Wed 16:15 H53

High-pressure polymorphism as a step towards high density structures of LiAlH₄ — XIAOLI HUANG, DEFANG DUAN, FANGFEI LI, LU WANG, GANG WU, BINGBIN LIU, and ●TIAN CUI — State Key Laboratory of Superhard Materials, College of Physics, Jilin University, Changchun 130012, P. R. China

Ternary aluminum hydrides could be an extremely efficient energy storage system owing to their high gravimetric and volumetric hydrogen densities. Of these, LiAlH₄ is a prominent hydrogen-storage material with 10.6 wt% theoretical hydrogen content and thus has recently received much attention. The search for polymorphism with high volumetric hydrogen densities is a key resource for hydrogen storage materials. The great interest in high pressure phase transformations of LiAlH₄ has been aroused by a theoretical prediction of a new high pressure phase. However, the crystal structures as the key to understand the intriguing high pressure behavior of LiAlH₄ remained elusive for several decades. In order to clearly explore the behavior of LiAlH₄ under high pressure, we have investigated the high pressure structures of

LiAlH₄ by a joint theoretical and experimental study. And we have uncovered two crystal structures (β -LiAlH₄ and γ -LiAlH₄) as metastable low-energy polymorphs, which are not reported in previous literatures. The first phase transition is accompanied by the local structure change from a distorted AlH₄ tetrahedron into a distorted AlH₆ octahedron, which contributes to a large volume collapse with 20%. This new structure may show completely different hydrogen storage properties if stabilized by chemical substitution at ambient pressure.

15 min. coffee break

MM 42.4 Wed 16:45 H53

Hydrogen-assisted actuation with nanoporous palladium — ●SHAN SHI^{1,2}, JÜRGEN MARKMANN^{1,2}, and JÖRG WEISSMÜLLER^{1,2} — ¹Institut für Werkstofforschung, Werkstoffmechanik, Helmholtz-Zentrum Geesthacht, Geesthacht — ²Institut für Werkstoffphysik und -technologie, Technische Universität Hamburg-Harburg, Hamburg

Nanoporous (np) metals made by electrochemical dealloying exhibit a three dimensional metal network with high specific surface area, which couples the entire material behaviour to surface effects and specifically to electrocapillary effects that induce stress in the network. While dealloying has been demonstrated for many transition metals, studies requiring homogeneous and monolithic np samples have remained restricted to nanoporous gold and gold-based alloys. Based on a systematic optimization of master alloy composition, electrolyte, as well as temperature and potential of corrosion we here demonstrate the preparation of mm-size homogeneous monolithic np palladium (Pd) samples. Thermal coarsening allows to adjust the characteristic ligament size between 30 and 300 nm. Pd readily dissolves hydrogen, which results in volume expansion. We explore the influence of electrocapillary coupling at the surface and of hydrogen alloying in the bulk on the effective macroscopic mechanical strain of np-Pd during electrochemical potential cycles. A remarkably large reversible strain amplitude (about 3.4%), fast response time, and good stability of our np-Pd actuator emphasizes the prospects of np-Pd as a novel functional material.

MM 42.5 Wed 17:00 H53

Surface stress charge response of nickel in alkaline solutions — ●CHUAN CHENG and JÖRG WEISSMÜLLER — Institut für Werkstoffphysik und Werkstofftechnologie, Technische Universität Hamburg-Harburg, 21073 Hamburg, Germany

Charge induced reversible strain was recently found in nanoporous structured nickel upon cyclic potential triggering in alkaline solutions [1,2]. Different from metallic actuators with clean metal surfaces, the surface of Ni is covered with several nanometers thick Ni(II) passive layer, which can cause reversible volume change during Ni(II)/Ni(III) redox reactions. The situation becomes even more complex as different types of Ni(II) can be formed on Ni surface, which exhibit opposite signed volume change when they are oxidized into Ni(III). In this work, surface stress charge response of Ni in alkaline solutions will be characterized by an in situ electrochemical cell. Ni thin film is sputtered on one side of a Si cantilever. Charge induced surface stress in Ni, which causes bending of the cantilever, was measured by a laser-based setup. The surface stress charge coefficients at both capacitive double layer region and the redox region are obtained. This work will provide a fundamental understanding of Ni based electrochemical actuators.

References:

1. M. Hakamada, S. Matsumura, and M. Mabuchi, Mater. Lett. 70, 132 (2012).
2. C. Cheng and A. H. W. Ngan, ACS Nano 9, 3984 (2015).

MM 42.6 Wed 17:15 H53

Tunneling current calculations across diamondoid-functionalized electrodes: impact on biosensing — GANESH SIVARAMAN¹, RODRIGO G. AMORIM², RALPH H. SCHEICHER³, and ●MARIA FYTA¹ — ¹Institute for Computational Physics, University of Stuttgart, Germany — ²Departamento de Física, Universidade Federal Fluminense, RJ, Brazil — ³Department of Physics and Astronomy, Materials Theory, Uppsala University, Sweden

Attaching specific molecules to a pair of opposing metal electrodes is known to enhance tunneling current signals measured across them.

This functionalization of electrodes can make them more selective in sensing and detecting DNA molecules translocating between the electrode gap. Diamondoids are tiny hydrogen-terminated diamond-like cages which can be produced in a variety of sizes and can be selectively chemically modified, showing a high potential as functionalization units. Here, we focus on the quantum-transport properties of diamondoid-functionalized Au(111) break-junctions. For the functionalization, different diamondoids are considered and the tunneling cur-

rent signals arising from different DNA units (the nucleobases) in the break-junction are investigated. We report on the read-out characteristics and the sensitivity of the functionalized electrodes to identify the four DNA nucleobases and their mutations. Such electrodes can be embedded in nanopores which are able to electrophoretically thread DNA. Our results indicate that a device based on diamondoid-functionalized electrodes could have a high potential in sequencing DNA with a strong impact in nanopore research and biosensing methodologies.