MM 41: Computational Materials Modelling VI - Dislocations

Time: Wednesday 11:30–13:00 Location: IFW D

MM 41.1 Wed 11:30 IFW D

Dislocation mediated diffusion mechanisms of carbon in α-iron — •Gh.Ali Nematollahi, Blazej Grabowski, Dierk Raabe, and Jörg Neugebauer — Max-Planck Institut für Eisenforschung, D-40237 Düsseldorf, Germany

Experimental observations have revealed that dislocations can provide "diffusion short circuits", i.e., impurities can use the distorted lattice around dislocations to diffuse faster than in the perfect bulk region. This phenomenon is usually referred to as pipe diffusion. These accelerated diffusion paths help to redistribute impurities faster, especially in heavily deformed materials that contain high dislocation densities. This has important consequences e.g. for carbon redistribution in severely deformed pearlite - a steel with the highest strength among nanostructured materials. In the present study, empirical potentials in conjunction with the nudged elastic band method are used to study carbon diffusion in the vicinity of edge, screw and mixed dislocation in bcc iron. Our results show that there are low carbon diffusion barriers of *0.2 eV (vs. 0.8 eV in bulk) for all three dislocation types. For edge dislocations the results are not fully conclusive as it is technically difficult to stabilize such a dislocation due to the low Peierls barrier. For screw dislocations the low diffusion barrier is perpendicular to the dislocation line prohibiting pipe diffusion. Finally, for mixed dislocations, the low diffusion barrier is parallel with the dislocation line and is the only type that explains the experimentally proposed accelerated short circuit diffusion.

MM 41.2 Wed 11:45 IFW D

Effects of carbon interstitials on Fe dislocation core mobility using atomistic-continuum coupling — •Karthikeyan Chockalingam, Rebecca Janisch, and Alexander Hartmaier — ICAMS, Ruhr-Universität Bochum, Universitätsstr. 150, Bochum, Nordrhein-Westfalen 44801

Besides iron, carbon is the most significant alloying element in steel. It has been observed that carbon segregates to dislocation cores to form so-called Cottrell clouds. This is energetically favorable due to the low solubility of C in the iron matrix and the release of strain at the dislocation core. The carbon clouds pin the dislocations, resulting in an increase in yield strength. To better understand the influence of carbon on dislocation core mobility, its influence on edge and screw dislocation was investigated. We found that the relative increase in critical stress is higher for an edge dislocation than for a screw dislocation.

For this analysis we implemented an atomistic-continuum framework in which the dislocation core is modeled atomistically, and the material away from the dislocation a core is described in a continuum-elasticity finite-element approach. Thus, the atomistic domain is restricted to a small region around the core, resulting in a significant reduction of the number of atoms required to model a dislocation. Initially we use an embedded atom method (EAM) type potential for the interatomic interactions, but the coupled framework is not limited to a particular choice of interaction and can also be used in combination with ab-initio methods.

MM 41.3 Wed 12:00 IFW D

Understanding H-embrittlement on the atomic scale: Multiscale modeling of homogenous dislocation nucleation — •Gerard Leyson, Blazej Grabowski, and Jörg Neugebauer — Max-Planck-Straße 1, 40237 Düsseldorf, Germany

Hydrogen enhanced local plasticity (HELP) is one of the proposed mechanisms by which hydrogen induces embrittlement in metals. A promising methodology to explore the HELP mechanism is through nano-indentation experiments, wherein the effect of hydrogen on the pop-in load is precisely measured. Using the Ni-H system as a model system, an analytic model is developed to quantify the effect of hydrogen on the Homogenous Dislocation Nucleation (HDN) assumed to be responsible for the reduction of the pop-in load. The model takes atomisitic inputs, such as hydrogen-hydrogen interaction and the effect of realistic dislocation cores, into account. The hydrogen binding energy and the local hydrogen concentration were calculated self-consistently. Unlike previous analyses, the model takes into account the complex nature of the dislocation field around the loops, as well as the discrete nature of the atomic lattice. In doing so, it addresses some shortcomings of previous models stemming from the continuum description of the dislocation line energy and the interaction of the dislocation with the external stress field. The onset of HDN as a function of bulk hydrogen concentration and temperature was quantified. Our results show that about 10-100 H atoms are sufficient to stabilize a dislocation loop in the presence of realistic shear stresses and allows for a quantitative description of the experimentally observed pop-in effects.

MM 41.4 Wed 12:15 IFW D

Metadislocation core structure in the ε-Al-Pd-Mn phases — Benjamin Frigan and •Hans-Rainer Trebin — Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany

In the past we have energy optimized the bulk structures of the ε-phases and the 16 Å decagonal phase of Al-Pd-Mn using density functional theory (DFT) and classical molecular dynamics. All phases consist of columns of pseudo-Mackay icosahedra (PMI) whose projections form tilings of hexagons, pentagons and nonagons in the ε-phases and several other tiles in the decagonal phase.

Most parts of the metadislocation cores in the ε-phases display the same cluster arrangements as in the bulk phases. Nevertheless, in small sections of the cores the usual cluster description fails. Recent microscopy images indicate that the central parts contain $1/\tau$ shorter PMI-PMI next-neighbor distances. The structure of these novel cluster intersections has been resolved with DFT calculations using the smallest possible approximant which contains such interpenetrating PMI clusters.

We present a full structure description of the metadislocation cores F_3 and F_5. Embedded in bulk structures of ε-phases the cores have been relaxed using a combination of classical molecular dynamics and a Monte Carlo method where the chemical species were randomly flipped.

MM 41.5 Wed 12:30 IFW D

Dislocation – grain boundary interactions in aluminum: insights from atomistic simulations on bi-crystalline and nanocrystalline samples — •Julien Guénolé, Aruna Prakash, and Erik Bitzek — Department of Materials Science and Engineering, Institute I: General Materials Properties, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen, Germany

The interactions between dislocations and grain boundaries (GB) are a dominating factor in the plasticity of nanocrystalline metals. Atomistic simulations have played a key role in improving our understanding of the atomic scale processes that govern dislocation–GB interactions. However, most studies so far have been performed on either quasi-2D bicrystal set-ups with straight dislocation lines or on unrealistic nanocrystalline samples generated by Voronoi tessaltation. In both cases, the dislocations interact with planar GBs.

Here, we present results of controlled studies on dislocations interacting with GBs in model bi-crystalline samples as well as in more realistic nanocrystalline samples. The deposition process of curved dislocations is compared to the absorption of straight dislocations in a quasi-2D set-up. In addition, the stress-signature of the absorbed dislocation is analyzed. The results are compared with the absorption and pinning of dislocations at curved and planar GBs in nanocrystalline samples with controlled GB network topology. 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 41.6 Wed 12:45 IFW D

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

Single crystalline Ni-base superalloys are key materials for turbine blades in modern gas turbines. The microstructure of these alloys consist of cubic γ' precipitates of Ni_3Al in the $L1_2$ crystal structure embedded in a γ-matrix of fcc Ni. The interaction of dislocations in the γ channels with the γ' precipitates is a main factor for the superior strength of these alloys even at high temperatures. The cutting of the dislocations from the γ channels into the precipitates is governed

by processes at the atomic scale. However, only few atomistic simulations of the dislocation behavior at the γ/γ'- interface have so far been performed. Here we report on a detailed study of screw and 60° dislocations interacting with a planar γ/γ'-interphase boundary in a quasi-two dimensional set-up. Static calculations as well as molecular dynamic calculations were performed to determine the critical penetration stress and to study the interaction of the channel dislocations with the misfit dislocation network. In addition, the interaction of dislocations with a curved interphase boundary was studied in a fully 3D set-up modeling an experimental microstructure obtained by 3D Atom Probe Tomography. The results of the simulations are discussed in the framework of a multiscale modeling approach to study the mechanical behavior and stability of Ni-based superalloys.