MM 42: Mechanical Properties I

Time: Wednesday 15:45–18:00 Location: TC 010

MM 42.1 Wed 15:45 TC 010

A first principles investigation of zinc induced embrittlement at grain boundaries in bcc iron — •Mira Todorova[1], Klaus-Dieter Bauer[2], Kurt Hingerl[2], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf, Germany — [2]Zentrum für Oberflächen- und Nanoanalytic, Universität Linz, Altenberger Str. 69, 4040 Linz, Austria

Using density-functional theory calculations we study the embrittling behaviour of liquid Zn in the $\Sigma3[111]60°$ and the $\Sigma5[100]36.8°$ symmetric tilt grain boundaries in bcc iron (ferrite). Investigating Zn induced changes in the energetics of the grain boundaries and their associated free surfaces we utilise both the canonical Griffith model and the grand canonical Rice-Wang formulation to evaluate the difference between the calculated grain boundary energies and the surface energies of their corresponding surfaces. We find that Zn wetting can reduce the cohesive strength of the interface by up to 40% and that the critical nominal bulk Zn concentration at which grain boundary weakening starts is almost two orders of magnitude lower in a grand-canonical model compared to the canonical case. The obtained results will be critically reviewed and discussed in the context of the embrittling behaviour of liquid zinc.

K.-D. Bauer, M. Todorova, K. Hingerl and J. Neugebauer, Acta Materialia (submitted).

MM 42.2 Wed 16:00 TC 010

Absorption of dislocations in grain boundaries: atomic scale information for mesoscale models — •Julien Guénolé, Aruna Prakash, and Erik Bitzek — Department of Materials Science an Engineering, Institute I, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen, Germany

Dislocation-grain boundary (GB) interactions play an important role in the plastic deformation of polycrystalline materials, in particular for nanocrystalline metals. Advanced models for the mechanical behavior of nanocrystalline metals therefore need to take GBs explicitly into account. Several approaches to include GBs into mesoscale models (dislocation dynamics, strain gradient plasticity models, ...) were recently suggested. Such GB models need information, like the conditions for dislocation absorption, the change of dislocation stress fields after absorption, or on how much dislocation content can be absorbed. Atomistic simulations are uniquely positioned to provide such information and advance our understanding on dislocation-GB interactions.

Here we present results of carefully controlled studies of dislocations interacting with GBs in model bicrystalline samples. The mechanisms during dislocation-GB interaction are studied in quasi-2D and fully 3D samples. The stress and energetic signatures of the absorbed dislocations are analyzed and a novel approach to model the effect of the dislocation absorption on the dislocation stress field is proposed. A primary aim of the current study is to provide a better understanding of the role of absorbed dislocation content in the GB on the pinning and nucleation of other dislocations.

MM 42.3 Wed 16:15 TC 010

Atomistic Simulations of Dislocation-Interface Interactions in the γ/γ' Microstructure in Ni-base Superalloys — •Aruna Prakash, Julien Guénolé, Juan Wang, and Erik Bitzek — Materials Science and Engineering, Institute I, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen, Germany

Single crystal Ni-base superalloys are characterized by an ordered $L1_2$ γ'-phase (comprising mostly of Ni_3Al) that precipitates as cuboidal particles in the face centered cubic (fcc) γ-channels comprising mainly of Ni. The interaction of dislocations in the channels with γ' precipitates plays an important role for the high-temperature mechanical properties of Ni-base superalloys. To date, most atomistic simulations concerning dislocation interface interactions in such materials have been performed with simplistic quasi-2D geometries. Here we report on simulations performed with a full 3D setup obtained by a novel approach that facilitates the reconstruction of experimental microstructures obtained from atom probe tomography. The reconstructed sample allows us to study the interaction of the relevant dislocations (screw and 60 degree) with a realistic curved interphase boundary, both in samples with ideal stoichiometric chemical composition and with concentration gradients of specific atoms. Static calculations as well as molecular dynamic calculations were performed to determine the interaction of the channel dislocations with the misfit dislocation network. The results of the simulations with the above setup are compared with those from a canonical quasi 2D approach and a 3D model and are discussed in the framework of a multiscale approach.

MM 42.4 Wed 16:30 TC 010

Modeling nanoporous gold: on the influence of nodal shifting and ligament size distribution — •Bao-Nam D. Ngô[1,2], Alexander Stukowski[2], Jürgen Markmann[1,3], Karsten Albe[2], and Jörg Weissmüller[1,3] — [1]Institut für Werkstoffforschung, Werkstoffmechanik, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — [2]Technische Universität Darmstadt, Fachbereich Material- und Geowissenschaften, Fachgebiet Materialmodellierung, Darmstadt, Germany — [3]Institut für Werkstoffphysik und Werkstofftechnologie, Technische Universität Hamburg-Harburg, Hamburg, Germany

We present a study of the influence of topology on mechanical behavior of nanoporous gold – a promising material for applications in actuation, catalysis and sensing, as well as a model candidate for study of plasticity at nanoscale. Using molecular dynamics, two topological descriptors were investigated: nodal shifting and ligament diameter distribution. For that purpose, we first studied a highly symmetric diamond-like structure – an idealized structure proposed recently by Finite Element Modeling. Then we gradually altered the topology of this symmetric structure in two different directions: randomly displacing its nodal positions and changing its ligament diameter distribution. Relevant mechanical properties investigated include macroscopic stress-strain behavior, deformation-induced structural changes, evolution of effective Young's modulus, and evolution of defect densities. Our results show that both topological descriptors are important and strongly affect the mechanical properties of nanoporous gold.

15 min. break

MM 42.5 Wed 17:00 TC 010

Refined statistical work hardening and recovery model for Aluminium alloys — •Volker Mohles[1], Volker Pankoke[1], Philipp Schumacher[2], and Benjamin Milkereit[2] — [1]RWTH Aachen University, Institute of Physical Metallurgy and Metal Physics, Aachen, Germany — [2]University of Rostock, Chair of Materials Science, Rostock, Germany

A new statistical work hardening and recovery model for aluminium alloys called 4IVM (4 Internal Variables Model) has been developed. Like its established predecessor (3IVM+) it calculates the evolution of dislocation densities during plastic deformation and derives the corresponding flow curves in a wide range of temperatures and strain rates. In order to improve the physical basis and its applicability, the new model considers four densities of dislocations as material state variables: mobile dislocations (ρ_{mob}), dipole dislocations (ρ_{dip}), locked dislocations (ρ_{lock}), and subgrain boundary dislocations (ρ_{sub}). These dislocation types have distinctly different properties, in reality and in the model, with respect to generation, annihilation, direct impact on the flow stress, and the overall dislocation density evolution. Moreover their cores and strain fields differ. In future this allows to introduce specific dependencies on segregation by foreign solved atoms. The new model is validated by comparing simulated flow curves to measured ones. For this, binary Al-Si alloys have been prepared and compression tested in varying precipitation states. Compared to its predecessor, 4IVM offers improved flow curve predictions.

MM 42.6 Wed 17:15 TC 010

Work hardening of Cu based conductors by deformation under cryogenic conditions — •Jens Freudenberger[1], Felix Thiel[1,2], Alexander Kauffmann[1,3], and David Rafaja[2] — [1]IFW Dresden — [2]TU Bergakademie Freiberg — [3]KIT

Cu-Ag-Zr alloys show a beneficial combination of high mechanical strength and good electrical conductivity making these materials suitable for a variety of applications, which strongly rely on this combination of properties. The mechanical as well as electrical properties of Cu-Ag-Zr alloys are strictly related to their microstructure, which can be adjusted by manufacturing processes. This study shows the effect

of cryogenic wire drawing of dynamically recrystallized Cu-Ag7-Zr0.3 alloys on its microstructure in comparison to material which has been deformed at room temperature. The different microstructural features such as grain size, dislocation density as well as precipitate size and their morphology were assessed. In addition, the formation of mechanical twins during cryogenic deformation is reflected. The mechanical and electrical properties of the alloy are explained upon the observed microstructure.

MM 42.7 Wed 17:30 TC 010

Deformation mechanisms of nano-twinned Ag wires and Cu — •Aaron Kobler[1,2], Thorsten Beuth[1], Markus Moosmann[1], Thomas Schimmel[1], Horst Hahn[1,2], and christian Kübel[1,3] — [1]Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — [2]Technische Universität Darmstadt (TUD), Jovanka-Bontschits-Straße 2, 64287 Darmstadt, Germany — [3]Karlsruhe Nano Micro Facility (KNMF), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Introducing nanotwins into the material is one possible approach to increase ductility and achieve high strength. However, the deformation mechanisms that govern the high strength and high ductility are still unresolved as twin boundaries can act as both barriers and sources for dislocations. For the materials strength, twin boundaries play a similar role as grain boundaries in ufg and nc metals, i.e. decreasing the twin spacing generally results in increased strength. We present Ag nanowires with twin planes parallel to the <112> wire axis. Using indentation experiments, we investigated the deformation mechanisms of individual nanowires. Further, we present in-situ tensile tests inside the TEM in combination with orientation mapping of nanotwinned Cu. In both cases we see a clear orientation dependent plastic deformation that we will analyze with respect to the underlying mechanisms.

MM 42.8 Wed 17:45 TC 010

Influence of alloying elements on the fracture strength of iron — •Sankari Sampath and Rebecca Janisch — ICAMS, Ruhr Universität Bochum, 44780 Bochum

Studying crack nucleation is the first step of understanding the fracture behavior of a material. With ab-initio density-functional theory calculations of fracture strength we identify possible nucleation sites for brittle cracks. In ferritic iron potential candidates are the well known {001} cleavage planes as well as different interfaces in the microstructure. The strength of both can change considerably with impurity or alloying element content, in our case silicon and carbon. Detailed studies on the strengthening effect of C on the interface structures and the embrittling nature of Si at the grain boundaries are available. In this work, the co-doping effects of both Si and C are of special interest. To identify the weakest type of interface or cleavage plane, and to investigate the influence of alloying elements on its strength, different model structures were created. The energy of formation of interstitial C in the single crystal as well as at the interfaces in the presence or absence of Si gives an insight on the expected composition of grain boundaries in Fe-Si-C alloys. The subsequent calculations of fracture strength with one or both type of elements reveal interesting non-linear effects.