MM 21: Interface Controlled Properties, Nanomaterials and Microstructure Design

Time: Wednesday 15:45–18:30 Location: H22

MM 21.1 Wed 15:45 H22

Plateau-Rayleigh-type failure mode of porous films and interconnects near massive substrates: mitigation strategies — •Gideon Henkelmann[1], Xinyan Wu[2], and Jörg Weissmüller[1,3] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Germany — [2]Institute of Optical and Electronic Materials, Hamburg University of Technology, Germany — [3]Institute of Hydrogen Technology, Helmholtz-Zentrum hereon, Geesthacht, Germany

Nanoporous thin films are under study as functional materials for actuation, photonics, catalysis, energy storage and as semiconductor interconnects. However, these thin films tend to self-detach from their substrate. The same failure mode is also observed in sintered silver paste, a widely used electronics interconnect material. In this work, we discuss the origin of the underlying instability. Based on those insights, we derive a mitigation strategy that depends on gradient in porosity. Combining experiment with kinetic Monte Carlo simulation, we validate the strategy and optimize the composition profile. An exponential gradient is found optimum, and this is rationalized by theory. Our approach greatly improves the structural stability of nanoporous thin films, enabling their more reliable use in advanced applications.

MM 21.2 Wed 16:00 H22

Compressive behavior and connecting topology of monolithic nanoporous niobium — •Seoyun Sohn[1,2], Shan Shi[3,1], Jürgen Markmann[1,2], Stefan Alexander Berger[1], and Jörg Weissmüller[2,1] — [1]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, 21502 Geesthacht, Germany — [2]Institute of Materials Physics and Technology, Hamburg University of Technology, 21073 Hamburg, Germany — [3]Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technology, 21073 Hamburg, Germany

This study investigates the mechanical behavior of nanoporous (NP) Nb fabricated through liquid-metal dealloying, with an eye on the role of structure size and topology. Results from X-ray nanotomography and macro-compression tests confirm that coarsening degrades yield strength and that Young's modulus deviates from scaling laws previously developed for NP Au made by dealloying in aqueous media. Our analysis reveals that the scaled genus, a measure of network connectivity, of NP Nb observed from the tomographic reconstructions is lower than what has been reported for NP Au. This reduced connectivity provides an obvious explanation for the low modulus of NP Nb. Furthermore, the structural dispersion implies that additional structural descriptors should be acknowledged to account for the mechanical differences between liquid-metal dealloyed materials and those synthesized via conventional aqueous dealloying.

MM 21.3 Wed 16:15 H22

Unravelling the metal-support interaction of sub-monolayer Pt thin films on manganese oxide via photoelectron spectroscopy — •Manuela Arztmann[1], Raul Garcia-Diez[1], Johannes Frisch[1], and Marcus Bär[1,2,3,4] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany — [2]Energy Materials In-Situ Laboratory Berlin, Germany — [3]Helmholtz-Institut Erlangen-Nürnberg für Erneuerbare Energien, Germany — [4]Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

In heterogeneous catalysis, metal-support interactions (MSI) have been shown to greatly influence the selectivity and activity of catalysts, with reducible supports as preeminent examples. The various oxidation states accessible for manganese oxide allow to accommodate different amounts of oxygen vacancies, making it a promising support with tunable properties for catalysis. Studies show that the oxidation state of manganese is closely linked to its promoter capabilities in catalysis, though the MSI is not well understood so far. In this 'in-system' study, the chemical and electronic structure of the interface between Pt and manganese oxide was investigated by XPS/UPS as a function of Pt surface coverage. The thin film model catalysts were prepared by e-beam evaporation in a system directly connected to the XPS/UPS setup, enabling precise control of the Pt thickness from sub-monolayer levels to thick metal-like Pt layers, allowing for a systematic study of the property evolution in the near surface region without leaving vacuum conditions. Our results reveal an enhanced reduction of the manganese oxide with increasing Pt surface coverage indicating significant MSI.

MM 21.4 Wed 16:30 H22

Optical and electrical properties of borophene and borophene/silicon junction — •yaser abdi[1,2], masoud taleb[1], alireza eskandari[2], zahra alavi[2], mohsen moayedi[2], and nahid talebi[1] — [1]Institute of Experimental and Applied Physics, Kiel University, 24118 Kiel, Germany — [2]Department of Physics, University of Tehran, 1439955961 Tehran, Iran

Borophene, a 2D monolayer of boron atoms, possesses unique properties that have led scientists to conclude that it could be an excellent alternative to graphene in future electronic device applications. In this talk, which is based on our recent work on synthesis [1] and characterization [2] of optical [3] and electrical properties of borophene and borophene/silicon Schottky junction, I will discuss about the growth of borophene using a chemical vapor deposition approach and investigation of its optical and electrical behaviors. Leveraging advanced deep-subwavelength cathodoluminescence spectroscopy, we reveal the extreme anisotropic optical response of borophene in the visible range[3]. Finally, direct growth of borophene on silicon to make Schottky junction will be explained and some opto-electrical measurements will be presented. The optoelectronic response of a borophene/silicon-based detector is approximately ten times higher than that of detectors fabricated by transferring 2D materials onto silicon, due to the excellent junction formed by the direct growth of borophene on silicon.

[1] ACS Applied Materials & Interfaces 2021 13 (7), 8844-8850 [2] ACS Applied Nano Materials 2024 7 (11), 13712-13719 [3] arXiv preprint arXiv:2404.13609v2

MM 21.5 Wed 16:45 H22

Atomistic computer simulations of the influence of grain boundary phases on segregation — •Tobias Brink, Dongjin Kim, and Gerhard Dehm — Max Planck Institute for Sustainable Materials, Düsseldorf, Germany

The properties of polycrystalline materials are often strongly affected by grain boundary (GB) segregation. Segregation energies, in turn, strongly depend on the available segregation sites and their atomic environments in the GB. At the atomic level, however, GBs are not only distinguished by their macroscopic, crystallographic parameters: different GB phases (or "complexions") can coexist even along the same GB and consequently affect available segregation sites. Similar as for bulk phases, the equilibrium atomic structure and chemistry of GBs changes based on temperature, pressure, concentration, chemical potential, etc.

Here, we investigate Ag segregation to [111] tilt GBs in Cu with hybrid molecular dynamics/Monte Carlo computer simulations using EAM potentials. These GBs are of interest because they exhibit two GB phases, "pearl" and "domino". Depending on the misorientation, either the pearl or the domino phase can more easily accommodate Ag segregants. As a consequence, the GB phases not only display distinct segregation behavior, but the stability of the GB phases is now also a function of the Ag excess concentration. An outlook on the effects of other segregants will be given and comparisons to experimental results will be discussed.

MM 21.6 Wed 17:00 H22

Characterizing the strength and stability of grain boundaries in Ni alloys by atomistic simulations — Reyhaneh Ghassemizadeh, •Daniel F. Urban, and Christian Elsässer — Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany

When increasing the in-service performance of engineering metallic materials, interfaces such as phase or grain boundaries (GB) may act as the weakest links. For the nickel-base superalloy Alloy 718 intergranular cracking can be a relevant damage mechanism as result of high-temperature fatigue in an oxygen-rich environment. The reliable prediction of the adhesion and mechanical stability of interfaces between two grains in a microstructure of a material from atomistic calculations remains a challenge. A possible approach to systematically address this issue is an idealized cleavage simulation analyzed in terms of the Rose-Ferrante-Smith universal binding energy relationship (UBER) which results in a measure for the ideal work of separation and the maximum tolerable normal strain. With this approach, we analyze the stability

of GBs in Alloy 718 using density functional theory calculations and thereby distinguish the influence of the different alloying elements on the strength of these interfaces. Furthermore, we systematically examine the influence of oxygen at the GBs and thereby shed light on the respective segregation-induced embrittlement in polycrystalline Ni systems. Our results can be used to parametrize traction separation laws used in finite element modelling, allowing for microstructure-sensitive modelling of fatigue crack formation and growth.

MM 21.7 Wed 17:15 H22

Ce-doped Ni-based nanocrystal ribbons for Near-Perfect Infrared Absorbers — •Timuçin Emre Tabaru[1], Ali Karatutlu[2], Iremnur Duru[1], and M. Fatih Kilicaslan[3] — [1]Department of Electrical Electronics Engineering, Sivas University of Science and Technology, 58000 Sivas, Turkey — [2]Institute of Materials Science Nanotechnology and National Nanotechnology Research Center (UNAM) Bilkent University Ankara 06800, Türkiye — [3]Department of Engineering Fundamental Sciences, Sivas University of Science and Technology, 58000 Sivas, Turkey

Absorption properties of Ni-based ribbons prepared with a composition of 75 % Ni, 10 % Cr, 8 % Si, 5 % Fe, 2 % B, and %1 Ce-doped were investigated in the infrared region. The ribbons were prepared by melt spinning, and the samples exhibited a nanocrystalline structure due to rapid solidification. The total absorbing effectiveness of the Ni-based ribbons reached a maximum of about %93 at 3-5 *m midwave infrared (mid-IR) window when the ribbons were doped with Ce causing an approximate 5% improvement in the mid-IR absorption. Overall, the composite films provide over 80% IR absorption at the wavelengths from 3 *m to 25 *m. Due to the superparamagnetic behavior of the Ni-based composite film suggesting a decrease in electrical conductivity, a high impedance allows such high IR absorption over a large EM spectrum. This indicates that Ce-doped Ni composite film can be a good candidate for thermal emitters and infrared imaging, and for integrating into small-pixel uncooled infrared detectors.

MM 21.8 Wed 17:30 H22

Tracking the emergence and persistence of abnormal grain growth in the commercial aluminum alloy AA5252 using 3D X-ray microscopy — •Helmuth-André Schulz-Harder[1], Jules M. Dake[1], Wolfgang Ludwig[2], Haixing Fang[2], Pierre-Olivier Autran[2], Karolína Gutbrod[1], Markus Ziehmer[1], Madlen Atzen[1], Thomas Wilhelm[3], Volker Schmidt[3], and Carl E. Krill III[1] — [1]Institute of Functional Nanosystems, Ulm University, Germany — [2]The European Synchrotron (ESRF), Grenoble, France — [3]Institute of Stochastics, Ulm University, Germany

The origin of abnormal grain growth (AGG) remains unclear despite decades of investigation, even though this phenomenon has far-reaching implications for a wide range of industrial applications. A significant challenge lies in the scarcity of time-resolved 3D data on AGG. To address this, we acquired a time series of 3D maps of the commercially available aluminum alloy AA5252 using synchrotron-based diffraction-contrast tomography (DCT). The reconstructed grain maps reveal the presence of extreme abnormal grains, the evolution of which could be observed over time and traced back nearly to the point of emergence. To further explore the influence of second-phase particles (known to be present in AA5252) on the growth of abnormal grains, we conducted complementary phase-contrast tomography (PCT) measurements. The combination of these datasets provides new insight into the locations where abnormal grains emerge and the mechanism(s) driving their persistent growth advantage.

MM 21.9 Wed 17:45 H22

Direct Laser Writing of metallic material utilizing the principle of sensitized triplet-triplet upconversion — •Kristin E. J. Kühl[1] and Georg von Freymann[1,2] — [1]University of Kaiserslautern-Landau, 67663 Kaiserslautern — [2]Fraunhofer Institute for Industrial Mathematics ITWM, 67663 Kaiserslautern

Direct Laser Writing (DLW) is a versatile technique for fabrication of microstructures, which is constantly evolving. Conventional DLW uses two photon absorption to form polymers from monomers via a photochemical reaction. Current research is leaning towards new materials, such as different kinds of metal which satisfy different demands on the physical properties of structures like electric conductivity or ferromagnetism, as well as the application of different photochemical reactions to provide more opportunities in the implementation of the printing process.

In this talk a novel approach to Direct Laser Writing of metallic materials is presented. For this purpose, photochemical compounds and principles were investigated via different methods and applied in a home built setup for Direct Laser Writing. A sensitized triplet-triplet annihilation upconversion process (sTTA-UC) is used to generate the energy required for the photochemical reduction of nickel. Since efficient sTTA-UC is usually limited to deoxygenated materials, a solvent is used that has the property of generating a local deoxygenated area upon excitation by a sensitizer. These three processes are combined to enable Direct Laser Writing of 2D nickel structures.

MM 21.10 Wed 18:00 H22

Friction coefficient and work function investigation of transition-metal dichalcogenide — •Malik Al naabi, Shuyu Huang, Antoine Hinaut, Ernst Meyer, and Thilo Glatzel — University of Basel, Basel, Switzerland

Despite extensive research on the tribological properties of MoS2,the frictional characteristics and electronic properties of other members of the transition-metal dichalcogenide (TMD) family have remained relatively unexplored. To understand the effect of the chalcogen on the tribological behavior of these materials and gain broader general insights into the factors controlling friction at the nanoscale, we compared the friction force behavior for a nanoscale single asperity sliding on MoS2, MoSe2, WS2, and WSe2, in bulk using friction force microscopy (FFM). Additionally, we used Kelvin probe force microscopy (KPFM) to investigate the work function. All the materials were cleaved in the nitrogen glovebox.

MM 21.11 Wed 18:15 H22

Nano-scale precipitations in NiTi-based alloys after laser powder bed fusion: FIB/STEM and APT analyses — •Farzad Khodabakhshi[1], Raphael Freundl[2], Eric A. Jägle[2], and Gerhard Wilde[1] — [1]University of Muenster — [2]Universität der Bundeswehr München

Phase formation and nano-scale precipitation during laser powder bed fusion (LPBF) of a NiTi/Nb powder mixture were characterized throughout the matrix of NiTi using advanced microscopy techniques. The study employed focused ion beam (FIB) preparation combined with scanning transmission electron microscopy (STEM) and atom probe tomography (APT). Different nano-scale phases formed through in situ alloying and their interfacial coherence with the NiTi-based alloy were examined using atomic-scale high-resolution microscopy. Subsequent nano-scale elemental mapping and chemical analysis were performed by APT. The results indicated significant changes in the contributions of in situ formed phases when altering the fraction of niobium. Low fractions of Nb can modify the intrinsic structure of NiTi precipitates. Changing the grain boundary energy helps shift these precipitates toward the interiors of grains rather than remaining at the boundaries. Conversely, increasing the niobium fraction towards the eutectic composition results in the formation of a new structure comprised of precipitates with a specific ternary composition within the NiTi alloy matrix due to LPBF deposition.