

MM 14: Topical session: Interface-Controlled Microstructures: Mechanical Properties and Mechano-Chemical Coupling - Electro- and mechano-chemical coupling

Time: Monday 15:45–17:15

Location: BAR 205

MM 14.1 Mon 15:45 BAR 205

Electrocapillary coupling at metal surfaces from first principles — ●ANJA MICHL¹, JÖRG WEISSMÜLLER^{2,3}, and STEFAN MÜLLER¹ — ¹Hamburg University of Technology, Institute of Advanced Ceramics — ²Hamburg University of Technology, Institute of Materials Physics and Technology — ³Helmholtz-Zentrum Geesthacht, Institute of Materials Research, Materials Mechanics

The surface stress f of metallic surfaces reacts sensitively to excess charge q . This response can be characterized by the electrocapillary coupling parameter $\varsigma = df/dq$. Due to their high surface-to-volume ratio, nanoporous metals respond with a macroscopic deformation to electric charging in electrolyte, which makes these materials interesting alternatives to conventional actuators. Exploiting a Maxwell relation, we have determined ς in terms of the response of the work function to in-plane strain for several metal surfaces, focusing mainly on the response of sp-bonded metals. It is found that aluminum surfaces exhibit positive coupling coefficients, whereas the other sp-bonded metals show the usual negative sign known from previous experimental and theoretical studies of clean transition metal surfaces. In addition, we investigate the impact of excess charge on surface structure and bonding via ab-initio simulation of metal surfaces in an external electric field in order to gain further insight into the underlying mechanisms. Both the direct effect on the surface stress via charging of the bonds and the indirect effect resulting from the charge-induced relaxation will be analyzed and discussed in relation to the trends of the determined coupling coefficients.

MM 14.2 Mon 16:00 BAR 205

Curvature induced stress and phase-boundary diffusion — ●RAPHAEL SCHIEDUNG, REZA KAMACHALI, INGO STAINBACH, and FATHOLLAH VARNIK — Ruhr Universität Bochum, Interdisciplinary Centre For Advanced Materials Simulations, Bochum, Deutschland

The multi-phase-field approach is generalized to treat diffusion, driven by mean curvature, parallel to surfaces between a condensed phase and its vapor as well as diffusion parallel to boundaries between condensed phases, 'phase-boundary diffusion'. Additionally, we present a treatment of surface-tension/energy for elastic bodies within the multi phase-field framework. The model is validated against the Young-Laplace law for the pressure gradient across the interface of spherical bodies and the prediction of Neumann's triangle relation for the force equilibrium at triple junctions. It is applied to thermal grooving and to the solid state sintering process of two spheres.

MM 14.3 Mon 16:15 BAR 205

Grain boundary diffusion of ions and electrons through a film or scale — ●MARKUS TAUTSCHNIG, NICHOLAS HARRISON, and MICHAEL FINNIS — Imperial College London, London SW7 2AZ, UK

A model for ionic and electronic grain boundary transport through thin films, scales or membranes with columnar grain structure is introduced. The grain structure is idealized as a lattice of identical hexagonal cells - a honeycomb pattern. Reactions with the environment constitute the boundary conditions and drive the transport between the surfaces. Time-dependent simulations solving the Poisson equation self-consistently with the Nernst-Planck flux equations for the mobile species are performed. The model is used to interpret alumina membrane oxygen permeation experiments. The simulation results provide a complete description of the measurements and insight into the microscopic processes underpinning the oxygen permeation of the membrane. Most notably, the hypothesized transition between p-type and n-type ionic conductivity of the alumina grain boundaries as a function of the applied oxygen gas pressure is observed in the simulations. The range of validity of a simple analytic model for the oxygen permeation rate, similar to the Wagner theory of metal oxidation, is quantified by comparison to the numeric simulations. The coupling between the defect fluxes and the stress state at the grain boundaries is discussed. The three-dimensional model we develop here is readily adaptable to problems such as transport in a solid state electrode, or corrosion scale growth.

MM 14.4 Mon 16:30 BAR 205

Oxygen adsorption on strained transition metal surfaces: An ab initio study of mechano-chemical coupling — ●GREGOR FELDBAUER, ANJA MICHL, and STEFAN MÜLLER — Hamburg University of Technology, Institute of Advanced Ceramics, Germany

Mechanical deformation can affect the adsorption and reaction processes of reactants on surfaces. Thus, by straining catalytically active surfaces their reactivity as well as selectivity can be influenced, which is of high importance, for example, in the field of heterogeneous catalysis. Here, transition metal surfaces, like Pd(111) and Ir(111), interacting with atomic oxygen are used as model systems. At first, the adsorption characteristics, e.g. the energetics, are investigated within the framework of density functional theory (DFT). The most favourable adsorption configurations are identified via the cluster expansion approach using DFT input data. Secondly, for various favourable oxygen configurations at the transition metal surfaces biaxial strain is applied in the surface plane to obtain the response of the adsorption energetics. Particularly, the coupling parameter between strain and adsorption energies is of interest to allow for a comparison with experiments. The coupling parameter is affected by the oxygen coverage as well as the occurrence of oxygen incorporation.

MM 14.5 Mon 16:45 BAR 205

Electrical modulation of the Poisson's ratio of nanoporous metals — ●LUKAS LÜHRS¹, BIRTHE MÜLLER¹, and JÖRG WEISSMÜLLER^{1,2} — ¹Institute of Materials Physics and Technology, Hamburg University of Technology — ²Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht

Nanoporous metals exhibit significant surface induced property modifications that are rendered possible by their large surface area to volume ratio. Among these materials nanoporous gold (NPG) appears an ideal model material due its high chemical stability and tunable surface area. Owing to its decisive electro mechanical coupling, electrical modulation of the strength and flow stress, elastic modulus, creep behavior and crack propagation have been demonstrated. However, the reliance of the lateral deformation behavior of NPG towards electrical tuning remains unclear.

In this contribution we study the influence of electrical modulation on the transverse mechanical coupling of NPG by the investigation of a metal/electrolyte hybrid material. We present experiments of NPG under compression testing in 1 M HClO₄ while varying the applied electrical potential, E . Our results show considerable changes of the plastic Poisson's ratio, ν_P , with E . We link these findings to the surface tension, γ , a capillary force that promotes a tension/compression asymmetry in the material. As γ depends on E , we show that the plastic lateral expansion behavior is governed by surface effects. In this line of argument we interpret the earlier reported ligament size dependence of ν_P .

MM 14.6 Mon 17:00 BAR 205

Size effects on hydrogen electrosorption in nanoporous Pd-Cu alloys — ●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. Electrochemical hydrogen electrosorption into bulk and surface of np-palladium-copper (np-PdCu) alloys results in reversible macroscopic expansion/contraction which can be monitored by in-situ dilatometry. This has been demonstrated to be an actuation mechanism and will be used to study the thermodynamics of the Pd-Cu-H system. Here, we fabricated mm-sized homogeneous monolithic np-PdCu samples by electrochemical dealloying. By thermal annealing after the synthesis, the characteristic ligament size was adjusted between 10 nm and 300 nm. Then we explored the influence of ligament size on both actuation performances (response time and strain amplitude) and thermodynamics (hydrogen solubility and hysteresis).