MM 49: Computational Materials Modelling VII - Grain boundaries & Interfaces

Time: Thursday 10:15–11:45 Location: IFW D

MM 49.1 Thu 10:15 IFW D

Theoretical study of hydrogen trapping and diffusion at grain boundaries in nickel — •Davide Di Stefano[1], Matous Mrovec[1,2], and Christian Elsaesser[1,2] — [1]Fraunhofer IWM, Freiburg, Germany — [2]Karlsruhe Institute of Technology, Karlsruhe, Germany

A correct description of hydrogen diffusion in metals is a prerequisite for understanding the phenomenon of hydrogen embrittlement. It is known that H mobility in metals is strongly affected by lattice defects such as vacancies, dislocations or grain boundaries. It is however rather difficult to investigate local diffusion and trapping of H at these nanoscale defects by experimental means.

In this theoretical study, we explore the interaction of H with several grain boundaries (GBs) in Ni at the atomic scale using first principles calculations based on density functional theory (DFT). Our results are that GBs with open structural units act as trapping sites for H and provide also easy diffusion pathways for H. In contrast, GBs with close-packed structures similar to that of bulk fcc Ni do not trap H but act instead as barriers for H. In order to obtain information about H diffusion on long time and length scales, we developed a kinetic Monte Carlo model that can utilize the DFT results to calculate effective diffusion coefficients of polycrystalline microstructure.

MM 49.2 Thu 10:30 IFW D

Ab-initio study of hydrogen trapping by kappa-carbides in an austenitic Fe matrix — •Poulumi Dey[1], Roman Nazarov[2], Tilmann Hickel[1], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany — [2]Lawrence Livermore National Laboratory 7000 East Avenue, Livermore, CA 94550

Experimental studies demonstrated that fine dispersed precipitates of carbides increase the tensile strength of steels and may act as deep trapping sites for hydrogen. In this regard, homogeneously distributed nano-sized kappa-carbides (Fe,Mn)3AlC, have been found to play an analogous role in a new class of high strength Fe-Mn-Al-C steels. However, much less is known about the efficiency of these carbides in trapping hydrogen in these steels. We thus perform a quantitative analysis of hydrogen solution enthalpies within kappa-carbide precipitates employing density functional theory (DFT). While the solubility of hydrogen is low in perfect kappa-carbide, the presence of hydrogen makes the formation of vacancies energetically favourable, which inturn act as effective trapping sites for hydrogen. Further, motivated by the experimental investigations, we investigate the trapping of hydrogen at the interface between kappa-carbide and the austenitic matrix. Our results show that the interface is a potential trapping site for hydrogen and also a nucleation point for subsequent fracture in the material.

MM 49.3 Thu 10:45 IFW D

Ab-initio prediction of the critical thickness of a precipitate in molybdenum — •Sankari Sampath and Rebecca Janisch — ICAMS, RUB, Bochum, Germany

The precipitation of new phases in a host metal or metallic alloy has a strong influence on the mechanical properties of the material. This precipitation leads to the formation of an interface that can be coherent, semi-coherent or incoherent with the host material. The calculation of coherent interface energies based on atomistic models is well established, but semi-coherent interfaces still present a challenge. Current approaches usually combine ab-initio data and continuum elasticity methods, while we now present a model for a semi-coherent interface completely based on ab-initio density functional theory calculations.

Our example is a metastable Mo-C phase, the body-centered tetragonal structure, which exists as a semi-coherent precipitate in body-centered cubic molybdenum. For the coherent interface, a standard supercell approach is used. The energy of the semi-coherent interface is calculated taking into account different contributions from the elastic strain energy stored in the precipitate, the misfit energy due to the misfit dislocation, and the chemical energy due to the bonding at the interface. By comparing the energy of a coherent with that of a semi-coherent precipitate as a function of thickness, we predict a critical thickness of the precipitate before it becomes semi-coherent that agrees well with the experimental observation.

MM 49.4 Thu 11:00 IFW D

Hot or cold: A guide on how to determine an optimal simulation temperature in the Potts model for normal grain growth — •Dana Zöllner — Institut für Experimentelle Physik, Otto-von-Guericke- Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

The simulation temperature in the Monte Carlo Potts model of grain growth is not correlated to any real experimental temperature and has originally been introduced into the simulation purely to activate thermal fluctuations that roughen the grain boundaries and prevent an unphysical lattice effect - namely the pinning of grain boundaries and their junctions to the underlying lattice.

In the present work it is shown that in the Monte Carlo Potts model there is for a given implementation of the simulation algorithm and a given set of lattice parameters a one-to-one correspondence between the simulation parameters γ and m representing the specific grain boundary energy and mobility in the simulation algorithm and the phenomenological parameters in the equation of motion only for one certain simulation temperature, T_opt. In particular, it is discovered that only the use of T_opt reproduces the curvature driven kinetics of normal grain growth, e.g., the von Neumann-Mullins-relation, correctly.

MM 49.5 Thu 11:15 IFW D

Atomistic simulation of a severe plastic deformation-induced "high-energy" state of grain boundaries — •Lisa Neier[1], Sergiy Divinski[1], Anantha Padmanabhan[2], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Westfälische-Wilhelms-Universität, 48149 Münster — [2]University of Hyderabad, India

A comparison of microstructures and properties in materials subjected to the later stages of severe plastic deformation or steady-state superplastic flow indicates several unexpected similarities especially with respect to the interface response on the deformation, such as grain boundary (GB) sliding events, which lead to a suppression of dislocation activity. Making use of this idea, we propose to describe the experimentally observed "high-energy" (or "non-equilibrium") state of general high-angle GBs in SPD-processed materials in terms of the concept of shear localization in the interfaces and choosing oblate spheroids of a few atomic diameters size as the basic units of sliding. Atomistic simulations of these special GBs are performed. The coupling of grain boundary motion in normal direction to a shear deformation parallel to the grain boundary plane is investigated for these special grain boundaries in comparison to those of different relaxed high angle grain boundaries. Furthermore thermal equilibrium fluctuations of the grain boundaries during the MD simulations are used to calculate the grain boundary stiffness and analyze the influence of grain boundary structure and shear localization on the fluctuation spectrum.

MM 49.6 Thu 11:30 IFW D

Driving force and temperature dependence of grain boundary motion — •Christian Brandl[1], Danny Perez[2], Timothy C. Germann[2], and Oliver Kraft[1] — [1]Karlsruhe Institute of Technology, Institute of Applied Materials, Karlsruhe, Germany — [2]Los Alamos National Laboratory, Theoretical Division, Los Alamos, USA

The motion of interfaces - in particular grain boundaries (GBs) - is a fundamental mechanism of microstructure formation at high temperature and long time scales (annealing, coarsening). Moreover GB motion is also shown to be a deformation mechanism occurring at high stresses and relative low temperatures as in deformation studies of nanocrystalline metals and shock loading. Using MD simulations and transition search methods (string method), we report on the interface motion of an asymmetric GB in Cu to elucidate the role of atomistic structure (morphology) and velocity-driving force relation (mobility) as function of temperature. We show that the GB velocity as a function of temperature and driving-force shows distinct regimes of dynamics regimes ranging from pinning-depinning transition at low temperature, through rare-event dynamics of critical kink-pair disconnection nucleation along intrinsic GB dislocations to approximate temperature independent GB velocities. We will discuss the observation in the context of necessary ingredients for a mesoscale model of interface motion, which incorporates the atomic scale interface structure and the different regimes of driving-force and temperature.