Multiscale approaches to hydrogen-assisted degradation of metals

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Hydrogen embrittlement (HE) is a serious and costly industrial problem that affects many commonly-used structural metals. Given the wide range of service environments in which hydrogen may occur or be produced, this represents a very serious threat to the structural integrity of machinery and infrastructure in many industries. Despite having been studied for several decades, there is still little consensus regarding the underlying mechanisms for HE. Recently-developed theoretical and experimental methods, which enable the evaluation of the influences of hydrogen on the mechanical behaviour of metals at the nano-scale, are helping to elucidate new aspects of these mechanisms. However, there remains an urgent need to develop tools for the prediction of the reliability and lifetime of materials and components affected by hydrogen. Critical to achieving this goal is the development of accurate descriptions of hydrogen-microstructure interactions under conditions relevant to those occurring in service. Since these interactions occur at all length scales, this poses a true multiscale challenge.

The International Symposium on Multiscale Approaches to Hydrogen-Assisted Degradation of Metals at the 2014 TMS Annual Meeting and Exhibition in San Diego was organised with the aim of promoting the exchange of ideas and information regarding the application of cutting-edge theoretical and experimental methods to industrial problems involving hydrogen-assisted degradation of metals. A particular focus of the symposium was multiscale modeling (e.g. coupled atomistic, mesoscopic and macroscopic descriptions of hydrogen transport and damage mechanisms) as well as integrated theoretical and experimental approaches to hydrogen-microstructure interactions (e.g. the application of experimental methods for model validation and determination of modeling parameters). The symposium brought together leading researchers in the field of HE, as well as representatives from a broad range of industries that provided vital insights into the impact of HE. A total of 32 presentations were given during the 4 day meeting. The following 5 articles are based on presentations that were selected in order to show the diversity of topics covered at the symposium.

Reese et al. [1] provide an overview of an experimental program at Airbus Group, which is aimed at evaluating the susceptibility of pulse-plated (PP) Ni to HE. This material is used in the fabrication of the Vulcain2 and Vinci rocket engines, which power the main and upper stage of the Ariane5 satellite launcher, respectively. Due to the nature of the PP process, some hydrogen may be incorporated into the material during deposition. Depending on the process parameters used, this hydrogen, in combination with residual stresses resulting from welding, may result in HE. Though this does not pose an immediate problem, there is a need to better understand the influences of microstructure and process parameters on the susceptibility of PP-Ni to HE. The study is part of a wider EU-funded program called “MultiHy” (Multiscale modelling of hydrogen embrittlement), which aims to develop advanced multiscale models to assist companies to better understand how HE occurs during manufacture and service.

Rajagopalan and Thirumalai [2] review recent and forthcoming publications in which HE of two commonly-used pipeline steels, X65 and X80, was investigated using advanced analytical techniques. Analysis of the deformation substructures under the fracture surfaces using transmission electron microscopy (TEM) and the observation of nanovoids on the fracture surfaces using high resolution scanning electron microscopy (SEM) led the authors to propose that the mechanism for HE involves vacancy-induced nanovoid nucleation and growth. The results are also discussed in the context of other recent theoretical and experimental studies that highlight the critical role of vacancies in the mechanism(s) for HE. The authors also provide an overview of HE-related challenges in the oil and gas industry.

Lawrence et al. [3] provides an example of the application of nano-mechanical test methods to the investigation of the influence of hydrogen on dislocation interactions. Nanoindentation tests were performed on commercially-pure Ni after charging in gaseous hydrogen. The nucleation and interaction of dislocations from the indented area were then studied using scanning probe microscopy (SPM). The indentations were made close to grain boundaries and twins in order to study the influence of hydrogen on dislocation pile-ups and transmission across grain boundaries. It was found that hydrogen charging resulted in an increase in the plastic zone size and an increase in spacing between slip steps. This is consistent with a reduction in cross slip and an increase in dislocation mobility due to hydrogen, as purported by the hydrogen enhanced localised plasticity (HELP). The influence of hydrogen on slip transmission was largely dependent on the east of slip within the adjacent grains and the grain boundary misorientation.

Dadfarnia et al. [4] present a finite element (FE) modeling approach that may be used to predict the influence of HE on crack propagation rates in bolt-loaded fracture mechanics samples. The approach is based on a stepwise crack propagation mechanism, with each step requiring the crack opening stress in some characteristic distance ahead of the crack tip being greater than some threshold value, which is given as a function of the hydrogen concentration. The model is used to predict crack velocity vs. stress intensity factor (V-K) curves that are qualitatively consistent with experiments. The sensitivity of the model to the various input parameters was systematically evaluated.

Finally, Hickel et al. [5] outlines the applicability of various atomistic modeling methods to the study of HE. Recent studies involving atomistic calculations of hydrogen-microstructure interactions are reviewed. First principles density functional theory (DFT) simulations were used to evaluate the influences of interstitial and substitutional impurities on the diffusivity and solubility of hydrogen in bulk BCC and FCC Fe phases as well hydrogen trapping at vacancies, grain boundaries and various precipitates. Due to their high computational cost, DFT calculations are limited to structures containing relatively small numbers of atoms. For studies of hydrogen interactions in complex systems over long time scales, it is necessary to employ complementary simulation techniques and methodologies such as classical interatomic potentials or kinetic Monte Carlo.

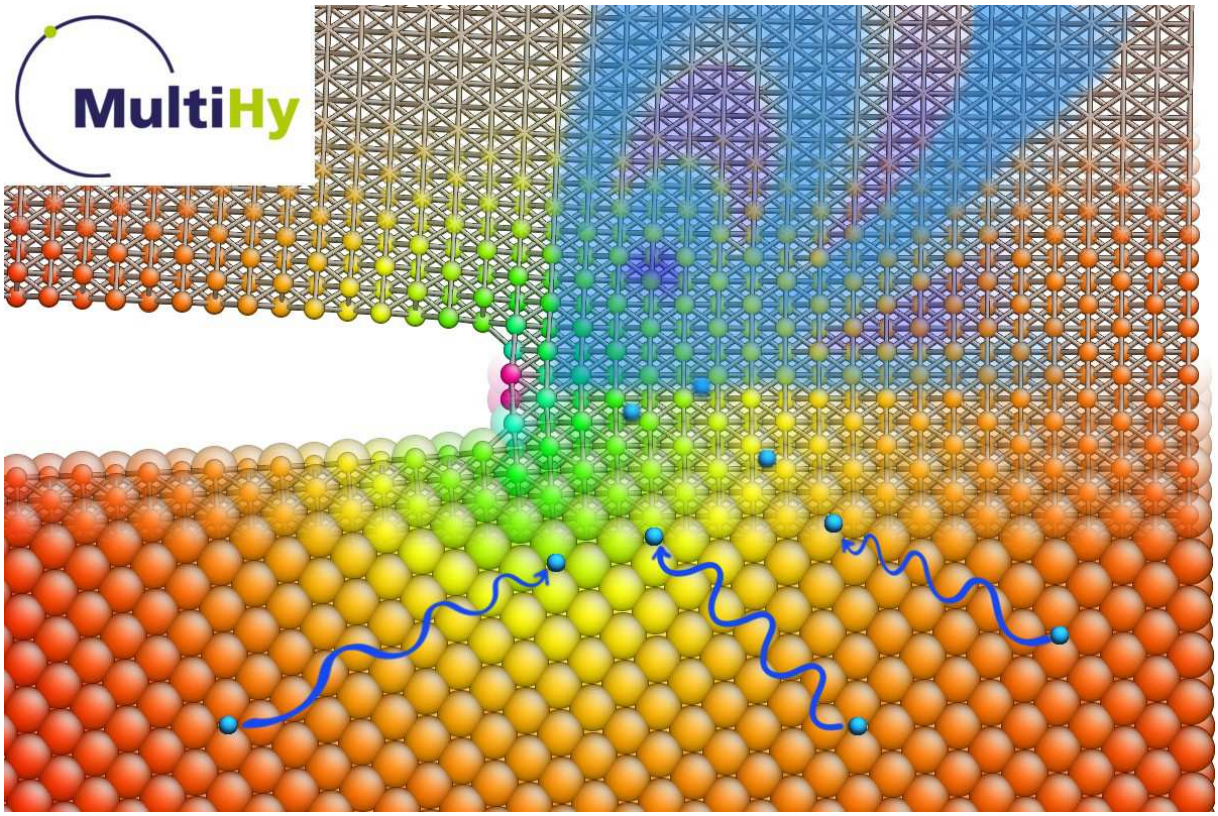

Figure 1: Modelling of hydrogen embrittlement is a true multiscale challenge.

References

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