MM 3: Topical session (Symposium MM): Hydrogen in Materials

Hydrogen interactions with defects

Hydrogen in Materials organized by Astrid Pundt (Institute of Materials Physics, U Göttingen, Germany) and Tilmann Hickel (MPI Eisenforschung, Düsseldorf, Germany).

Time: Monday 10:15–13:15 Location: H 0107

Topical Talk MM 3.1 Mon 10:15 H 0107

Effects of hydrogen on plasticity and fracture in iron—atomic level to mesoscale theory — •Anthony Paxton — King's College London, London, UK

The phenomenon of hydrogen embrittlement involves processes at all time and length scales. At the smallest scales it must be recognised that the proton in magnetic α-Fe acts as a quantum particle even at room temperature [1]. It is necessary to take into account proton quantum effects if one is not to make errors of factors of two or three in calculations involving trapping and diffusion problems. On the other hand the frequently discussed concepts of hydrogen induced localized plasticity (HELP) and hydrogen enhanced decohesion (HEDE) can only be discussed meaningfully at the mesoscale level and above. Here I will describe our recent work in which we have used magnetic tight binding [2] and density functional theory results as inputs into calculations of dislocation velocity and cohesive strength as functions of stress, temperature and hydrogen concentration in magnetic iron [3, 4]. I may also speculate on certain paradoxes surrounding the theory of elastic shielding of dislocations by hydrogen and on how hydrogen may act to localise plasticity.

1. A. T. Paxton and I. H. Katzarov, *Acta Mater.*, **103**, 71 (2016)
2. A. T. Paxton and C. Elsässer, *Phys. Rev. B*, **82**, 235125 (2010)
3. I. H. Katzarov, D. L. Pashov and A. T. Paxton, *Phys. Rev. Materials*, **1**, 033602 (2017)
4. I. H. Katzarov, and A. T. Paxton, *Phys. Rev. Materials*, **1**, 033603 (2017)

Topical Talk MM 3.2 Mon 10:45 H 0107

Hydrogen-assisted failure in Ni-based superalloy 718 studied under in situ hydrogen charging: The role of localized deformation in crack propagation — Zahra Tarzimoghadam[1], •Dirk Ponge[1], Jutta Klöwer[2], and Dierk Raabe[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]VDM Metals GmbH, Altena, Germany

We investigated hydrogen embrittlement (HE) of Ni-base superalloy 718 after different heat treatments by slow strain rate tensile testing under continuous electrochemical hydrogen charging. Hydrogen-assisted cracking mechanisms were studied by electron backscatter diffraction (EBSD) analysis and electron channeling contrast imaging (ECCI). Fracture in hydrogen-charged samples was dominated by localized deformation. Non-uniform hydrogen concentrations and plastic instabilities arise at the impingement of slip bands on grain boundaries and at intersecting slip lines. Transgranular cracking was caused by shear localization assisted by hydrogen-enhanced localized plasticity (HELP) along slip planes. Intergranular cracking was due to grain boundary triple junction cracking, slip-localization at grain boundaries, and delta/gamma interface cracking. Observations on the overaged state confirmed that the delta-phase promotes HE by initializing micro-cracks from delta/gamma interfaces. Hydrogen-enhanced strain-induced vacancy (HESIV) mechanism also assisted the ductile intergranular and transgranular fracture. The failure mechanism is explained based on hydrogen-enhanced formation of strain-induced vacancies, nano-void nucleation and coalescence during deformation.

30 min. break

MM 3.3 Mon 11:45 H 0107

Ab-initio study of the role of kappa carbides as potential hydrogen traps in advanced high-strength steels — •Poulumi Dey[1], Tobias A. Timmerscheidt[2], Dimitri Bogdanovski[2], Jörg von Appen[2], Tilmann Hickel[1], Richard Dronskowski[2], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany — [2]Institute of Inorganic Chemistry, RWTH Aachen University, 52056 Aachen, Germany

Hydrogen embrittlement is one of the major challenges for Fe based materials such as high-Mn steels. Addition of Al to high-Mn steels is known to reduce their sensitivity to hydrogen-induced delayed fracture which motivated us to investigate possible trapping effects related to the presence of Al in the grain interior employing density-functional theory (DFT). The role of Al-based kappa carbide precipitates is investigated to understand the relevance of short-range ordering effects. As H tends to occupy the same positions as C in these precipitates, the interaction and competition between both interstitials is studied via DFT-based simulations. Our study reveals that the interstitials tend to increase the lattice parameter leading to a net increase of the trapping capability despite the fact that the individual H-H/C-H chemical interactions are generally repulsive. An increased Mn content is shown to enhance H trapping due to attractive short-range interactions. Another short-range ordering that is favorable for H trapping is found at the interface between an Fe-matrix and the carbide. The study further shows that the trapped H atoms subsequently yield a decohesion at the interface, which may be one reason for the observed failure.

MM 3.4 Mon 12:00 H 0107

Atomistic modelling of hydrogen cosegregation at grain boundaries in iron and nickel — •Eunan J. McEniry, Tilmann Hickel, and Joerg Neugebauer — Department of Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

The behaviour of hydrogen at structural defects in metallic alloys is well-known to play a key role in the mechanical stability of such materials. As a result, the energetics and kinetics of hydrogen in the vicinity of grain and phase boundaries have been extensively studied via atomistic simulation, in order to understand mechanisms of hydrogen-induced decohesion. The emphasis of this work is the critical interplay of hydrogen with additional elements present in the material.

Using atomistic simulations, we have performed high-throughput calculations of the cosegregation behaviour of H, B, C, and N at selected grain boundaries in Fe and Ni. Due to the large number of configurations that must be considered, we have employed tight-binding approaches to enable the efficient and accurate description of the thermodynamics of light element cosegregation. Having obtained segregation profiles at the chosen grain boundaries as a function of bulk concentration and temperature, we employ both thermodynamic analysis as well as simulated mechanical testing to assess the impact of segregants on the structural stability of the grain boundaries.

MM 3.5 Mon 12:15 H 0107

Hydrogen embrittlement of Tungsten induced by Deuterium Plasma: Insights from Nanoindentation Test — •Xufei Fang[1], Arkadi Kreter[2], Marcin Rasinski[2], Christoph Kirchlechner[1], Steffen Brinckmann[1], Christian Linsmeier[2], and Gerhard Dehm[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Structure and Nano-/ Micromechanics of Materials, Max-Planck-Str. 1, 40237 Düsseldorf, Germany — [2]Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung - Plasmaphysik, Partner of the Trilateral Euregio Cluster (TEC), 52425 Jülich, Germany

Hydrogen exposure has been found to result in metal embrittlement. We use nanoindentation experiments to study the mechanical properties of single crystalline and polycrystalline tungsten subjected to deuterium plasma. The results exhibit a decrease in the pop-in load and increase in hardness on exposed tungsten sample due to the presence of deuterium. These findings agree with the defactant theory that explains the decrease of the load required for dislocation nucleation. The hardness increase is also discussed based on the solid solution strengthening effect.

MM 3.6 Mon 12:30 H 0107

Hybrid QM/MM study of the effect of hydrogen on dislocation glide in tungsten — •Petr Grigorev and James Kermode — Warwick Centre for Predictive Modelling, School of Engineering, University of Warwick, Coventry CV4 5AL, United Kingdom

In this study we use a hybrid musltiscale approach, namely quantum mechanics/molecular mechanics (QM/MM) [1], combining an accurate local QM description of the dislocation core atoms with a classi-

cal model for the rest of the system. We apply a recently developed QM/MM implementation of the virtual work principle [2] to compute energy barriers. The effect of H atoms in the material on the dislocation core structure together with the energetics of interaction of H with dislocations are investigated. The obtained results are analysed by comparison with pure DFT studies from literature [3, 4, 5] together with machine learning based Gaussian Approximation Potential (GAP) model [5].

[1] N. Bernstein, J. R. Kermode, and G. Csányi, Rep. Prog. Phys. 72, 026501 (2009). [2] T. Swinburne, J. R. Kermode, Phys. Rev. B. 96, 144102 (2017). [3] L. Dezerald, D. Rodney, E. Clouet, L. Ventelon, F. Willaime, Nat. Commun. 7, 11695 (2016) [4] A. Bakaev, P. Grigorev, D. Terentyev, A. Bakaeva, E. E. Zhurkin, Y. A. Mastrikov, Nucl.Fusion 57, 126040 (2017) [5] W. Slachta, A. Bartók and G. Csányi, Phys. Rev. B. 90, 104108 (2014).

MM 3.7 Mon 12:45 H 0107

DFT study of absorption and migration of hydrogen and oxygen in MAX phases — •Daniel F. Urban[1], Francesco Colonna[2], and Christian Elsässer[1,2] — [1]Fraunhofer IWM, Freiburg, Germany — [2]University of Freiburg, FMF, Germany

MAX phases are ternary metal carbides and nitrides with multi-layered crystal structures and mixed metallic-covalent bonding. They have very good thermal, chemical, and mechanical properties which make them potentially suitable as corrosion protection coatings for high-temperature energy-conversion devices such as solid oxide fuel cells. To assess the capability of MAX phases as diffusion barriers for hydrogen and oxygen, we investigate absorption and migration of H and O atoms in a variety of MAX-phase carbides and nitrides by means of first-principles calculations based on density functional theory. The resulting calculated formation and migration energies indicate that MAX-phase coatings can act as protective diffusion barriers for both hydrogen and oxygen, but with different migration mechanisms [1].

[1] F. Colonna, C. Elsässer, RSC Advances 7, 37852 (2017)

MM 3.8 Mon 13:00 H 0107

New approaches for in-situ nanoindentation of hydrogen charged alloys: insights on bcc FeCr alloys — •Jazmin Duarte Correa, Xufei Fang, Steffen Brinckmann, and Gerhard Dehm — Max-Planck-Institut für Eisenforshung GmbH, 40479 Düsseldorf, Germany

Understanding hydrogen-microstructure interactions in metallic alloys is needed to prevent hydrogen embrittlement. The failure mechanisms that initiate at the atomic scale with hydrogen absorption and interaction with trap binding sites, can be studied independently by nanoindentation; in-situ charging the sample with hydrogen avoids the formation of concentration gradients due to desorption. Two custom electrochemical cells were built for hydrogen charging while nanoindenting the sample: front-side charging with sample and indenter tip immersed into the electrolyte, and back-side charging where the analyzed region is never in contact with the solution. We discuss the advantages and disadvantages of both approaches during the study of the hydrogen effect on homogeneous nucleation of dislocations in bcc FeCr alloys. A reduction in the pop-in load indicating the yield point with the increase of hydrogen content and formation of multiple pop-ins during nanoindentation provided evidence for the decrease in the resolved shear stress and enhanced dislocations nucleation. Although a similar trend is observed for both strategies, a more pronounced effect is noticed by front-side charging, likely due to surface degradation.