MM 5: Topical Session Interface Dominated Phenomena - Poster

Time: Tuesday 10:00–12:45 Location: P

MM 5.1 Tue 10:00 P

Temperature and chemical bonding effects on the brittle-to-ductile transition in metal-metalloid glasses — •Daniel Şopu[1,2], Franco Moitzi[1], and Jürgen Eckert[1,3] — [1]Erich Schmid Institute of Materials Science of the Austrian Academy of Sciences, Leoben, Austria — [2]Technische Universität Darmstadt, Darmstadt, Germany — [3]Montanuniversität Leoben, Leoben, Austria

The relationship between the deformation behavior of metal-metalloid glasses and their intrinsic properties is studied using large-scale molecular dynamics simulations. The influence of composition and temperature on the tensile deformation behavior of amorphous PdSi alloys is investigated. A transition from cracking perpendicular to the loading direction to shear banding can be achieved by increasing the temperature or decreasing the amount of silicon. A decrease in silicon content leads to fewer covalent bonds and, therefore, lower activation barriers for shear transformation zones and, consecutively, a high probability for shear band formation. On the other hand, at low temperatures these barrier cannot be overcome and cracking will dominate over shear banding. In this case, high activation barriers for local relaxation impedes stress redistribution into the glassy structure and, finally, cracking occurs. Additionally, the cracking path also depends on the degree of homogeneity. A corrugated fracture surface similar to experiment can be formed due to crack defection and cavitation ahead of the crack tip in chemically inhomogeneous samples. In contrast, a sharp cleavage-like fracture occurs for more homogeneous samples.

MM 5.2 Tue 10:00 P

Enabling materials design of ionic systems with automated corrections: AFLOW-CCE — •Rico Friedrich[1,2], Marco Esters[1], Corey Oses[1], Stuart Ki[1], Maxwell J. Brenner[1], David Hicks[1], Michael J. Mehl[1], Mahdi Ghorbani-Asl[2], Arkady Krasheninnikov[2], Cormac Toher[1], and Stefano Curtarolo[1,3] — [1]Center for Autonomous Materials Design, Duke University, USA — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [3]Materials Science, Electrical Engineering, Physics and Chemistry, Duke University, USA

Materials databases such as AFLOW [1] leverage *ab initio* calculations for autonomous materials design. The predictive power critically relies on accurate formation enthalpies - quantifying the thermodynamic stability of a system. For ionic materials such as oxides and nitrides, standard DFT leads to errors of several hundred meV/atom [2,3].

We have recently developed the "coordination corrected enthalpies" (CCE) method yielding highly accurate room temperature formation enthalpies with mean absolute errors down to 27 meV/atom [3]. Here, we introduce AFLOW-CCE [4]: a tool where users can input a structure file and receive the CCE corrections, or even the CCE formation enthalpies if pre-calculated LDA, PBE or SCAN values are provided. The results can be used for the design of *e.g.* 2D materials.

[1] S. Curtarolo *et al.*, Comput. Mater. Sci. **58**, 218 (2012).
[2] V. Stevanović *et al.*, Phys. Rev. B **85**, 115104 (2012).
[3] R. Friedrich *et al.*, npj Comput. Mater. **5**, 59 (2019).
[4] R. Friedrich *et al.*, Phys. Rev. Mater. **5**, 043803 (2021).

MM 5.3 Tue 10:00 P

Molecular Dynamics study of the influence of microstructure on reaction front propagation in Al-Ni multilayers — •Fabian Schwarz and Ralph Spolenak — Laboratory for Nanometallurgy, Department of Materials, ETH Zürich, CH-8093 Zürich, Switzerland

Reactive multilayers can be used for energy storage as well as releasing large amounts of heat in a short time. We use Molecular Dynamics (MD) simulations to study the influence of the crystal structure on the reaction front propagation in Al-Ni multilayers. Different microstructures, namely amorphous, single crystal, columnar grains and randomly oriented grains of varying size are investigated. The effect of the microstructure on the propagation speed is studied and compared to existing experimental results. Furthermore, MD simulations allow to study the inter-diffusion of the Al and Ni layers. We found that crystallinity has a significant impact on the front propagation speed, which is likely related to different diffusion mechanisms. The more disordered the individual layers become, e.g. by increasing the grain boundary density, the higher is the resulting propagation speed.

MM 5.4 Tue 10:00 P

Grain boundary segregation and precipitation in an Al-Zn-Mg-Cu alloy — •Huan Zhao[1], Baptiste Gault[1,2], Liam Huber[1], Wenjun Lu[1], Nicolas Peter[1], Dirk Ponge[1], and Dierk Raabe[1] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — [2]Department of Materials, Royal School of Mines, Imperial College London, London, United Kingdom

High-strength Al-Zn-Mg-Cu alloys are highly susceptible to intergranular embrittlement, which severely limits their lifetime. In this talk, I will present our recent work on the effect of solute segregation in the precipitation behavior at grain boundaries (GBs) compared to grain interiors. Solute segregation could accelerate the precipitation behavior at GBs, which causes the formation of coarse precipitates and precipitate free zones along GBs. Furthermore, the interplay of solute segregation and the local structure at GBs has been considered. We show that faceting occurs at GBs and that the distinct segregation and precipitation behavior occurs within the same GB. Investigations on the solute distribution inside the precipitates, matrix, and at GBs related to SCC resistance in Al-Zn-Mg-Cu alloys will also be discussed.

MM 5.5 Tue 10:00 P

On the role of rotational twin boundaries in lamellar TiAl on the deformation behavior — •Ashish Chauniyal and Rebecca Janisch — ICAMS, Ruhr-University Bochum, 44780 Bochum, Germany

Twin boundaries in lamellar TiAl alloys have a determining influence on their mechanical properties. During deformation, the twin boundaries prevent easy glide of dislocations, thereby contributing to strengthening. In nano-scale lamellae, twin boundaries can cause considerable dislocation pileups which contribute to strengthening, but compromise ductility. To maintain deformability, it is desirable to have movement of dislocations and sufficient dislocation sources to nucleate new dislocations. In this regard, the twin boundaries in lamellar TiAl are special as the tetragonality of the γ phase ($L1_0$) leads to several variants of rotational twin boundaries by rotating in steps of 60° around the [111] axis. While a $\gamma/\gamma_{180°}$ boundary is fully coherent, $\gamma/\gamma_{60°}$ and $\gamma/\gamma_{120°}$ boundaries exhibit a lattice misfit at the interface, which can result in coherency or semi-coherency. For a coherent interface a residual coherency stress is generated within the lamallae which can have a profound influence during deformation. For a semi-coherent interface, misfit dislocations at the interface can act as nucleation sources. In this work we model these interfaces atomistically and compare their deformation behavior by carrying out large scale atomistic simulations. Our simulations reveal the mechanisms of dislocation nucleation and propagation in lamellar layers with rotational twin boundaries.

MM 5.6 Tue 10:00 P

High hydrogen mobility in an amide-borohydride compound studied by quasielastic neutron scattering — •Neslihan Aslan[1], Sebastian Busch[1], Wiebke Lohstroh[2], Claudio Pistidda[3], and Martin Müller[1,4] — [1]German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Hereon, Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technical University Munich (TUM), Garching, Germany — [3]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany — [4]Institute of Materials Physics, Helmholtz-Zentrum Hereon, Geesthacht, Germany

The hydrogen storage performance of reactive hydride composites Mg(NH2)2 + 2 LiH can be significantly improved by the addition of LiBH4 and the subsequent formation of the amide-borohydride compound Li4(BH4)(NH2)3 during hydrogen release. To understand the chemical behaviour and atomic motions of Li4(BH4)(NH2)3, we present an in situ phase analysis with X-ray synchrotron diffraction and quasielastic neutron scattering (QENS) during heating.

Li4(BH4)(NH2)3 melts at 494 K and the crystallization of a second phase is detected and identified as LiNH2. In molten phase, the neutron measurements confirm a long-range diffusive motion of hydrogen-containing species with the diffusion coefficient $D \sim 10^{-6}\,\frac{\mathrm{cm}^2}{\mathrm{s}}$. In solid phase, localized rotational motions are observed that have been attributed to (BH4)- tetrahedra units mainly undergoing rotations around C_3 axes.

MM 5.7 Tue 10:00 P

Substrate-Induced Anisotropic Superconductivity in Layered Materials: the role of Nonlocal Coulomb Interactions and Band Hybridisation — •Manuel Simonato[1], Anand Kamlapure[1], Emil Sierda[1], Manuel Steinbrecher[1], Umut Kamber[1], Elze. J. Knol[1], Peter Krogstrop[2,3], Mikhail I. Katsnelson[1], Alexander Khajetoorians[1], and Malte Rösner[1] — [1]Institute for Molecules and Materials, Radboud University, Nijmegen 6525AJ, Netherlands — [2]Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, 2100 Copenhagen, Denmark — [3]Microsoft Quantum Materials Lab Copenhagen, 2800 Lyngby, Denmark

We investigate how anisotropic substrate materials, such as black-phosphorus (BP), can affect the properties of layered superconductors (SC), both via dielectric screening of the Coulomb interaction and via band hybridization. We employ generic lattice models to describe the SC in BCS theory and utilize Thomas-Fermi screening theory for the Coulomb interactions. The SC-substrate hybridization is studied by means of an effective two-band model, which yields an extension of conventional BCS theory in the Nambu-Gorkov formalism. We derive a new gap equation, from which the effective gap and other SC properties are evaluated. Our predictions for the spectral density function show great qualitative agreement with experimental data for thin Pb films on BP substrates.

MM 5.8 Tue 10:00 P

Sampling the parameter space of grain boundaries with a sequential sampling technique - Atomistics meets statistics — •Timo Schmalofski[1], Martin Kroll[2], Holger Dette[2], and Rebecca Janisch[1] — [1]ICAMS, Ruhr-University Bochum, 44780 Bochum, Germany — [2]Department of Mathematics, Ruhr-University Bochum, 44780 Bochum, Germany

The grain boundary energy is a function of five degrees of freedom (DOF). Two DOF describe the inclination of the grain boundary plane and the remaining three DOF the misorientation between both grains (one for the misorientation angle and two for the rotation axis). The sampling of this grain boundary energy space or even subspaces of it has been shown to be very challenging due to the so-called "cusps", steep energy minima at special misorientations and/or inclinations. Several approaches have been tried to sample energy subspaces, but they mostly need a large amount of datapoints for sufficient accuracy, and in addition an a-priori knowledge of the positions of the energy cusps. Therefore, in this work, statistical methods are combined with atomistic simulations and a sequential sampling technique is designed. In this presentation this technique will be introduced and compared to a regular sampling technique, to prove its advantages when sampling a whole subspace with a minimal amount of datapoints and discovering unknown cusps automatically. The presentation will focus on the sampling of only one dimensional subspaces of symmetrical tilt grain boundaries to prove the concept, but the application can be generalized towards multidimensional subspaces.

MM 5.9 Tue 10:00 P

The methods of neutron diffraction intensity calculation — •Anastasiia Kuznetsova[1], Jie Luo[2], Hareesh Chavana[3], Veronika Reich[1], Sebastian Busch[1], and Martin Müller[4] — [1]GEMS at MLZ, Hereon, Lichtenbergstr. 1, 85748 Garching b. München, Germany — [2]ILL, 71 avenue des Martyrs, 38000 Grenoble, France — [3]ICG Place Eugene Bataillon, Bat. 15, 34095 Montpellier, France — [4]Hereon, Max-Planck-Str. 1, 21502 Geesthacht, Germany

Neutron diffraction intensity on a crystal is commonly calculated as crystal's structure factor squared. The SASSENA program, suitable for atomic movement modeling, and the Debye formula, applicable for any material, not obligatory a periodic one, were tested for calculation of diffraction on crystalline powders. Mono- and biatomic structures of cP, bcc, and fcc crystal lattices of two different sizes each were used as model crystals. Furthermore, for Po, which data on scattering length were not listed, it was set artificially and also varied. The first method sums up reflections from all crystalline planes for the same Q-vector; the second one takes into account both crystalline structure and atomic motions; the third one spherically averages all possible orientations of the system. The resulting curves were juxtaposed and for Debye formula, the intensities were also correlated with structure factors squared and plotted against Q to obtain some kind of dependence. Given their results' difference, one has to choose a proper calculation method and to justify their choice. Due to some Q-dependence of intensities ratios the presence of some explanation for the divergence among the results of both formulas was assumed.

MM 5.10 Tue 10:00 P

Broadband coupling of fast electrons with high-Q whispering gallery mode resonators — •Niklas Müller, Vincent Hock, Christopher Rathje, Nora Bach, Holger Koch, and Sascha Schäfer — Institute of Physics, University of Oldenburg, 26129 Oldenburg, Germany

The inelastic interaction of fast electrons with spatially confined intense light fields has recently enabled new techniques in ultrafast transmission electron microscopy (UTEM), enabling the coherent control of free-electron states. Advanced quantum control scenarios, including electron-light entanglement and non-trivial electron/photon counting statistics, become accessible if non-classical light states are applied. However, to mitigate the reduced coupling strength when considering few-photon-states, novel concepts for coupling electrons to high-Q optical resonators are required. Here, we demonstrate the excitation of high-Q whispering gallery modes in a silica microfiber taper in a transmission electron microscope by relativistic electrons (200 keV) passing close to the fiber surface. The evanescent electric field of the passing electron induces a femtosecond electric polarization in the silica, which can be decomposed into optical whispering gallery modes (WGM). The dtected coherent cathodoluminescence spectra consist of octave-spanning frequency combs with narrow-bandwidth peaks. By probing the WGM resonances for different distances from the taper apex, we demonstrate that the peaks within the comb exhibit a frequency spacing inversely scaling with the local fiber circumference. Q-factors up to 700 a measured, depending on the local taper angle.

MM 5.11 Tue 10:00 P

Large scale process for adjustable resonances as a versatile platform for SERS — •Marcel Below and Jörg Schilling — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06108 Halle, Germany

Samples on cm^2-scale with hexagonal lattices of gold nanoscatterers were created with different controlled periods by using three-beam interference lithography. The resulting nanoscatterers have an elliptical shape and the size of their semi-axes is linked to the period of the lattice.

Spectral transmission measurements show two broad drops of transmission at different wavelengths depending on the polarization of the light. These are identified as single particle plasmonic resonances and can be shifted from the visible to the mid-IR with increasing size of the nanoscatterers. FEM simulations reveal that both plasmonic resonances are caused by the shape of the individual nanoscatterers.

Additionally, considerably sharper and asymmetric drops of transmission, known as Fano resonances, were observed. These Fano resonances are caused by an overlap of the single particle plasmonic resonance of each nanoscatterer and the collective response of the lattice.

When a sample is immersed in a solution of 4-MBA molecules, the molecules bond to the surface of the gold nanoscatterers. Subsequent Raman measurements show a clear SERS signal and a strong dependency on the polarization of the excitation laser. These results present a possible route for large area SERS substrates with tunable plasmonic resonances.

MM 5.12 Tue 10:00 P

Influence of oxygen on the development of facets on the ligaments of nanoporous gold — •Ulrike Dette[1], Stefan A. Berger[1], Ling-Zhi Liu[2], Jürgen Markmann[1,3], and Jörg Weissmüller[3,1] — [1]Institut für Werkstoffmechanik, Helmholtz-Zentrum Hereon — [2]Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences — [3]Institut für Werkstoffphysik und Werkstofftechnologie, Technische Universität Hamburg

Even at comparably low temperatures, gold atoms diffuse on the surface of ligaments in nanoporous gold and create facets. Defects and residual silver act as pinning points for the diffusion and thus the facets. For a better understanding of the faceting mechanism and the role of oxygen in it, we annealed nanoporous gold in argon atmosphere at 500°C for 3 h with different oxygen partial pressures controlled by an electrolyzer. We used samples with and without residual silver on the surface. The results show that the higher the oxygen level the stronger the faceting and bigger the ligament size. Therefore, oxygen does support the faceting of nanoporous gold and the coarsening of the ligaments during annealing. We additionally found that the more

residual silver on the surface the more silver clusters are formed during annealing and the smaller the facets become. It confirms that residual silver does act as a pinning point for the facets.

MM 5.13 Tue 10:00 P

Revealing highly stable copper based alloys using active learning — •Angel Diaz Carral[1], Azade Yazdan Yar[1], Siegfried Schmauder[2], and Maria Fyta[1] — [1]Institute for Computational Physics (ICP), Universität Stuttgart, Allmandring 3, 70569, Stuttgart, Germany — [2]Institut für Materialprüfung, Werkstoffkunde und Festigkeitslehre (IMWF), Pfaffenwaldring 32 70569, Stuttgart, Germany

Copper based alloys, due to their high electrical conductivity and high strength, are of great importance for electric and electronic applications such as connectors or lead frames. To this end, we investigate the stability of Cu-Ni-Si-Cr alloys, that is copper alloys with nickel, silicon and chromium impurities. Through computational means, we scan a large number of impurities' concentration and configurations. A relaxation-on-the-fly active learning algorithm is applied in order to investigate the influence of this scanning and reveal the alloys of higher stability. The latter are used at a next step in larger scale simulations in order assist the design of alloys with pre-selected properties. Here, we mainly focus on the first part, the learning process and the stable alloy structures. We discuss the efficiency of this approach, the predictions that can be made and the impact in designing alloys.