MM 26: Interface Controlled Properties and Nanomaterials: Grain Boundaries and Stability, Spectroscopy and Interatomic Potentials

Time: Wednesday 10:15–13:00 Location: SCH A 216

MM 26.1 Wed 10:15 SCH A 216

Grain-boundary segregation effects on bicrystal Cu pillar compression — •Tobias Brink, Mohammed Kamran Bhat, James Best, and Gerhard Dehm — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf

It is well known that segregation to grain boundaries (GBs) can modify the mechanical properties of metals, leading for example to improved strength, but also to detrimental effects like embrittlement. Despite this, the nanoscale mechanisms of these changes are currently not fully understood. Here, we present the results of atomistic computer simulations of bicrystalline Cu pillar compression and corresponding micromechanics experiments. The experiments show that Ag segregation to the GB increases the yield stress of the pillars, but only slip traces observed post mortem hint towards the mechanisms. We prepared segregated GB structures with combined molecular dynamics/Monte-Carlo simulations by matching the resulting excess Ag concentration to atom probe tomography results. The virtual nanopillars were cut from this material and varying amounts of dislocation loops were inserted in order to model the pre-existing dislocation networks in the experiment. Switching the atomic types of the segregants between Ag and Cu allowed us to model the exact same pillar and dislocation network with and without segregation, thereby enabling an investigation of the mechanisms underlying the experimentally observed strengthening.

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MM 26.2 Wed 10:30 SCH A 216

When grains go wild! Tracing microstructural outcomes back to possible mechanisms for abnormal grain growth — •Carl E. Krill III[1], Elizabeth A. Holm[2], Jules M. Dake[1], Ryan Cohn[2], Karolína Holíková[1], and Fabian Andorfer[1] — [1]Ulm University, Ulm, Germany — [2]Carnegie Mellon University, Pittsburgh, PA, USA

Usually, the coarsening of a polycrystalline material is a civilized affair, with adjacent grains swiping atoms so surreptitiously that relative growth rates remain moderate, and the mutual boundary stays smooth. In some cases, however, certain participants in this competition give free rein to an innate hunger for growth! The result is a subpopulation of large, "abnormal" crystallites embedded in a matrix of much smaller grains, whereby the abnormal/matrix interface can be anywhere from perfectly flat to fractally convoluted. The formation of such a microstructure is the telltale signature of abnormal grain growth (AGG). Although the most prominent feature of AGG is the shape of the abnormal grains, simulations indicate that the mechanism of AGG is encoded to a greater extent in the morphology of the interfaces between abnormal and matrix grains. Based on this finding, we propose a scheme for inferring the possible mechanism(s) underlying any experimentally observed case of (sufficiently extreme) AGG, and we illustrate our phenomenological method with experimental examples taken from the literature. Surprisingly, in the most clear-cut cases of AGG we have encountered, microstructural outcomes point to boundary-to-boundary mobility variation as the sole governing factor.

MM 26.3 Wed 10:45 SCH A 216

Influence of precipitates during anodization of aluminum alloys studied by TEM at cryogenic temperatures — •Lydia Daum, Stefan Ostendorp, Martin Peterlechner, and Gerhard Wilde — Westfälische-Wilhelms-Universität, Münster, Germany

Aluminum alloys with predefined alloying elements are chosen regarding their performance in certain areas of industrial applications due to their hardness, strength and corrosion resistance. Precipitates such as Mg2Si and dispersoids, e.g. enrichments of Mn in EN * AW6xxx alloys hinders the formation of ordered anodic aluminum oxides (AAOs) as achievable using high-purity aluminum samples.

The focus of this work is on correlating the structural and chemical properties of precipitates within AAOs and at the interface to the alloy. Due to geometry and size of the precipitates, transmission electron microscopy (TEM) is performed at selected areas. Measuring the same properties inside an Al 6xxx alloy close to the interface provides information about the contribution of the segregations during anodization. Previous scanning transmission electron microscopy (STEM) studies have shown that cryogenic temperatures can partially reduce the beam damage in electron beam sensitive materials as organics or AAOs [1]. In this study, the sample is also characterized by nanobeam diffraction pattern analysis and electron dispersive X-ray spectroscopy at cryogenic temperatures.

[1] A. M. Jasim, X. He, Y. Xing, T. A. White, and M. J. Young. ACS Omega 6.13 (2021), 8986-9000.

MM 26.4 Wed 11:00 SCH A 216

Disconnection-mediated migration of interfaces: continuum modeling and applications — •Marco Salvalaglio[1], Caihao Qui[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, China — [3]Department of Mechanical Engineering, The University of Hong Kong, Pokfulam Road, Hong Kong SAR, China

We present a model for the motion of arbitrarily curved interfaces that respects the underlying crystallography of two phases/domains meeting at an interface and is consistent with microscopic mechanisms of interface motion, i.e., migration of disconnection (line defects in the interface with step and dislocation character) [1]. The equation of motion for interface migration under the influence of a wide range of driving forces is discussed with the aid of numerical simulations [1,2]. A diffuse interface framework is also used to handle complex morphology and deliver proof of concept for microstructure evolution [2]. Recent results achieved with this model, concerning grain boundary morphologies, the competition among thermodynamic and kinetic effects, and grain rotation will be illustrated. [1] J. Han et al. Acta Materialia 227, 117178, (2022). [2] M. Salvalaglio et al. Acta Materialia 227, 117463, (2022).

MM 26.5 Wed 11:15 SCH A 216

Simulated mechanical deformations on graphene oxide — •Javier Rojas-Nunez[1], Samuel Baltazar[1], Eduardo Bringa[2], and Alejandra Garcia[3] — [1]Physics Department and CEDENNA, Universidad de Santiago de Chile (USACH), Santiago, Chile — [2]Laboratorio de síntesis y modificación de nanoestructuras y materiales bidimensionales, Centro de Investigación en Materiales Avanzados, Nuevo León, México — [3]CONICET & Facultad de Ingeniería, Universidad de Mendoza, Mendoza, Argentina

The better understanding of nanomaterial properties will be a key factor to tailor and enhance properties of new materials. Graphene oxide in particular can be synthesized with different oxidation levels in order so gain similar properties to its deoxidized counterpart, graphene. Through the molecular dynamic simulations, the atomistic behavior of a tri-layer graphene membrane under mechanical indentation will be studied in this work.

This work will study a highly oxidized graphene oxide tri-layer that will be indented with a repulsive spherical indentator. The modeling of the membrane will generate single layer graphene oxide candidates to pick the lowest energy configuration and later stack this layer over itself. The final tri-layer was used for the indentation simulation, where the young modulus was reproduced with decent similarity to experimental results.

The atomistic analysis of the indentation process suggest an important role of epoxide groups in the mechanical deformation of the membrane.

15 min. break

MM 26.6 Wed 11:45 SCH A 216

Atomic cluster expansion for Ag-Pd — •Yanyan Liang, Matous Mrovec, Yury Lysogorskiy, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Germany

Binary alloys of silver and palladium have recently attracted attention due to their importance in catalysis and nanotechnology. However, the binary Ag-Pd system lacks reliable and efficient interatomic potentials that provide an accurate description of structural and thermodynamic properties, in particular for atomistic simulations of nanoparticles. In this work, we present an atomic cluster expansion (ACE) parametrized

for binary Ag-Pd. We show that the Ag-Pd ACE potential provides an ab-initio accurate description of elastic, structural and thermodynamic properties of both, elements as well as their compounds. We demonstrate the computational efficiency and the applicability of our ACE for atomistic investigations of complex phenomena in Ag-Pd nanoparticles.

MM 26.7 Wed 12:00 SCH A 216

Spin-orbit interactions in plasmonic crystals probed by site-selective cathodoluminescence spectroscopy — Masoud Taleb[1], •Mohsen Samadi[1], Fatemeh Davoodi[1], Maximilian Black[1], Janek Buhl[2], Hannes Lüder[2], Martina Gerken[2], and Nahid Talebi[1,3] — [1]Institute of Experimental and Applied Physics, Kiel University, Germany — [2]Integrated Systems and Photonics, Faculty of Engineering, Kiel University, Germany — [3]Kiel, Nano, Surface, and Interface Science, Kiel University, Germany

The study of spin-orbit coupling (SOC) of light is crucial to explore the light-matter interactions in sub-wavelength nanostructures with broken symmetries. Herein, we explore the SOC in a plasmonic crystal, both theoretically and experimentally. Cathodoluminescence (CL) spectroscopy combined with the numerically calculated photonic band structure reveals an energy band splitting that is ascribed to the behavior of light in the plasmonic crystal where the inversion symmetry is locally broken. By shifting the impact position of the electron beam throughout a unit cell of the plasmonic crystal, we show that the emergence of the energy band splitting strongly depends on the excitation position of the surface plasmon (SP) waves on the crystal. Moreover, we exploit angle-resolved CL and dark-field polarimetry to demonstrate polarization-dependent scattering of SP waves interacting with the plasmonic crystal. Our study gives insight into the design of novel plasmonic devices with polarization-dependent directionality of the Bloch plasmons.

MM 26.8 Wed 12:15 SCH A 216

Soft and Hard X-ray Circular Dichroism in Valence-Band and Core-Level Momentum Microscopy — •O. Tkach[1,2], O. Fedchenko[1], K. Medjanik[1], Y. Lytvynenko[1], S. Babenkov[1], D. Vasilyev[1], Q.L. Nguyen[3], T.P. Vo[4], T.R.F. Peixoto[5], A. Gloskovskii[5], C. Schlueter[5], M. Hoesch[5], D. Kutnyakhov[5], M. Scholz[5], L. Wenthaus[5], N. Wind[5,6], S. Marotzke[5], A. Winkelmann[7], J. Minar[4], K. Rossnagel[5,8], H.-J. Elmers[1], and G. Schönhense[1] — [1]Univ. Mainz — [2]SSU, Ukraine — [3]SLAC Nat. Accel. Lab., USA — [4]Univ. West Bohemia, Czech — [5]DESY Hamburg — [6]Univ. Hamburg — [7]AGH Univ., Poland — [8]Univ. Kiel

We introduce full-field mapping of the circular dichroism texture in X-ray momentum microscopy. I(EB,k) energy-momentum space tomography with both soft and hard X-rays at PETRA-III yields CDAD patterns. Kinetic energies of up to >7 keV and a large k-field-of-view enable capturing of structural information via XPD Kikuchi patterns, which show pronounced asymmetries. Patterns at different azimuthal angles exhibit sharp zero lines, when the helicity vector lies in a mirror plane. Similar zero lines also appear in the XPD patterns of core levels, as exemplified for Ge 3p, Si 2p and various W core levels at hv = 6 keV. Calculations using Bloch-wave approach and one-step photoemission show good agreement with experiment. In order to disentangle the contributions of the photoexcitation (intrinsic part) from the Kikuchi process (extrinsic), XPD has been implemented in the Munich SPRKKR package, unifying one-step model of photoemission and multiple scattering theory.

MM 26.9 Wed 12:30 SCH A 216

Direct writing of three-dimensional nano-superconductors — •Elina Zhakina[1], Markus König[1], Sebastian Seifert[1], Amalio Fernández-Pacheco[2], Paul Simon[1], Wilder Carrillo-Cabrera[1], and Claire Donnelly[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany — [2]Institute of Nanoscience & Materials of Aragón CSIC-University of Zaragoza, Zaragoza, Spain

In recent years, superconductivity and vortex matter in curved 3D nanoarchitectures have become a vibrant research avenue because of the rich physics of the emerging geometry- and topology-induced phenomena [1]. However, the fabrication of such architectures is still challenging. Currently, fabrication techniques of innovative three-dimensional (3D) nano-objects are being developed [2].

Here, we present a new route to fabricating superconducting 3D nanoarchitectures by focused electron-beam-induced-deposition [3] of tungsten, allowing for the realisation of complex 3D superconducting geometries with a critical temperature on the order of 5 K. We observe a geometrical effect of the 3D nanoarchitecture, namely, the angular dependence of the upper-critical magnetic field that is not possible in bulk superconductors. This method unveils a wide perspective in experimental studies of the dynamics of topological defects in curved 3D nanoarchitectures.

[1] V. M. Fomin et al, Appl. Phys. Lett. 120, (2022) [2] R. Corboda et al, Beilstein J. Nanotechnol, 11, (2020) [3] L. Skoric et al, Nano Letters 20 (2020)

MM 26.10 Wed 12:45 SCH A 216

Influence of a p-n Heterojunction on the Diffusive Transport in Tungsten Trioxide Thin Films — •Jan L. Dornseifer[1,2], Markus S. Friedrich[1,2], and Peter J. Klar[1,2] — [1]Institute of Experimental Physics I, Justus-Liebig-University, Giessen, Germany — [2]Center for Materials Research (ZfM), Justus-Liebig-University, Giessen, Germany

Tungsten trioxide (WO_3) is (typically) an n-type semiconductor and a prominent electrochromic material. It changes its optical properties when charge carriers are inserted. Due to its excellent electrochromic properties, WO_3 is the most commonly used functional material in so called "smart" windows which are a promising technology for significantly lowering the energy consumption for building climatization. Industrially manufactured polycrystalline WO_3 thin films were coated with p-type nickel monoxide (NiO_x) thin films by ion beam sputter deposition. In order to investigate the diffusive transport of hydrogen in WO_3 thin films influenced by a p-n heterojunction, spatially and temporally resolved optical transmission measurements are conducted on NiO_x/WO_3-heterostructures during the potentiostatic coloration of the WO_3 thin films. Spatial and temporal diffusion profiles determined by analyzing these measurements indicate that the lateral propagation of hydrogen in NiO_x coated WO_3 films is accelerated. In addition, an increased transmittance is observed in the colored state. To describe these findings, a model is set up based on an increase in hydrogen concentration inside the WO_3 layer outside the space-charge region formed at the NiO_x/WO_3 interface.