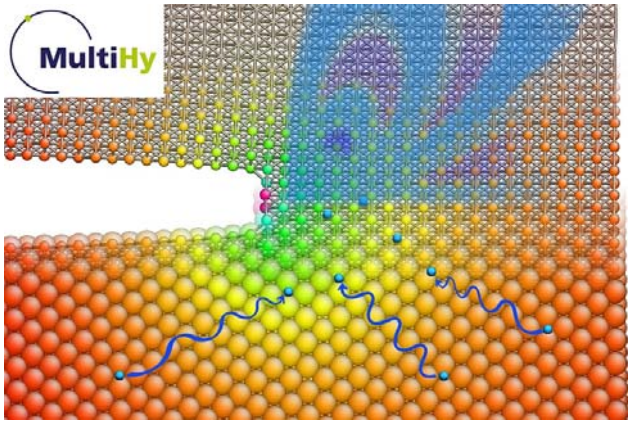
MultiHy Update

The newsletter of the EU FP7 project MultiHy

November 2011 – April 2012

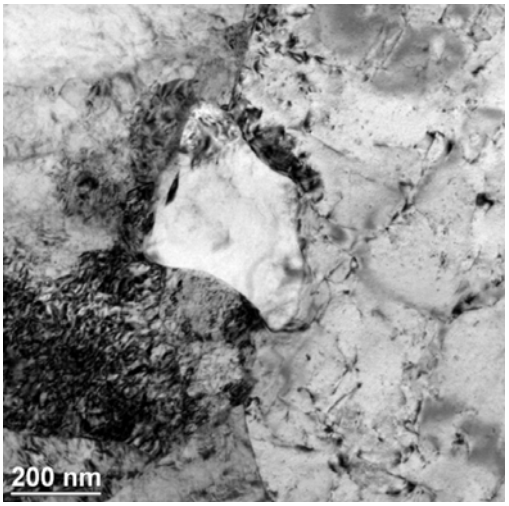
Dear friends and colleagues,

Once again it's my pleasure to report on the progress of the EU Project "MultiHy". Just over one year has passed since the project began and activities in most work packages are now progressing at full pace. During the first six months we focused our efforts primarily on the fabrication of model materials and components (WP1.1), which was the first important step in the project and potential bottleneck for the other work packages. With most of the materials and components fabricated, we turned our attention during the last six months to characterising the microstructures of the model materials (WP1.2) and the collection of process parameters and in-service data (WP3) that will serve as boundary conditions for our numerical models. This period also saw the commencement of finite element modelling activities in WP6 (continuum and specimen modelling), as well as considerable advancements in WP4 (atomistic modelling) and WP5 (KMC calculations and constitutive laws of diffusion). We have also concerned ourselves with the fabrication of outstanding materials and components that have been delayed; however, sufficient materials have been available such that other work packages have not been affected. Thus, experimental work aimed at determining modelling parameters (WP2) has continued unabated.



Modelling of H-diffusion in real engineering materials is a true multiscale challenge!

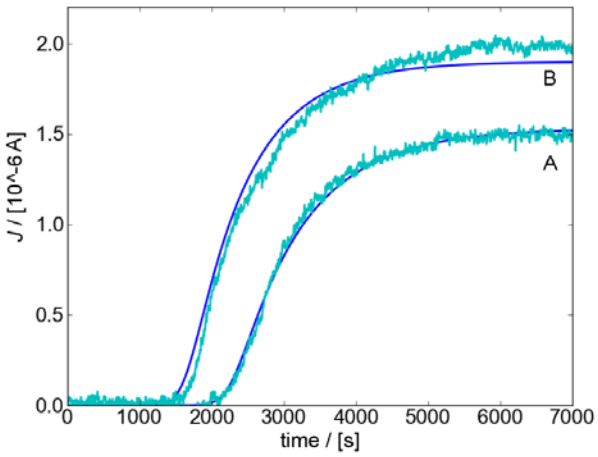
In WP1 (microstructural characterisation and micromechanical testing), all but a few of the model materials and components have been made available to partners for use in experiments. In our first case study, CS1 (delayed H cracking of pulse-plated nickel), fabrication of the final "intermediate" material was performed between March and April, 2012. Microstructural characterisation of some model materials in CS2 (H-assisted degradation of automotive AHSS's) and CS3 (H-assisted RCF in wind turbine bearings) provided some unexpected results; some of our model steels did not meet microstructural requirements and, consequently, have been re-fabricated. TEM-analysis of the model steels in CS2 revealed the presence of Ti-carbides in the TKSE-concept steels but failed to find pure Nb-carbides in the VAS-concept steels. Consequently, we have been forced to re-evaluate out modelling approach; modelling of H trapping in the VAS-concept steels will focus on secondary microstructural changes caused by Nb-addition rather than on the carbides themselves. A key focus of the next six months shall be the analysis of the collected microstructural data its correlation with the experimental results in order to refine our modelling approach.



TEM image of a TiC particle in one of the "TKSE-concept" model steels.

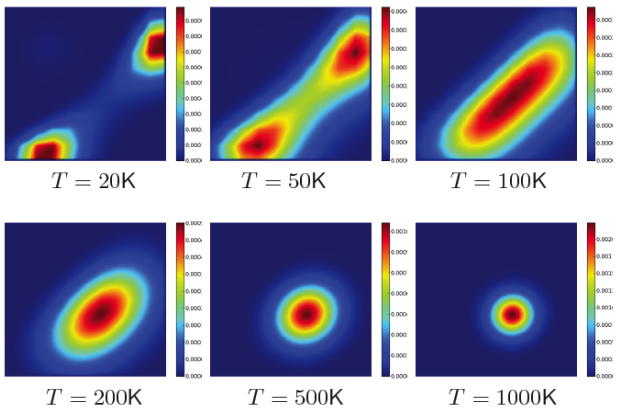
In WP2 (experimental determination of modelling parameters) we have continued electrochemical permeation tests and commenced in-situ tensile testing of the model steels in CS2. Fracture mechanics testing of the PP-Ni materials in CS1 has also begun. Rolling-contact fatigue testing in CS3 is scheduled to begin in mid-July.

A large volume of data pertaining to manufacturing conditions resulting in HE in all CS's has been collected from existing data or new measurements as part of WP3. For example, we have measured H concentrations in our model steels as well as commercial variants at various stages in the production cycle.



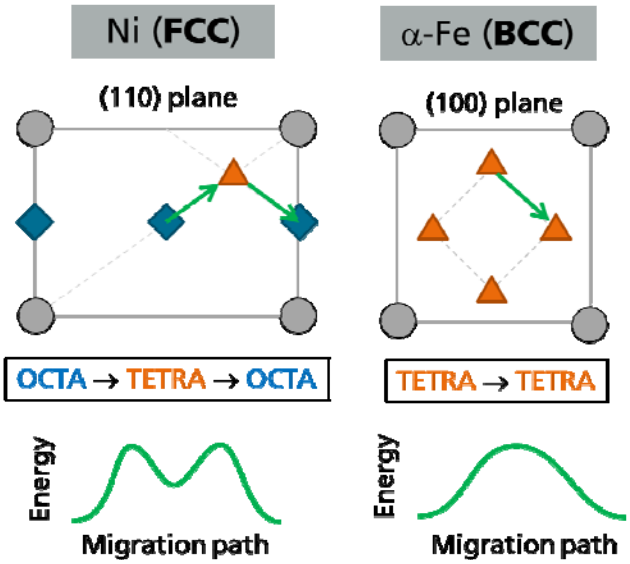
1st (A) and 2nd (B) permeation curves for one of our model steels fitted with FE-model.

The first task in WP4, *ab initio* calculations of the strain dependence of the energetics of H in bulk Fe and Ni, has been completed. A key outcome of atomistic calculations is that quantum effects cannot be neglected. Consequently, our modelling approach has been adapted according to the extra resources required to consider these effects. We have also applied our tight-binding model for H in Fe to the calculation of trap depths for H-vacancy complexes. This model will next be applied to H trapping by extended defects. In WP5 we have calculated diffusion coefficients for H in Fe as a function of vacancy concentration using our kinetic Monte Carlo model. We have also decided on a generalised set of constitutive laws of diffusion, following a detailed literature review and discussions between partners. These are now in the final stages of implementation in the form of sub-routines for the commercial finite element software ABAQUS. A critical issue at the moment is the prioritisation of modelling work in WP4. Thus, the analysis of results from WP1-3 and the transfer of information between partners will become increasingly vital as we move beyond generic modelling to the characterisation of H trapping by specific microstructural features and defects in the following months.

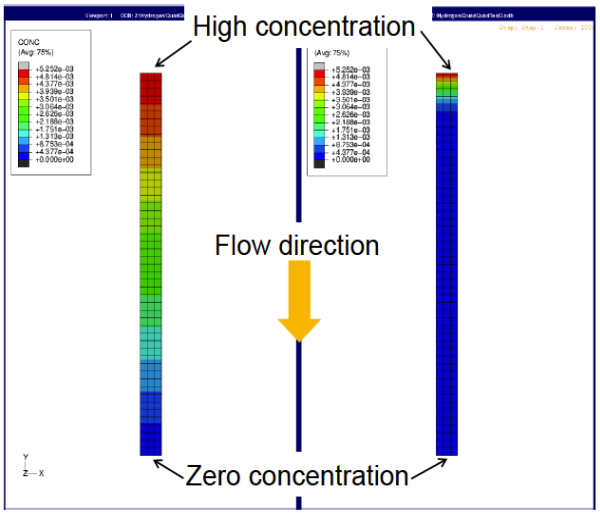


Position probability density of a proton in bcc Fe when the particle's "centroid" is placed at the saddle point between two tetrahedral sites.

FE modelling of H diffusion in WP6 is underway, though the focus so far has primarily been the development of models that will be used to resolve the experimental permeation curves and thermal desorption spectra into trapping parameters. In future, these models will enable us to directly relate the outcomes of our atomistic calculations to experimental results, thus forming a powerful tool to validate the modelling framework. Several meetings were also held at the beginning of 2012 in Munich and Madrid with the aim of defining the scope of specimen and component models in each CS and encouraging dialogue between partners providing input data and those carrying out the modelling work. Consideration has also been given to the unification of modelling approaches used by different partners, i.e. the adoption by all of the constitutive laws being implemented in WP5.



Schematic picture of minimum energy pathways between the equilibrium H interstitial sites in fcc Ni (left) and bcc Fe (right).



2D simulation of H diffusion in the presence (right) and in absence (left) of traps using ABAQUS.

The second full consortium meeting was held at Queen' University of Belfast in April and was attended by all partners. One of the outcomes of the meeting was that partners shall begin considering possibilities for exploitation of project outcomes leading up to the next meeting in 2013. Ideas for limited licensing of FE codes have been discussed.

Another key focus of the next six months will be applying our models to more specific microstructural aspects of our materials and begin linking models at different scales, e.g. by incorporating atomistic results into our FE-models for permeation and TDS tests and correlating our predictions with experimental results. We are hoping to present some of our initial results at the International Hydrogen Conference in Wyoming, USA, and the Materials Science and Engineering Congress in Darmstadt, Germany, in September. I look forward to seeing some of you there!

Best wishes

Nick Winzer

MultiHy Coordinator

The MultiHy consortium poses for a photo at the 2nd annual meeting at Queen's University of Belfast, April, 2012.

Contact: Dr. Nicholas Winzer
Fraunhofer Institute for Mechanics of Materials IWM
Wöhlerstraße 11, D-79108 Freiburg, Germany
Email: multihy@iwm.fraunhofer.de
Web: www.multihy.eu