MM 25: Interface Controlled Properties, Nanomaterials and Microstructure Design IV

Time: Tuesday 11:45–13:00 Location: C 230

MM 25.1 Tue 11:45 C 230

Automatic exploration of elementary processes with adaptive kinetic Monte Carlo — •King Chun Lai, Sebastian Matera, Christoph Scheurer, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin

Lattice kinetic Monte Carlo (kMC) is very efficient for the simulation of rare event controlled dynamics but requires prior knowledge about the network of elementary processes. Currently, constructing such a network heavily relies on human intuition, which has its limitations in complex scenarios. We address this with a newly developed adaptive kMC (akMC) framework to automatically explore the reaction space. Elementary processes are identified solely on the basis of their energetics and without human bias. A key feature of our akMC framework is the on-the-fly labeling of local atomic environments, which is used to speed up the process searching algorithm. Demonstrating on island migration on Pd surfaces, we employ this labeling to structure the obtained elementary processes. Intriguingly, the process exploration readily identifies a number of non-trivial elementary steps, which involve collective motion of multiple atoms in a single event. Long time scale kMC simulations including these collective processes highlight the shortcomings of prevalent human-generated fixed process lists which typically center on intuitive single-atom events.

MM 25.2 Tue 12:00 C 230

Rapid Metal-Induced Crystallization and Layer Exchange via Flash Lamp Annealing — •Max Stöber[1], Matthias Zschornak[2], Hartmut Stöcker[1], Felix Bräuer[1], and Dirk C. Meyer[1] — [1]Institut für Experimentelle Physik, TU Bergakademie Freiberg, Leipziger Straße 23, 09596 Freiberg — [2]Technische Physik, Hochschule für Technik und Wirtschaft Dresden, Friedrich-List-Platz 1, 01069 Dresden

DC sputtered Si layers are crystallized in the presence of a thin aluminum layer on a copper foil substrate. The energy for the reaction was provided by the means of Flash Lamp Annealing (FLA) technique with a pulse duration of 1 ms. X-Ray diffraction and scanning electron microscopy revealed structural changes, namely metal-induced crystallization and layer exchange. Above a certain flash energy the formation of a metastable intermetallic alloy was observed. The final synthesis result is an intermetallic alloy layer in between two metal layers, which can be refered to as a self-assembled sandwich structure. The metastable phase is "frozen in" due to rapid quenching. Some properties of the intermetallic layer can be fine-tuned by the flash lamp parameters. Understanding the fundamental processes involved may lead to interesting applications in heterostructured functional material systems.

MM 25.3 Tue 12:15 C 230

Nano-scale investigation of fractal abnormal grains and grain boundaries in Pd-Au using atom probe tomography — •Johannes Wild[1], Torben Boll[1,2,3], Fabian Andorfer[4], Svetlana Korneychuk[2,3], Jules M. Dake[4], Dorothée Vinga Szabo[1,2,3], Stefan Wagner[1], Carl E. Krill III[4], and Astrid Pundt[1,2] — [1]Institute for Applied Materials (IAM-WK), Karlsruhe Institute of Technology — [2]Institute of Nanotechnology (INT), Karlsruhe Institute of Technology — [3]Karlsruhe Nano Micro Facility (KNMFi), Karlsruhe Institute of Technology — [4]Institute of Functional Nanosystems, Ulm University

Nanocrystalline (NC) Pd-Au prepared by inert gas condensation exhibits fractal abnormal grain growth during heat treatment. The resulting microstructure is characterized by a bimodal grain size distribution with micrometer-sized grains (FG) embedded in a matrix of NC grains (NG). To elucidate this unusual manifestation of grain growth, we extracted sharp tip samples from FG and NG bulk regions, as well as from the FG-FG and FG-NG interface regions and analysed them with a LEAP 4000X HR atom probe. The NG region exhibited an O content that was multiple times higher in comparison with the FG region. Cluster analysis confirmed the presence of a multitude of O-rich clusters in the NG, but not in the FG region. Furthermore, the reconstructions of the boundary regions revealed an unexpected diversity of host and contamination element distributions at the FG-FG and FG-NG interfaces.

MM 25.4 Tue 12:30 C 230

Positive and Negative Structured 3D Nano Current Collectors Based on AAO Templates Applied for Sodium Metal Anodes — •Mo Sha and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

The uncontrollable dendrite growth leads to safety issues during plating/stripping processes, severely restricting the practical application of sodium metal batteries (SMBs). 3D nano current collectors exhibit great potential for stabilizing the Na anode by homogenizing the electric field and Na ion flux distribution. Herein, 3D nanopore arrays (NPAs) and 3D nanorod arrays (NRAs) current collectors with opposite structures have been prepared with the AAO-template-assisted method. As current collectors for SMBs, both 3D NPAs and 3D NRAs have better electrochemical performance than 2D foil, demonstrating the great potential of 3D nanostructured current collectors based on AAO templates for SMBs. Compared with 3D NRAs, 3D NPAs have better electrochemical performance at a certain depth, with a long cycling stability of 1000 cycles at 1 mAh*cm-2 and 1 mA*cm-2 and a small nucleation potential of about 2 mV.

MM 25.5 Tue 12:45 C 230

effect of crack-tip geometry on crack-interface interactions in molecular dynamics studies of fracture in Ti-Al alloys — •Onur Can Şen[1,2] and Rebecca Janisch[2] — [1]IMPRS SusMet, Max-Planck-Institut für Eisenforschung GmbH — [2]ICAMS, Ruhr-Universität Bochum

The fracture behavior of lamellar Ti-Al alloys is strongly influenced by the twin interfaces in the microstructure. Molecular dynamics (MD) simulations are a valuable tool to systematically study crack-interface interactions with atomistic resolution, but their results are often criticized as being too academic. Experimental validation is difficult, because controlling the initial notch orientation is very challenging and the crack tip is never as sharp as in the typical MD set-ups. We investigate this issue by studying crack-tip interface interactions at various coherent and semi-coherent interface types in nano-lamellar Ti-Al, using different crack configurations to differentiate the effects of the microstructure from those of the crack geometry. Results show that the semi-coherent pseudo twin (PT) interface is the strongest barrier for crack propagation while the coherent true twin (TT) interface is the weakest. The initial crack orientation has a bigger influence on this effect than the aspect ratio of the microcrack. The stress shielding behavior of the interfaces is also found to be strongly dependent on the initial crack configuration, however, the coherent TT interface remains the most effective interface in terms of shielding in all cases.