MM 35: Interfaces

Segragation

Time: Wednesday 11:45–13:00 Location: H 0107

MM 35.1 Wed 11:45 H 0107

Strain-controlled electrocatalysis on gold thin film — •Xinyan Wu[1], Matthias Graf[2,3], and Jörg Weissmüller[1,3] — [1]Institute for Materials Physics and Technology, Hamburg University of Technology, Hamburg — [2]Institute for Electronic and Optical Materials, Hamburg University of Technology, Hamburg — [3]Insitute for Materials Technology, Helmholtz-Zentrum Geesthacht, Geesthacht

It is well known that the elastic deformation of a surface in its tangent plane modifies adsorption enthalpies. The observation is particularly relevant in heterogeneous catalysis, where strain - for instance in pseudomorphic active layers - is recognized as a means of tuning the reactivity and selectivity. Yet, quantifiable experimental observations of the impact of strain for catalysis are exceedingly rare. In other words, the field lacks a quantitative experimental database. Here, we use Dynamic Electro-Chemo-Mechanical Analysis (DECMA) in order to investigate the impact of strain on the electrocatalytic methanol oxidation on planar gold surfaces as a model reaction. Our approach works with a cyclic elastic strain applied to the surface and it detects modulations in the surface state and in the reaction current by means of a lock-in technique. In this way, DECMA affords quantifying the coupling between mechanics and reactivity as a function of the overpotential. In this way, the coupling strength can be explored separately for each reaction step.

MM 35.2 Wed 12:00 H 0107

Vacancy behaviour at FePt/MgO interface — •Petr Sestak[1,2], Miroslav Cerny[1,2], and Mojmir Sob[1,2,3] — [1]Institute of Physics of Mater., Academy of Sci. of CZ — [2]Central European Institute of Technology, Brno, CZ — [3]Faculty of Science, Masaryk University, Brno, CZ

Interfaces between two phases represent important parts of material structure. They have a significant effect on mechanical and magnetic properties. In particular, they can attract material defects like vacancies or dislocations. Moreover, vacancies located at interfaces can also serve as a place where impurities segregate. In our study we present ab initio simulations of formation of vacancies at the FePt/MgO interface. We analyze vacancy formation energy as a function of distance from the interface, the effect of vacancies on magnetic and mechanic properties and interaction between vacancies close to the interface.

MM 35.3 Wed 12:15 H 0107

Atom probe tomography of grain boundary segregation in the FeCr system — •Helena Solodenko, Patrick Stender, Sebastian Eich, and Guido Schmitz — Institute for Materials Physics, University of Stuttgart, Heisenbergstraße 3, 70569 Stuttgart, Germany

Nanocrystalline materials have unique properties. This is due to the small grain size and high amount of interfaces, like grain boundaries (GB) or even triple junctions (TJ). Unfortunately, nanocrystalline materials are not thermally stable. The high amount of interfaces usually leads to a high interfacial excess energy, which is reduced by grain growth. A chance to overcome this problem is segregation of solutes to GBs, which can lower the interfacial energy and thus the driving force for grain growth. Density functional theory and experimental data suggest that the iron-chromium (Fe-Cr) system is expected to show exceptional thermodynamic behavior, which was also recently predicted by atomistic simulations based on a thermodynamically accurate embedded-atom potential. The key prediction is a distinctive negative GB energy for very specific compositions close to the phase boundary on the chromium-rich side, thus inhibiting grain growth. In this work, the segregation behaviour of Fe-Cr is investigated by atom probe tomography (APT). Nanocrystalline APT samples of a Cr(Fe) alloy with predefined compositions are produced by ion beam sputtering and focused ion beam. Reconstructed samples show strong segregation of the minority component Fe to Cr grain boundaries. The segregation isotherm is investigated at different compositions and compared with available atomistic studies.

MM 35.4 Wed 12:30 H 0107

Understanding chemical trends of solute-GB segregation by high-throughput analytics — •Liam Huber, Blazej Grabowski, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH

Microstructure evolution is critically influenced by solute interaction with grain boundaries (GBs). Depending on the mobility and driving force of solutes to segregate at GBs, even small additions of alloying elements may have a dramatic effect on microstructure evolution. We present high-throughput calculations of solute segregation to aluminium grain boundaries using a variety of available classical potentials. Using a cluster geometry unrestricted by periodic boundary conditions, we sample both high-symmetry boundaries commonly found in literature, as well as low-symmetry boundaries which are ubiquitous in real materials. We extract simplified descriptors based on the local structure and build models for predicting segregation energies on a per-site basis. To test the predictive capability of these models we apply data science techniques. We show that despite their relative simplicity these models deepen our physical understanding and provide novel insights into the nano-scale effects which influence solute-GB interaction. Based on this insight we discuss how to calculate model parameters a priori, leading to fit-free segregation predictions.

MM 35.5 Wed 12:45 H 0107

Mesoscopic simulations of grain boundary motion: influences on the Zener drag — •Volker Mohles — Interdisciplinary Centre for Advanced Materials Simulation ICAMS, Ruhr-Universität Bochum, Bochum, Germany

A new three-dimensional vertex model of grain boundary motion has been developed in which, for now, a single grain boundary is pushed through an array of particles in order to derive the Zener drag, i.e. the effective pinning force of these particles on grain boundaries. The spherical particles have a realistic size distribution and spatial arrangement. Like the grain boundary itself, the particle interfaces are described by a network of triangular facets, with the distinction that the nodes connecting the particle facets can only move tangentially along the surface of the prescribed particle shape. The model also accounts for the energy of the triple lines connecting the particles with the grain boundary. The simulations allow to derive the Zener drag as a function of the grain boundary energy, for now assumed to be independent of the grain boundary inclination, the triple line energy (constant), the mean particle size, and their volume fraction. The effects of varying size distribution and spatial arrangement are also tested. The results are compared to established formulations for the Zener drag.