MM 26: Computational Materials Modelling V - Fracture and Other Failure Mechanisms

Time: Tuesday 12:00–13:00 Location: TC 006

MM 26.1 Tue 12:00 TC 006

First principles study of brittle cleavage processes in FeTi — •Li-Fang Zhu[1], Martin Friák[1], Antje Schlieter[2,3], Uta Kühn[2,3], Jürgen Eckert[2,3], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]IFW Dresden, Germany — [3]Dresden University of Technology, Dresden, Germany

Thorough understanding of atomistic mechanisms that are responsible for brittle failure of materials is crucial for many engineering applications. We employ density functional theory calculations to study the brittle cleavage under loading mode I in an important structural intermetallics, FeTi, along [100], [110], [111] and [211] directions. The calculated energy vs. separation curves are found to follow universal binding energy behavior (see e.g. [1]) and allow to determine the corresponding surface energies γ, cleavage energy G_b, and theoretical strength σ_b. Relations between cleavage and elastic properties are explored by applying the generalized Orowan-Gilman model [2]. Our study shows that the brittle loading along the [110] direction has the lowest strain to fail, as well as lowest cleavage energy and theoretical strength. These findings indicate that the preferred fracture occurs in single crystal FeTi along the (110) plane. We also find an onset of magnetism in FeTi when increasing the distance between the cleavage planes and show how it is responsible for termination-specific surface energy reductions.

[1] J. H. Rose, J. R. Smith, J. Ferrante, *Phys. Rev. B* **28** (1983) 1835.
[2] E. Orowan, *Rep. Prog. Phys.* **12** (1949) 185.

MM 26.2 Tue 12:15 TC 006

Atomistic simulations of grain boundary fracture in tungsten bicrystals — •Johannes J. Möller and Erik Bitzek — Lehrstuhl WW1: Allgemeine Werkstoffeigenschaften, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Deutschland

Brittle crack propagation in polycrystals frequently occurs along grain boundaries. Understanding the influence of grain boundary character (misorientation, interface plane, atomic structure) on the fracture behavior is therefore important for modeling fracture of polycrystalline materials. Although atomistic simulations are ideally suited to investigate the details of grain boundary fracture, relatively few systematic simulation studies exist.

Here we present results of atomistic fracture simulations in symmetrical low-Σ tilt grain boundaries in tungsten modeled by the Finnis-Sinclair potential. The fracture behavior (brittle crack advance, dislocation emission, twinning) and the critical stress intensity factors K_{Ic} were determined by molecular statics simulations.

Asymmetrically oriented slip systems lead to different fracture behavior in opposing crystallographic propagation directions. The simulations show that K_{Ic} for brittle fracture along grain boundaries can also dependent on the crack propagation direction and can be larger than the K_{Ic} for brittle fracture in single crystals of the corresponding orientation. The results are discussed in terms of thermodynamic and kinetic aspects, and the concept of grain boundary trapping is introduced. Finally, consequences for mesoscopic models of grain boundary fracture are addressed.

MM 26.3 Tue 12:30 TC 006

Carbon at Σ5 STGB in molybdenum - from ab-initio results to traction-separation law — •Arshad Tahir, Rebecca Janisch, and Alexander Hartmaier — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr University Bochum, Germany

Grain boundaries play an important role during plastic deformation and failure of poly-crystals. The presence of point defects, line defects or segregated second phase particles at the grain boundaries affect their mechanical properties, which in turn alter the hardness or fracture toughness of the poly-crystals favorably or adversely. In case of the bcc transition metals, which are the materials of interest for high temperature applications, grain boundaries and segregated impurities at grain boundaries play a vital role as well. Therefore, a sigma-5 (310)[001] Σ5 STGB present in molybdenum (Mo) has been atomistically investigated and the results are being used for fracture prediction at continuum scale.

The atomistic calculations were performed using the VASP employing GGA to DFT. After the initial convergence tests for the optimization of k-point meshing and energy cut-off of the plane wave basis set, a Σ5 (310)[001] STGB structure was constructed, relaxed and stable translation states along [310], [-130] and [001] were obtained. With this model uni-axial tests loaded perpendicular to the grain boundary plane having different C contents were performed. From these results, traction separation data has been derived that is being used for the parameterization of cohesive zone model to predict fracture of Mo bicrystals at continuum level using finite element analysis.

MM 26.4 Tue 12:45 TC 006

Ab-initio Study on Liquid Metal Embrittlement in the Fe/Zn System — •Klaus-Dieter Bauer[1], Mira Todorova[2], Kurt Hingerl[1], and Jörg Neugebauer[2] — [1]Center for Surface and Nanoanalytics, Johannes Kepler University Linz, Austria — [2]Department for Computational Materials Design, Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

In the manufacturing of high quality steels products, processing steps and costs can be saved by hot-forming (already) coated steel plates. For galvanized sheets however, a degradation of workpieces' quality is observed, caused by *Liquid Metal Embrittlement* (LME) of the steel bulk coming in contact with the liquid zinc phase. To get insight into the mechanism of LME in the Fe/Zn system we perform density-functional-theory calculations, considering the [111]Σ3 and [110]Σ5 tilt grain boundaries in bcc iron (ferrite). Investigating the applicability of the Griffith model, we compare the interface energies of the grain boundaries and associated surfaces for different Zn coverages. Our results show Zn wetting to stabilize the grain boundaries, and even stronger the associated surfaces, yet not sufficiently to cause spontaneous surface formation. This is compatible with the outcome of experiments performed at Voestalpine AG.