MM 3: Topical Session Interface-Dominated Phenomena - Defect Structures and Mechanical Properties

Time: Monday 13:30–15:00 Location: H2

MM 3.1 Mon 13:30 H2

Imaging the Deformation-Induced Accumulation of Defects in Nanoporous Gold — •Maowen Liu[1] and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology — [2]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Hereon

Nanoporous gold (NPG) provides a model material for studying small-scale deformation and the mechanical behavior of network solids. While studies of nanopillars indicate dislocation starvation, the strain hardening of NPG suggests dislocation accumulation. Yet, the approach to confirm that latter process by direct experimental observation, namely transmission electron microscopy (TEM), is impaired by the need to distinguish native defects in the microstructure from artifacts due to sample slicing or thinning. Here, we report a TEM study of the defect structure in electron-transparent NPG leaf deformed by rolling. The results confirm that plastic deformation significantly enhances the defect density. Specifically, twins are formed on several crystallographic planes, and their interaction forms Lomer-Cottrell locks. This inhibits dislocation escaping from NPG, thus avoiding the dislocation starvation scenario that is often considered in the "smaller is stronger" context of small-scale plasticity. Instead, strain-hardening is apparently linked to accumulation and interaction of twins.

MM 3.2 Mon 13:45 H2

How the interface type manipulates the thermomechanical response of nanostructured metals: A case study on nickel — •Oliver Renk[1], Verena Maier-Kiener[2], Christian Motz[3], Daniel Kiener[2], Jürgen Eckert[1], and Reinhard Pippan[1] — [1]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, Austria — [2]Montanuniversität Leoben — [3]Saarland University, Germany

The presence of interfaces with nanoscale spacing significantly enhances the strength of materials, but also changes the rate controlling processes of plastic flow. Due to the confined grain volumes, intragranular dislocation-dislocation interactions are replaced by emission and absorption of dislocations from and at the interfaces. Both processes not only depend on the interfacial spacing, but also on the interface structure. The present study attempts to rationalize this effect by investigating the thermomechanical behavior of samples consisting of three different interfaces. Nickel samples with predominant fractions of low- and high-angle as well as twin boundaries with a similar average spacing of 150 nm are investigated using high temperature nanoindentation strain rate jump tests. Depending on the interface structure, hardness, strain rate sensitivity and apparent activation volumes evolve different with temperature. While in case of high-angle boundaries for all quantities a pronounced thermal dependence is found, the other two interface types behave almost athermal. These differences can be rationalized based on the different interfacial diffusivity, affecting the predominant process of interfacial stress relaxation.

MM 3.3 Mon 14:00 H2

Atomistic simulation study of grain boundary migration for different complexions in copper — •Swetha Pemma[1], Rebecca Janisch[2], Gerhard Dehm[1], and Tobias Brink[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Interdisciplinary Centre of Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, 44780 Bochum, Germany

Grain boundary (GB) migration is significant to study the microstructural evolution which determines the properties of polycrystalline materials. Previous studies showed that the coupling between applied shear and GB migration differed for different complexions on the same GB. In this work, shear coupled grain boundary migration (SCGBM) of two complexions ("pearl" and "domino") observed experimentally in $\Sigma19b$ $\langle111\rangle$ tilt GBs in copper was investigated by molecular dynamics simulations. Effects of these complexions on the shear-coupling factor, critical shear stress for GB motion, and elementary GB migration mechanism were analysed. The coupling factors of the complexions were observed to be of same magnitude and sign for several temperatures and shear velocities. However, the critical shear stress differs by 31 % between pearl and domino, indicating a difference in activation barriers. Additionally, the precise atomistic mechanisms of SCGBM were examined using nudged elastic band calculations.

Acknowledgment: This result is part of a project that has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (Grant agreement No. 787446; GB-CORRELATE).

MM 3.4 Mon 14:15 H2

Prismatic slip in pure Magnesium with a Neural Network Potential — •Markus Stricker[1] and William A. Curtin[2] — [1]ICAMS, Ruhr-Universität Bochum, Germany — [2]LAMMM, EPFL, Lausanne, Switzerland

Studying fundamental mechanisms of deformation in metals and alloys requires dependable interatomic potentials because dislocations and cracks are above scales accessible with first-principles calculations. While classical potential forms like the modified embedded atom method (MEAM) have been successfully employed in many cases, non-fcc metals and almost all alloys are not modeled sufficiently quantitative. As a first step towards Mg-alloys we present a broadly applicable machine learned potential for pure Magnesium in the Behler-Parrinello neural-network framework trained on first-principles density-functional theory. We show that the potential predicts dislocation and crack structures very well and subsequently apply it to cross-slip of prismatic screw dislocations, which is not accessible to first-principles approaches. Prismatic slip is achieved by double-cross-slip of stable basal dislocations in steps of $c/2$ driven by a shear stress on the prismatic plane. The geometry of the observed process compares very well with the process deduced from experiments, the enthalpy barrier not. This mimics the stress-driven double-kink nucleation in bcc elements: the geometry of the mechanism is predicted well, but stress and activation barriers are overestimated by first-principles predictions.

MM 3.5 Mon 14:30 H2

Ab-initio study of the Mo/SiC interfacial adhesion — •David Sebastian Kasdorf and Karsten Albe — Fachgebiet Materialmodellierung, Institut für Materialwissenschaft, TU Darmstadt, Otto-Berndt-Str. 3, Darmstadt D-64287, Germany

Mo-Si-based alloys are a potential alternative to commercially available Ni-based superalloys for high-temperature applications. While the optimization of corrosion, oxidation and creep behavior of Mo-Si-based alloys are the object of current research efforts, also materials that could act as a thermal barrier coating (and possibly bond coats) need to be identified in order to maximize the temperature capabilities. Failure modes like delamination and fractures often happen at the interfaces between the metallic substrate and ceramic top coats as the interfacial adhesion presents the limiting factor of the fracture toughness in the materials system.

We performed first-principles calculations to study the ideal work of separation and theoretical strength of Mo/SiC interfaces. In those calculations, bcc Molybdenum acts as a representative for Mo-Si-based alloys as a Mo solid solution phase is common in those alloys. Similarly, β-SiC was chosen as the second part of the interface since it is a typical high-temperature crystallization product of Si-based ceramic coatings.

MM 3.6 Mon 14:45 H2

Unravelling the lamellar size-dependent fracture behavior of fully lamellar intermetallic γ-TiAl — •Anupam Neogi and Rebecca Janisch — ICAMS, Ruhr-University Bochum, 44780 Bochum, Germany

Strengthening of metals by incorporating nano-scale coherent twin boundaries is one of the important breakthroughs in overcoming the strength-ductility trade-off in recent years. Also, nano-scale twin boundaries in the nano-lamellar in lightweight Ti-Al alloys promise great potential, but their contribution to the deformation and fracture behavior needs to be better understood for designing optimum microstructures. To this end, we carry out linear elastic fracture mechanics informed, large-scale atomistic simulations of fully lamellar γ-TiAl, and find, that nano-scale lamellae are not only effective in improving the fracture toughness and crack growth resistance, but the lamellar size possesses a significant controlling role on the crack tip mechanisms. The fracture initiation toughness exhibits an increasing

trend with decreasing lamellar size until ∼3 nm. In this regime, the crack tip events are mostly dislocation-based plasticity. Below the critical lamellar size of ∼3 nm, the crack advances via a quasi-brittle manner, i.e., the cleavage of atomic bonds at the crack tip accompanied by some plasticity events, such as twin-boundary migration and dislocation nucleation. A layer-wise stacking fault energy-based analysis, including the quantitative analysis of dislocation barrier energy, elucidates the nano-scale lamellar size-dependent fracture behavior of γ-TiAl.