MM 30: Topical Session: Fundamentals of Fracture - Modelling Intergranular Fracture

Time: Wednesday 10:15–11:30 Location: H4

MM 30.1 Wed 10:15 H4

Ideal strength of grain boundaries in nickel with segregated sp-impurities — Miroslav Černý[1,2], •Petr Šesták[1,2], Petr Řehák[1,2], Mojmír Šob[1,3], and Monika Všianská[1,3] — [1]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [2]Faculty od Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — [3]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic

Grain boundaries (GB) represent extended planar defects with crucial effect on macroscopic strength of polycrystalline materials. In this first-principles study, we calculate the ideal tensile strength of Σ5(210) tilt GB in nickel under uniaxial loading perpendicular to the GB plane. A computational supercell containing 64 atoms is continually relaxed during the loading. Tensile strength of GB with segregated impurities (S and Al) is compared with that of the clean GB and with the results of previous studies. Differences in computed values demonstrate both the effect of impurities on the ideal strength and the importance of full lattice optimization during the simulation of tensile test.

MM 30.2 Wed 10:30 H4

Structure and stability of vacancies and Cr atoms at Fe Σ5 (210) grain boundary — •Tomasz Ossowski[1], Jan Kuriplach[2], Evgeny Zhurkin[3], Marc Hou[4], and Adam Kiejna[1] — [1]Institute of Experimental Physics, University of Wrocław, Poland — [2]Department of Low Temperature Physics, Charles University, Prague, Czech Republic — [3]Experimental Nuclear Physics Department, Saint-Petersburg State Polytechnical University, Russia — [4]Physique des Solides Irradiés et des Nanostrucutres CP234, Université Libre de Bruxelles, Belgium

The high-chromium ferritic/martensitic steels are promising materials for advanced reactors. They display high resistance to irradiation induced effects. On the other hand, Fe-Cr alloys serve as a model system to understand microscopic mechanism behind various processes occurring in real materials. One of such processes is the segregation/depletion of vacancies or Cr atoms at grain boundaries (GBs). In this contribution the density functional theory (DFT) and molecular dynamics (MD) results of vacancies and Cr atoms stability at the Fe Σ5(210) GB are presented. Using MD quenching at zero temperature we investigate possible structural modifications of this GB. We found different configurations of the GB and their energies. For these purposes, the state-of-the-art interatomic potentials were utilized. Configurations from MD were then relaxed by means of the DFT to confirm their stability. The most stable one was employed to investigate the Cr atoms and vacancies at the GB under consideration in order to have a first idea which sites attract or repel Cr atoms and vacancies.

MM 30.3 Wed 10:45 H4

Computational study of the intergranular fracture strength of transition metals in the presence of impurity atoms — •Arshad Tahir, Venkata Naga Sudheer Ganisetti, Rebecca Janisch, and Alexander Hartmaier — ICAMS, Ruhr University Bochum, Germany

Grain boundaries play an important role during plastic deformation and failure of poly-crystals. In case of the refractory metals e.g. molybdenum and tungsten which are the materials of interest in high-temperature applications, the reduction of strength due to grain boundary embrittlement is especially large. The presence of defects e.g. point defects at the grain boundaries affect their mechanical properties, which in turn alter the hardness or fracture toughness of poly-crystals favorably or adversely. Carbon as a point defect has been reported to increase the strength of bcc metals whereas hydrogen and oxygen are assumed to be detrimental for grain boundary strength. In order to investigate the strengthening and em-brittling nature of above mentioned impurity atoms at grain boundaries, a systematic study of a Σ 5 (310)[001] symmetrical tilt grain boundary (Σ5 STGB) in molybdenum, tungsten and iron has been carried out. Atomistic scale uni-axial mechanical tests with loads perpendicular to the grain boundary were performed for all the afore mentioned systems using ab-initio density functional theory calculations. From these results, traction separation data has been derived that is being used for the parameterization of cohesive zone model to predict the inter-granular fracture at continuum level using finite element analysis.

MM 30.4 Wed 11:00 H4

A Finite Element Analysis of the Fracture Behavior of Tungsten at the micro scale — •Christoph Bohnert[1,2], Nicola Julia Schmitt[2], Sabine Maria Weygand[1], and Oliver Kraft[2] — [1]Karlsruhe University of Applied Sciences, Department of Mechanical Engineering and Mechatronics, D-76133 Karlsruhe, Germany — [2]Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM), D-76344 Eggenstein-Leopoldshafen, Germany

Due to its high melting point tungsten has the potential to be used as a structural material in future energy applications. However, one of the challenges is to deal with the brittleness at room temperature, where the fracture behavior of polycrystalline tungsten is strongly influenced by the grain structure and texture as well as sample dimensions. The aim of the present work is to numerically analyze crack initiation and growth in single crystal tungsten microbeams and to relate it to corresponding experimental observations.

A finite element model was developed to study the fracture behavior of the cantilever at different crack orientations. As plastic deformation is observed at the crack tip, plastic deformation is implemented using a crystal plasticity approach which allows for specifying the crystal orientation. Crack initiation and growth are treated by using the cohesive zone method. Based on experimental oberservations, the material parameters are estimated, and the fracture model has been applied to simulate microbending tests. The simulations allow for comparison of the computed with the measured load displacement curves as well as details of the fracture process, ultimately at various length scales.

MM 30.5 Wed 11:15 H4

A high-resolution look at crack tip deformation — •Christoph Kords[1], Philip Eisenlohr[1], Arshad Tahir[2], Rebecca Janisch[2], and Franz Roters[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf, Germany — [2]ICAMS, Ruhr-University Bochum, 44780 Bochum, Germany

The deformation behavior around a pre-existing intergranular crack is simulated in a two-dimensional setting for a grain boundary in bcc Mo. The associated boundary value problem is solved at very high spatial resolution (millions of pixels) by means of a recently implemented spectral method based on fast Fourier transforms. The cohesive properties of the grain boundary are derived from ab-inito density functional theory calculations. Our interest focuses on the conditions under which the theoretical interface strength obtained from such atomistic calculations will be locally reached in the mesoscale simulation when dislocation-mediated crack tip plasticity is included. In this study we will investigate the influence of spatial resolution on the one hand and of the physical rigorousness of the crystal plasticity description on the other hand. To the latter end, three different crystal plasticity models are to be compared: a frequently employed (standard) power-law dislocation kinetics coupled with a phenomenological hardening description; a dislocation mechanics-based description considering dislocation densities and their reactions; and finally the same (second) model but with additional integration of the dislocation transport that is always associated with plasticity.