MM 23: Topical Session: Interface-dominated phenomena - Interactions at Interfaces

Time: Tuesday 11:45–13:00 Location: IFW A

MM 23.1 Tue 11:45 IFW A

Elastic Strain Effect in Electrocatalysis during Methanol Oxidation Reaction on Gold/Platinum Thin Films — •Xinyan Wu[1] and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany — [2]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany

It is well known that one effective method of enhancing the electrocatalytic performance is to tune the surface strain of nanomaterials, by which the adsorption enthalpies could be modified. However, quantifiable experimental observations of the impact of strain for reactivity of catalyst are still rare, which means this field lacks a quantitative experimental database. Here we explore a method, Dynamic Electro-Chemo-Mechanical analysis (DECMA), in order to investigate the impact of elastic strain on the electrocatalystic methanol oxidation reaction on gold and platinum thin film surface in alkaline solutions. In this way, coupling parameters such as potential-strain & and current-strain Λ coefficients are measured and suggest that tensile strain decreases the adsorption energy thus bring a strong binding between OHads and electrode. However, this stronger binding plays different roles on Au and Pt electrodes, which revealed different strain modulation mechanism in these two systems during methanol oxidation reaction(MOR). Pt electrode responses more strongly and oppositely as Au electrode towards external tensile strain, namely a compressive stain effect is more favourable on Pt electrode.

MM 23.2 Tue 12:00 IFW A

Structure and local electrical resistivity in copper grain boundaries — •Hanna Bishara, Matteo Ghidelli, and Gerhard Dehm — Max-Planck-Institut für Eisenforschung

Grain boundaries (GBs) are among the most significant microstructure defects influencing mechanical and functional properties of materials. The atomic structure at a GB is determined by the crystallography, composition and temperature as well as by the relative orientation between neighbouring grains. Still, the impact of structural characteristics of the GB on the various physical properties of the materials is not fully understood. Here, we aim to correlate the structural and electrical properties of GBs through in-situ local electrical measurements on well-defined GB planes.

To this aim Cu thin films are sputter-deposited and annealed to induce grain growth with final grain sizes of a few tens of micrometers. EBSD is used to identify the GB plane. Subsequently, FIB machining is employed to isolate specific GBs and their corresponding grains from the rest of film, to probe the electrical resistivity. The electrical resistivity measurements are conducted in-situ through 4-point-probe measurements using micro-manipulators and a nV sensitive voltagemeter. We report, for the first time, on direct resistivity measurements of different coincidence site lattice (CSL) and low angle GBs in Cu. Measured resistivities span for more than order of magnitude and match the predicted values by simulations. Deviation from predicted values are related to Ga segregation into GBs. The results provide a solid relation between structure and electrical properties of GBs.

MM 23.3 Tue 12:15 IFW A

Directionality of metal-induced crystallization and layer exchange in amorphous carbon/nickel thin film stacks — •Matthias Krause[1], Daniel Janke[1], Frans Munnik[1], Jaakko Julin[1], René Hübner[1], Jörg Grenzer[1], Christina Wüstefeld[2], David Rafaja[2], and Sibylle Gemming[1,3] — [1]Helmholtz-Zentrum Dresden- Rossendorf, 01328 Dresden, Germany — [2]Institute of Materials Science, TU Bergakademie Freiberg, Gustav-Zeuner-Straße 5, 09599 Freiberg, Germany — [3]Institute of Physics, TU Chemnitz, Reichenhainer Straße 70, 09126 Chemnitz, Germany

Metal-induced crystallization and layer exchange (LE) of amorphous carbon in thin film stacks with Ni were investigated as a function of the initial stacking order. Bilayer and triple layer stacks were exposed to heating ramps up to 700°C.

Turbostratic carbon formed during annealing. The degree of LE, quantified by ion beam analysis, is 95 % and 80 % for the outward and inward direction, respectively. Based on the calculation of surface and interface energies of the initial and final states, thermodynamic estimations pointed to the wetting of Ni grain boundaries by C atoms as the initial driving force for the LE and allowed a consistent understanding of the LE directionality and of the final thin film microstructure.

MM 23.4 Tue 12:30 IFW A

Atomistic simulation of nucleation during solidification in binary alloys — •Sarath Menon, Grisell Díaz Leines, Jutta Rogal, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität, Bochum

Advances in experimental methods such as fast scanning calorimetry have enabled the study of nucleation during solidification to obtain free energy barriers and reaction rates. Insight into the nucleation mechanism on an atomic scale, however, remains elusive due to the time and length scales of the process. In the case of binary alloy systems, the thermodynamic and kinetic quantities often depend on the concentration, phase separation and phase selection, leading to a complex nucleation mechanism. Here, we employ transition path sampling to calculate thermodynamic and kinetic quantities and to study nucleation mechanisms atomistically. An interesting class of materials are metal-semiconductor compounds. As a model system to approximate such a binary alloy, we use a two-component Stillinger-Weber potential that is able to capture the characteristic features of the phase diagram including the eutectic point. Our results provide information about the concentration dependence of nucleation kinetics and shed light on phase selection and separation during nucleation in binary alloys.

MM 23.5 Tue 12:45 IFW A

Interplay of grain boundaries, deformation and electromagnetic properties in iron silicon steel — •Martin Heller[1], James Gibson[1], Nora Leuning[2], Kay Hameyer[2], and Sandra Korte-Kerzel[1] — [1]Institute of Physical Metallurgy and Material Physics, RWTH Aachen — [2]Institute of Electrical Machines, RWTH Aachen

Iron-silicon electrical steel sheet is the most widely used material for iron cores of electrical machines like generators, motors or transformers. Although already ubiquitous, the demand will nevertheless rise in the future since electro-mobility is spreading rapidly. The magnetic properties of the electrical steel sheet directly influence the application performance. Hysteresis losses result from the movement of domain walls. Even though electrical sheet steel is generally used in a fully recrystallized state, it is the final stages of production involving cutting that introduce large plastic strains, and hence high local dislocation densities. These have been shown to cause significant loss in performance, due to pinning of domain walls by dislocations. This study aims to learn more about the evolving dislocation structures at specific grain boundaries during deformation. Thus, single-crystalline micropillars (2*m x 4*m) are milled in two adjacent grains and their corresponding bi-crystalline counterparts on the grain boundary. After compression mechanical data, slip traces and crystal rotation are further analysed to study the interaction of dislocations on individual slip systems and the grain boundary. In a next step, grain orientations, grain boundaries and evolved dislocation structures will be correlated with electromagnetic properties on the macroscale.