MM 30: Interface Controlled Properties, Nanomaterials, and Microstructure Design II

Time: Thursday 10:15–11:45 Location: SCH/A215

MM 30.1 Thu 10:15 SCH/A215

Statistics of Shear-Coupled Grain Growth in Polycrystals — •Marco Salvalaglio[1], Caihao Qiu[2], Jian Han[2], and David J. Srolovitz[3] — [1]Institute of Scientific Computing, TU Dresden, 01062 Dresden, Germany — [2]Department of Materials Science and Engineering, City University of Hong Kong, Hong Kong SAR — [3]Department of Mechanical Engineering, The University of Hong Kong, Pokfulam, Hong Kong SAR

Grain growth in polycrystals, the coarsening of crystalline domains with different orientations, is traditionally viewed as a capillarity-driven process governed by interfacial energy minimization. However, grain-boundary migration can also induce, and in turn couple to, shear deformation, making microstructure evolution sensitive to externally applied stress. At the microscopic level, this behavior arises from the motion of disconnections, steps with dislocation character constrained at grain boundaries. Using a multi-phase-field (PF) framework that incorporates disconnection flow through coarse-graining, we demonstrate that accounting for shear coupling enables realistic grain-growth behavior in single-component polycrystals. Simulations reproduce recent experimental observations of weak correlations between grain boundary velocity and curvature. We then use PF simulations to analyze key aspects of microstructure evolution, including grain-size distributions, grain-shape evolution, and statistical characterization of the evolving network.

MM 30.2 Thu 10:30 SCH/A215

Revealing nanovoids in growth-resistant regions of nanocrystalline Pd–Au using atom probe tomography — •Johannes Wild[1], Fabian Andorfer[4], Svetlana Korneychuk[2,3], Jules M. Dake[4], Dorothée Vinga Szabó[1,2,3], Stefan Wagner[1], Carl E. Krill III[4], and Astrid Pundt[1,2] — [1]Institute for Applied Materials, Karlsruhe Institute of Technology — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology — [3]Karlsruhe Nano Micro Facility (KNMFi), Karlsruhe Institute of Technology — [4]Institute of Functional Nanosystems, University of Ulm

Nanocrystalline Pd–Au produced by inert gas condensation (IGC) shows extreme abnormal grain growth (AGG) upon heat treatment. In some cases, narrow regions of residual nanocrystalline material resist coarsening entirely, persisting between abnormally grown grains exceeding 100 μm. We investigate these growth-stagnant regions using site-specific SEM/FIB lift-outs, atom probe tomography (APT) and TEM. FIB cross-sections reveal that these nanocrystalline regions are significantly more porous than the surrounding matrix, and APT reconstructions from them exhibit a strongly elevated density of OH-containing clusters, which are largely absent elsewhere. By analysing local ion-density variations during field evaporation into voids, we show that these OH clusters correspond to nanovoids in the material. Correlating porosity with grain morphology, we find that the most porous regions exhibit the strongest resistance to grain growth, indicating that nanoscale porosity is a key factor in stabilizing the nanocrystalline grain structure in IGC Pd–Au (manuscript submitted).

MM 30.3 Thu 10:45 SCH/A215

Vacancy-mediated extreme abnormal grain growth in inert gas-condensed nanocrystalline Pd–Au: when what's missing runs the show! — Fabian Andorfer[1], Johannes Wild[2], Jürgen Markmann[3,4], Markus Ziehmer[1], Jules M. Dake[1], Torben Boll[2], Dorothée Vinga Szabó[2,5,6], Stefan Wagner[2], Astrid Pundt[2,5], and •Carl E. Krill III[1] — [1]Inst. of Functional Nanosystems, Ulm University — [2]Inst. for Applied Materials, KIT — [3]Inst. of Hydrogen Technology, Helmholtz-Zentrum Hereon — [4]Inst. of Materials Physics and Technology, TUHH — [5]Inst. of Nanotechnology, KIT — [6]Karlsruhe Nano Micro Facility (KNMFi), KIT.

Inert gas-condensed Pd–Au exhibits extreme abnormal grain growth (AGG), marked by a small number of grains growing dendritically through a matrix of nanocrystallites, eventually reaching sizes of 100 μm or more. The triggers for rapid growth of abnormal grains (emergence) and for maintaining this growth advantage (persistence) remain unclear. Annealing under hydrogen accelerates emergence without altering grain morphology, suggesting that the ~ 5 vol% porosity inherent to inert gas condensation not only pins matrix/matrix grain boundaries (GBs) but also governs where and when abnormal grains emerge. In nano-Pd–Au, pores can coarsen by vacancy diffusion along GBs, with larger pores growing at the expense of smaller ones. Small-angle x-ray scattering measurements support such an evolution in pore-size distribution. Vacancy transport, rather than variations in boundary mobility, appears to establish the spatiotemporal conditions for AGG in this system.

MM 30.4 Thu 11:00 SCH/A215

Small-angle x-ray scattering of nanoporous gold - a discussion of the structure factor and its implications for local order — •Celina Passig[1,2], Jürgen Markmann[2,1], and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Germany — [2]Department Hybrid Materials Systems, Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany

Nanoporous gold (NPG) made by dealloying is a popular model system for studies of size and interface effects as well as microstructure evolution in nanomaterials. Here, we investigate to what extent information on the microstructural geometry may be obtained by Small-Angle X-Ray Scattering (SAXS). It is well established that NPG exhibits a sharp interference peak, indicative of a characteristic wavelength underlying its leveled-wave-like microstructure and, hence, of an exceptional degree of order. Remarkably, our measurements even reveal a secondary peak at larger wave number. We compare the experimental data to simulations for small-angle scattering of NPG generated (1) by kinetic Monte Carlo (KMC) studies of dealloying or (2) as leveled-wave structures. On that basis, we discuss in how far the secondary interference peak is intrinsic to the microstructure of idealized, uniform NPG and what information it provides on the geometry of that microstructure. Since the feature vanishes during coarsening, we inspect how this process affects the order of the ligament network.

MM 30.5 Thu 11:15 SCH/A215

Enhanced Field Emission Current Density in Chemically Engineered Multiwall Carbon Nanotube - Neodymium Oxide Heterostructures — •Anima Mahajan[1], Menaka Jha[2], and Santanu Ghosh[1] — [1]Department of Physics, Indian Institute of Technology, Hauz Khas, New Delhi -110016, India. — [2]Institute of Nano Science & Technology, Knowledge City, Sector-81, Mohali, Punjab-160062, India.

The MWCNT, neodymium oxide (Nd*O*), and MWCNT-Nd*O* heterostructure were successfully fabricated through a facile three-step synthesis process: the synthesis of MWCNT rods by the chemical vapor deposition technique, the synthesis of the Nd*O* nanoparticles by using the micellar-assisted solid-state route, and the fabrication of the MWCNT-Nd*O* heterostructure. Moreover, the MWCNT-Nd*O* heterostructure exhibits enhanced field emission properties, with a lower turn-on field of 2.4 V/*m compared to pure MWCNT and Nd*O*, which have turn-on fields of 3.6 and 3.8 V/*m, respectively. The emission current stability at a preset value of 6 V/*m over an 8-hour duration is found to be fairly good, characterized by current fluctuations within * 3% of the average value. The enhanced field emission (FE) performance of the MWCNT-Nd*O* heterostructure is attributed to its high enhancement factor (β) of ~3.3*10*.

MM 30.6 Thu 11:30 SCH/A215

Exploring Superconductivity in Misfit Nanodevices — •Sushmita Chandra and Claudia Felser — Nöthnitzer Str. 40, 01187 Dresden

Recently, MISFIT layered compounds (MLCs) have attracted considerable attention in the field of 2D materials due to their unique structure, crystallographic diversity, and chemical tunability. Typically, MLCs can be represented by the general formula [(MX)(1+δ)]m[(TX2)n] with m, n = 1, 2, 3, where M = Sn, Sb, Pb, Bi, rare-earth elements; T = Ta, Nb, Mo, etc., and X = S, Se, Te. The lattice mismatch between the distorted rock salt MX layers and hexagonal TX2 counterparts creates a strained interface in the MLCs which allows a charge transfer from one layer to another, leading to a wealth of fascinating physical phenomena and modulations in the electronic structure. Although MLCs have been extensively studied for their potential applications in thermoelectrics, the fabrication of nanodevices with single- or multilayer MISFIT crystals is a challenging task and has not been explored at all. In this talk, I will present the fabrication of nanodevices based on high-quality MISFIT single crystals. I will also correlate how the misfit strain is associated with the superconducting transition and affects the electronic transport in these natural van der Waals heterostructures.