MM 5: Hydrogen in Metals: Ab initio approaches

Time: Monday 10:15–11:45 Location: TC 006

Topical Talk MM 5.1 Mon 10:15 TC 006

Atomistic simulations of microstructural defects and their role in H trapping and diffusion — •Matous Mrovec[1], Davide Di Stefano[1], Christian Elsässer[1], Roman Nazarov[2], and Tilmann Hickel[2] — [1]Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany — [2]Max-Planck Institute for Iron Research, Düsseldorf, Germany

A correct description of hydrogen diffusion and trapping is prerequisite for understanding the phenomenon of hydrogen embrittlement. The macroscopic H diffusion in bulk materials has been studied extensively in the past both experimentally and theoretically. Nevertheless, the knowledge of microscopic diffusion processes, especially in distorted environments around crystal defects, is still limited. In this study we apply atomistic simulations to investigate the diffusion and trapping of hydrogen in Fe and Ni using accurate first-principles methods based on the density functional theory. Our results show that the diffusion barriers can indeed vary significantly in the vicinity of crystal defects, imperfections and interfaces. The calculations also confirm that a proper treatment of quantum effects is crucial for a reliable theoretical description of H diffusion, in particular for bcc Fe. Several examples of H trapping at grain and phase boundaries will be presented and analyzed.

MM 5.2 Mon 10:45 TC 006

Hydrogen at the ferrite-cementite and ferrite-austenite interfaces — •Eunan J. McEniry, Tilmann Hickel, and Jörg Neugebauer — Department of Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany

In the present contribution, detailed simulations of the hydrogen behaviour in the vicinity of the ferrite-cementite and ferrite-austenite interfaces have been performed. The effects of hydrogen trapping and diffusion, as well as the interaction of hydrogen with vacancies near the interface, have been studied. To elucidate more clearly the effect of hydrogen on the mechanical properties of the interfaces, a series of simulated tensile tests have been performed, which shed light on specific mechanisms of the hydrogen embrittlement effect.

The results of such simulations can also be used as benchmarks for large-scale atomistic simulations, in particular for the development of potentials based on the tight-binding approximation, so that hydrogen behaviour in the vicinity of extended defects, such as nanovoids and dislocations, can be simulated. The generation of such a model, and initial test calculations based upon it, will be demonstrated.

MM 5.3 Mon 11:00 TC 006

Hydrogen trapping at vacancies and hydrogen impact on vacancy diffusion and self-diffusion in Ni. — Yu Wang[1,2], Damien Connétable[2], and •Döme Tanguy[1] — [1]Institut Lumière Matière, UMR 5306, Université Lyon 1-CNRS, Villeurbanne, France — [2]CIRIMAT,UMR 5085, ENSIACET, Toulouse, France

We have performed EAM and DFT calculations of H segregation energies at vacancies in Ni. The maximum binding is 0.27eV and 0.4eV in the single and divacancy respectively, in good agreement with Fukai's Thermal Desorption Spectroscopy results. By a comprehensive calculation of the formation energy of VHn clusters (n=1 to 14), it was shown that segregation occurs mostly on the octahedral site (off-centered) in the vacancy (O1) with almost no O1-O1 interactions, strong O1-T1 (tetrahedral) repulsion and weak attractive O1-O2 interaction. Approximately constant effective pair interactions can be extracted from these formation energies. Together with the segregation energies in the dilute limit, they constitute a simple energetic model from which we can derive the equilibrium distributions and concentrations of VHn (analytical formulas are validated against Monte Carlo simulations). A good separation of timescales between H diffusion events and vacancy-metal exchanges enables a simple calculation of the diffusion coefficient of the clusters from the equilibium distribution and a limited set of barriers. H drastically slows down the vacancies, but this effect is overcompensated by the increase in equilibrium vacancies and finally Ni self-diffusion is markedly increased.

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MM 5.4 Mon 11:15 TC 006

Hydrogen embrittlement of a carbon segregated symmetrical tilt grain boundary in α-Fe — Arshad Tahir, •Rebecca Janisch, and Alexander Hartmaier — ICAMS, Ruhr-Universität Bochum, 44780 Bochum

The cleavage strength of a symmetrical tilt grain boundary (STGB) in body centred cubic (bcc) Fe is investigated by means of ab-initio calculations with respect to the effect of a varying number of C and H atoms at the grain boundary. Our results indicate that hydrogen enhanced decohesion of interfaces in Fe-C alloys could be understood as a co-segregation effect.

The calculated segregation energy for C shows that in a bcc Fe-C system with a sufficient amount of interstitial C, the C segregated state should be considered as the ground state of this interface. The work of separation as well as the tensile strength increase significantly with increasing C content. A partial exchange of C with hydrogen changes the cohesion enhancing elastic contribution of C to an embrittling contribution, and also reduces the beneficial chemical contribution to the cohesion. The reduction in strength amounts to almost 20% in the co-segregated case, and to more than 25% if C is completely replaced by H. Compared to the strength of the STGB in pure iron, however, the influence of H is negligible. Hence, H embrittlement of this interface can only be understood in the three component Fe-C-H system.

15 min. break