MM 45: Mechanical Properties and Alloy Design: e.g. Light-Weight, High-Temperature, Multicomponent Materials IV

Time: Wednesday 15:45–17:00 Location: C 230

MM 45.1 Wed 15:45 C 230

Ab initio insights into compositional dependence of TWIP and TRIP barriers of Ti-alloys — •David Holec[1], Johann Grillitsch[1], José Neves[2], and Thomas Klein[2] — [1]Department of Materials Science, Montanuniversität Leoben, 8700 Leoben, Austria — [2]LKR Light Metals Technologies, AIT Austrian Institute of Technology, 5282 Ranshofen, Austria

Advanced manufacturing, such as additive manufacturing, is a promising concept for a more material-efficient production route of components with complex shapes. However, this new technology also brings new challenges such as different microstructures and compositions. In this contribution, we will present a fundamental study on the impact of alloying species on transformation barriers in Ti-alloys. We employ ab initio methods to calculate the potential energy surface (PES) for a bcc-to-hcp transformation as a model for transformation-induced plasticity (TRIP), as well as stacking fault energies together with their barriers for different twinning mechanisms as a measure of the twinning-induced plasticity (TWIP). We present strategies for evaluating the alloying impact on those measures using a thermodynamics-based statistical averaging of various local configurations.

MM 45.2 Wed 16:00 C 230

Dislocation-mediated non-basal plasticity in topologically close-packed phases — •Zhuocheng Xie[1], Martina Freund[1], Wei Luo[1], Christina Gasper[1], Pei-Ling Sun[1], Siyuan Zhang[2], and Sandra Korte-Kerzel[1] — [1]Institute of Physical Metallurgy and Materials Physics, RWTH Aachen University, Kopernikusstraße 14, 52074 Aachen, Germany — [2]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, D-40237 Düsseldorf, Germany

Topologically close-packed (TCP) phases exhibit great promise as high-temperature structural materials, however, their notorious brittleness at room temperature limits their applications. The dislocation motion mechanisms in these complex alloys, especially on non-basal/{111} planes, remain poorly understood. We perform atomistic simulations to elucidate the deformation mechanisms of TCP phases and complement with experimental observations from nanomechanical testing at room temperature. Dislocation glide and cross-slip mechanisms among newly identified {11n} slip planes in cubic Laves phases and associated minimum energy paths are determined. Additionally, we unveil a new non-basal slip mechanism, namely the formation of (1-105) stacking fault by partial dislocation glide with a Burgers vector of 0.07[-5502], in μ-phases. This comprehensive exploration of dislocation dynamics not only contributes to a fundamental understanding of TCP phases but also paves the way for tailored design strategies to enhance their mechanical properties at room temperature.

MM 45.3 Wed 16:15 C 230

Anomalous brittleness of iridium: Atomistic insights from DFT and ACE simulations — •Minaam Qamar, Matous Mrovec, Yury Lysogorskiy, and Ralf Drautz — ICAMS, Ruhr University Bochum, Germany

The anomalous brittle nature of face-centered cubic (fcc) metal iridium has puzzled researchers for decades. We investigated fracture mechanisms in Ir using atomistic simulations based on density functional theory (DFT) and the atomic cluster expansion (ACE). ACE is a data-driven interatomic potential with a formally complete basis that can reach quantum accuracy while remaining highly computationally efficient. Both transgranular cleavage in perfect bulk and intergranular fracture along grain boundaries were examined. Detailed computational tensile tests for several grain boundaries were performed in parallel for Ir and Cu, which can be considered a prototypical ductile fcc metal. Subsequently, ACE parametrizations for both metals were employed in large-scale atomistic simulations of various fracture scenarios at finite temperatures and different loading conditions. We will present results of the simulations and discuss new insights into the intrinsic fracture behavior of Ir.

MM 45.4 Wed 16:30 C 230

Parameterising dislocation dynamics in Ni-based superalloys from atomistic simulations — •Geraldine Anis, Thomas Hudson, and Peter Brommer — University of Warwick, Coventry CV4 7AL, UK

Ni-based superalloys are important materials for high temperature applications. Nanoscale precipitates in their microstructure hinder dislocation motion, which results in an extraordinary strengthening effect at elevated temperatures. In the present work, we parameterise the motion of edge dislocations in pure face-centred cubic (FCC) Ni, which we use to represent an idealized γ phase in Ni-based superalloys. Molecular dynamics (MD) simulations with classical effective potentials were used to obtain edge dislocation trajectories, and the parameters of equations of motion were then fitted using Differential Evolution Monte Carlo (DE-MC) within a Bayesian framework. The reduced model accounts for dislocation-dislocation and dislocation-precipitate interactions, and the fitting procedure yields physically meaningful parameters. Using DE-MC sampling makes it possible to obtain parameter distributions and propagate uncertainties through the model, quantifying the uncertainty in its predictions: the dislocation positions and velocities. This work serves as a first step towards building a more comprehensive surrogate model that can describe the deformation behaviour of Ni-based superalloys, where the parameterisation approach employed here can offer a quantitative measure of the effect of precipitates on dislocation dynamics in these materials.

MM 45.5 Wed 16:45 C 230

Dislocation Crack Interactions in Tungsten — •Benedikt Eggle-Sievers and Erik Bitzek — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf

The fracture toughness of single crystalline Tungsten at low temperature is critically influenced by its microstructure. Understanding the underlying crack-microstructure interactions is therefore necessary to model and predict materials failure. In order to gain insight into the interactions of dislocations with crack tips, large-scale atomistic simulations are carried out. Screw dislocations are placed in the vicinity of a strain-controlled crack. In various crack systems screw dislocations that are attracted towards the crack tip have a strong tendency to cross-slip at the crack tip and glide along the crack front. Driving forces for this phenomenon as well as implications for fracture behaviour shall be discussed in this contribution.