MM 28: Mechanical properties

Strengthening Mechanisms

Time: Thursday 10:15–11:30 Location: H23

MM 28.1 Thu 10:15 H23

Parameterising edge dislocation trajectories in Ni-based superalloys with uncertainty quantification — •Geraldine Anis, Thomas Hudson, and Peter Brommer — University of Warwick, Coventry, United Kingdom

The extraordinary strength exhibited by Ni-based superalloys at high temperatures is attributed to the presence of nanoscale precipitates in their microstructure, which hinder dislocation motion. In our work, we study edge dislocation-precipitate interactions using Molecular Dynamics (MD) simulations with classical effective potentials. The motion of a pair of edge dislocations moving under shear between pure Face-Centred Cubic (FCC) Ni into Ni3Al with an L12 structure is simulated using MD, where Ni is used to represent an idealised γ solid solution phase and Ni3Al for the γ' precipitate phase. The obtained trajectories are parameterised and Differential Evolution Monte Carlo (DE-MC) is used to determine parameter distributions. These distributions are then used to quantify the uncertainty in the model outputs, namely the dislocations' positions and velocities. The present approach yields physically meaningful parameters and accordingly, offers a means of extracting quantitative information from the atomistic scale that can be used to inform larger length scale simulations of dislocations. Using DE-MC as a sampling approach also means that parameter uncertainties can be propagated through a hierarchy of multiscale models. We illustrate how such uncertainty propagation can be achieved by considering a dislocation mobility law with quantified uncertainties.

MM 28.2 Thu 10:30 H23

Atomistic Modelling of Solid Solution Strengthening in the Mg-Al-Ca System — •Erik Bitzek and Marvin Poul — MPI SusMat, Düsseldorf, Germany

Solid solution strengthening is one of the most important strengthening mechanisms for engineering alloys. It is caused by solutes impeding the glide of dislocations and is therefore best studied using atomistic simulations. While the interaction strength of individual solute atoms with dislocations in Mg has been well-studied with density functional density (DFT) calculations, the combined impact of multiple solute species on dislocation glide has not been extensively investigated. Furthermore, the prediction of the critical resolved shear stress requires additionally a statistical treatment and a continuum elastic model for the dislocation line.

Here we present atomistic simulations of basal dislocations gliding in Mg with different concentrations of Al, Ca, and mixtures of Al and Ca. These large-scale simulations were enabled by a newly-developed machine learning interatomic potential that allows for near-DFT accuracy. Using MD/MC simulations of different heat treatments, we show that Al-Ca clusters can form, which influence the solid solution strengthening by reducing the concentrations of individual solutes and through an antagonistic effect of Al and Ca on the stress field of these clusters.

MM 28.3 Thu 10:45 H23

Normal stress effect on the slip system of Mg alloys with long-period stacking ordered structures — •Naoki Uemura[1] and Ryosuke Matsumoto[2] — [1]Nagamori Institute of Actuators, Kyoto University of Advanced Science, Kyoto, Japan — [2]Department of Mechanical and Electrical Systems Engineering, Faculty of Engineering, Kyoto University of Advanced Science, Kyoto, Japan

Mg alloys with long-period stacking, which have a unique structure with synchronized concentration modulation and structural modulation are attracting attention for their high strength. Various studies are currently being conducted to understand their high mechanical properties and plastic deformation behaviors. We investigated the tensile and compressive dependence of the stacking fault energy (SFE) by using first-principles calculations for the Mg-Y-Zn system, which is a typical LPSO-Mg alloy. As with hcp-Mg, the change in SFE due to tensile and compressive loading was greater on the basal plane than on the prismatic plane. This work was supported by JST, CREST Grant Number JPMJCR2094, Japan.

MM 28.4 Thu 11:00 H23

Understanding crystal defects mechanisms with atomistic simulations and knowledge engineering — •Abril Azocar Guzman, Guojing Huang, and Stefan Sandfeld — Institute for Advanced Simulations, Materials Data Science and Informatics (IAS-9), Forschungszentrum Jülich GmbH, Aachen, Germany

Crystallographic defects play a key role for determining the physical properties of materials. Computational methods, such as density functional theory and molecular dynamics, have been widely used to investigate these defects and their mechanisms at the atomic scale. However, the application of these methods require increasingly complex workflows. To enable workflow and data reusability, as well as meaningful interpretation, it is crucial to ensure well-described (meta)data at each step of the workflow, from atomic structure to computed material properties. Our aim is to facilitate data-driven approaches in materials science by establishing semantic standards for representing material structures, including defects, simulation workflows, and calculated properties. Using this framework, datasets of crystal defects simulations can be generated in the form of a materials knowledge graph. We showcase the application for the study of hydrogen segregation at grain boundaries in iron and nickel, quantifying the influence of the local atomic environment on the energetics of the system. The resulting knowledge graph incorporates structure-property relationships and serves as a tool to understand defect mechanisms at the atomic scale. Additionally, it provides a robust data foundation for exploring the potential of emerging methods in the field of knowledge engineering.

MM 28.5 Thu 11:15 H23

Effect of Cold Work on the Microstructure and Properties of Hierarchical Nanoporous Metals — •Weiche Chang[1] and Shan Shi[2,1] — [1]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany — [2]Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technology, Hamburg, Germany,

Nanoporous metals with bicontinuous porous network, high specific surface area, and low density have shown promising applications as light-weight structural materials and high-performance functional materials in actuators, sensors, and various energy devices. Recently, monolithic hierarchical nanoporous gold (HNPG) has been tailor-made via a two-step dealloying method and has shown improved mechanical properties and much lower density than non-hierarchical nanoporous gold. The effects of ligament size and structural hierarchy on the strength of HNPG have also been well studied via macro- or micro-compression approaches. In this work, we further explore the role of cold working treatments before and after second step dealloying on the mechanical properties of HNPG using micropillar compression tests. Furthermore, HNPG with a controllable degree of anisotropy and a much wider range of solid fractions are obtained.