MM 9: Topical Session: Fundamentals of Fracture – Interface Fracture

Time: Monday 15:45–18:00 Location: SCH A 216

Topical Talk MM 9.1 Mon 15:45 SCH A 216

Modeling of grain boundary embrittlement phenomena in metallic materials — •Lorenz Romaner[1], Alexander Reichmann[1], Christoph Dösinger[1], Tobias Spitaler[1], Daniel Scheiber[2], Oleg Peil[2], Markus Alfreider[1], Michael Wurmshuber[1], and Daniel Kiener[1] — [1]Department of Materials Science, Montanuniversität Leoben, 8700 Leoben, Austria. — [2]Materials Center Leoben Forschung GmbH, 8700 Leoben Austria.

Intergranular embrittlement phenomena are of strong relevance for many technological materials including steels, nickel-based alloys, coinage metals or refractory metals. The decisive process is grain boundary segregation where solutes diffuse and enrich at grain boundaries thereby modifying their cohesive properties which can favor or impede crack propagation. We present a multi-scale simulation framework for grain boundary segregation employing atomistic, thermokinetic and data-driven computational methods and show how chemistry and propensity against crack propagation can be modeled from basic knowledge of composition and processing parameters. Validation examples with several experimental methods including atom probe tomography, high resolution transmission electron microscopy and micromechanical testing are presented. Furthermore, we discuss the potential of statistical learning methods to replace density functional theory simulations in future, in particular to address advanced phenomena such as concentration dependence and co-segregation.

MM 9.2 Mon 16:15 SCH A 216

Atomistic study of impurity-induced intergranular embrittlement in tungsten — •Pär A. T. Olsson[1,2], Praveenkumar Hiremath[2], and Solveig Melin[2] — [1]Materials Science and Applied Mathematics, Malmö University, SE-205 06 Malmö, Sweden — [2]Division of Mechanics, Materials & Components, Lund University, Box 118, SE-221 00 Lund, Sweden

In the present work we study the impact of phosphorus (P) impurities on the grain boundary strength of tungsten (W) by means of classical atomistic modelling to explore the role of impurities on the grain boundary (GB) embrittlement of W. To this end, we have fitted a new binary 2NN-MEAM potential for the W-P system that is designed to capture the embritteling potency of P in W GBs as predicted by means of density functional theory (DFT) modelling. Analysis of the GB work of separation and generalized stacking fault energy data derived from DFT and the 2NN-MEAM potential show that substitutional P-impurities reduce the resistance to both cleavage and slip. Mode I tensile and crack simulations reveal that the most dominant mode of GB failure is cleavage and that pristine GBs, which are initially ductile, on most accounts change to brittle upon introduction of impurities. Such tendencies are in line with experimentally observed correlations between P-impurity content and reduced ductility.

MM 9.3 Mon 16:30 SCH A 216

Characterization of the stability of metal/metal interfaces by atomistic simulations — •Daniel F. Urban, Reyhaneh Ghassemizadeh, and Christian Elsässer — Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany

The reliable prediction of the adhesion and mechanical stability of interfaces between two metal phases from density functional theory (DFT) calculations remains a challenge. One possible approach to systematically address this issue is an idealized cleavage simulation analysed in terms of the Rose-Ferrante-Smith universal binding energy relationship (UBER) which results in a measure for the ideal work of separation and the maximum tolerable normal strain. Another approach is the study of the gamma surface, i.e. the generalized stacking fault energy, as function of lateral displacement, which yields information on the critical resolved shear stress of dislocation motion. Here we systematically study coherent [111]-oriented interfaces between fcc metals in terms of the above mentioned methods. We analyze the interface energy in terms of coupled tensile and shear displacements which include the effect of the tension softening of the interface. Furthermore, the influence of an additional lateral mechanical strain on the two phases, as often present in experimentally grown thin layers, is examined.

15 min. break

MM 9.4 Mon 17:00 SCH A 216

The heterogeneous nature of grain boundary segregation and embrittlement — •Remi Dingreville — Sandia National Laboratories, Albuquerque NM, USA

Nanostructured materials are inherently unstable due to the high density of non-equilibrium defects that provide a substantial driving force for exaggerated or unexpected evolution. Departing from most mesoscale models for grain boundaries (GB), there is a clear recognition that GB properties, especially GB embrittlement and GB fracture, are not single-valued for a given material, but widely disparate depending on the configuration of the particular boundary and its neighboring grain. Taking this one step further, both GB character and GB defects control the GB embrittlement and fracture in response to mechanical, thermal, and irradiation stimuli. Each different type of stimuli perturb the GB character in distinctly different processes: e.g. stress causes elastic mismatch that tilts the energy barrier whereas strain drives specific dislocation content into the GB; non-implanting irradiation on the other hand creates local thermal spikes and atomic shuffling. In this presentation, I will discuss these effects on GB segregation and GB fracture properties from both a theoretical and atomistic perspectives.

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MM 9.5 Mon 17:15 SCH A 216

Modelling the grain boundary segregation of phosphorus in iron using thermodynamical approaches and Bayesian inference — •Alexander Reichmann[1], Christoph Dösinger[1], Daniel Scheiber[2], Oleg Peil[2], Vsevolod Razumovskiy[2], and Lorenz Romaner[1] — [1]Department of Materials Science, Montanuniversität Leoben, Austria — [2]Materials Center Leoben Forschung GmbH, Leoben, Austria

The chemistry and structure of grain boundaries (GBs) play a key role for understanding fracture in metallic alloys. Atomistic simulations provide a direct access to one of the key fundamental GB characteristics, the GB solute segregation energy. Experimentally, the solute segregation can be evaluated by measuring the GB solute concentration using a variety of techniques, one of which is the Auger electron spectroscopy. However, a direct comparison of experimentally measured GB solute excess and calculated GB segregation energy requires an additional step of conversion, which is a non-trivial task in many cases. As a result, calculated and measured data are not always found in good agreement with each other and often require an in-depth investigation. In this talk, we will present an approach for getting a consistent comparison between the calculated and experimentally measured data based on the Bayesian inference framework, which we use in combination with Markov chain Monte Carlo simulations for uncertainty quantification and model evaluation. We apply this framework to analyze phosphorus segregation in iron and evaluate theoretical and experimental data on GB excess.

MM 9.6 Mon 17:30 SCH A 216

Characterizing interface toughness in functional materials — •Eloho Okotete[1], Subin Lee[1], Steffen Brinckmann[2], and Christoph Kirchlechner[1] — [1]Institute for Applied Materials, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany — [2]Structure and Function of Materials (IEK-2), Forschungszentrum Jülch, 52425 Jülich, Germany

Interfaces are the backbones of functionality in emerging material systems for this new age. However, mechanical failure usually occurs in these interfaces leading to degradation of functional properties. Experimental methods to investigate the interface strength and its failure mechanisms include peel test, super layer test, or indentation test. These methods output qualitative data with huge experimental scatter and a lack of in-depth understanding of underlying mechanisms of failure. Small-scale mechanical testing using single and double cantilever beams makes it possible to extract quantitative data for interface properties of micro/ nanometer-sized films. However, these methods are prone to unstable crack growth, finite notch root radius, and other problems arising from testing geometries. In this talk, we propose a

new micro cantilever design that provides reliable quantitative interface toughness. Our initial finite element calculations showed the optimized geometry could propagate a pre-notch in a stable manner, which is essential to generate a natural crack front without FIB-induced damage/artifacts. This observation is validated with in situ experiments on the interface between a hard coating and silicon substrate.

MM 9.7 Mon 17:45 SCH A 216

Abnormal internal oxidation of grain boundary and its cracking behavior under mechanical stress in an FeCr alloy — •Kuan Ding[1], Xiao Shen[2], Siyuan Zhang[3], Jiejie Li[4], Enrico Bruder[1], Jianjun Li[4], Wenwen Song[2], Karsten Durst[1], James P. Best[3], and Xufei Fang[1] — [1]Department of Materials and Earth Sciences, TU Darmstadt, 64287 Darmstadt, Germany — [2]Steel Institute (IEHK), RWTH Aachen University, 52072 Aachen, Germany — [3]Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany — [4]School of Mechanical and Electrical Engineering, Central South University, 410083 Changsha, China

FeCr-based Ferritic stainless steels display great potential for applications as interconnects of solid oxide fuel cells at temperatures below 800 °C. Cr provides good oxidation resistance by forming a protective oxide layer to prevent the substrate from exposing to corrosive environment. However, grain boundaries (GBs) act as fast diffusion paths, and internal oxidation along the GB can form brittle oxide, which is prone to cracking under mechanical stresses. In this work, we investigated the abnormal growth of GB oxide at 600 °C in air and its impact on GB cracking in Fe-15wt.%Cr alloy. The microstructure and chemical characterization of the abnormal GB oxide revealed a layer of chromium oxide forming with a large penetration depth. To study the mechanical response, we conducted both ex-situ and in-situ micromechanical tests and simulation and observed the cracking behavior of the abnormal GB oxide. Our finding provides insights into improving the oxidation and fracture resistance through material design.