MultiHy Update

The newsletter of the EU FP7 project MultiHy

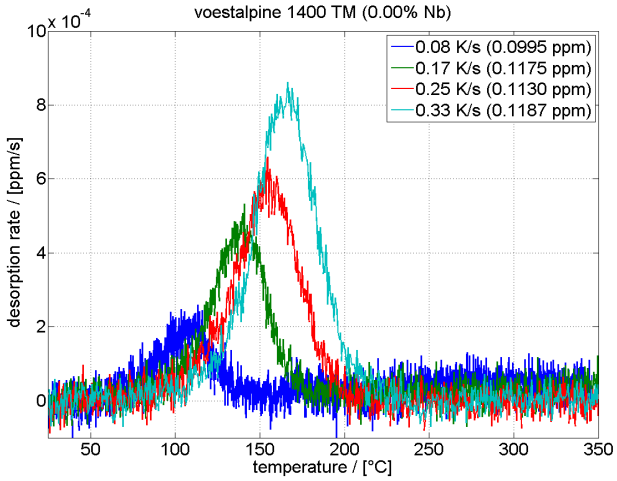
Issue 3, May – November 2012

Dear friends and colleagues,

Another six months have passed and once again it's my pleasure to report on developments in the EU project "MultiHy". The period since my last update has been a particularly critical one for the project, with our first major progress report as well as a number of key deliverables having been completed in the final months of 2012. With this largely out of the way, it's now time to report on some of the most important accomplishments of this period.

After having fabricated most of the model materials and components in the first year of the project, the next step was to analyse their microstructures in sufficient detail to provide a basis for simulations of hydrogen-microstructure interactions. In our first case study, CS1 (H-assisted cracking of the pulse plated Ni combustion chambers for the Ariane satellite launcher), microstructural analysis focused mainly on characterizing the density and misorientation of grain boundaries. Based on the results, numerical models of the grain structures at the atomistic and macroscopic levels were developed, which will be used in simulations of anisotropic hydrogen diffusion. In CS2 (H-embrittlement of advanced high strength steels), microstructural analysis focused primarily on characterising the distribution and morphology of Nb and Ti-carbides in our model materials. This resulted in some novel findings, such as the segregation of Mn and Cr at TiC particle interfaces. Microstructural analysis in CS3 (H-assisted rolling contact fatigue of wind turbine bearings) is largely complete, although analysis of one of the three model steels has been delayed due to its re-fabrication. The complete results of microstructural analysis are expected to be completed in the upcoming weeks.

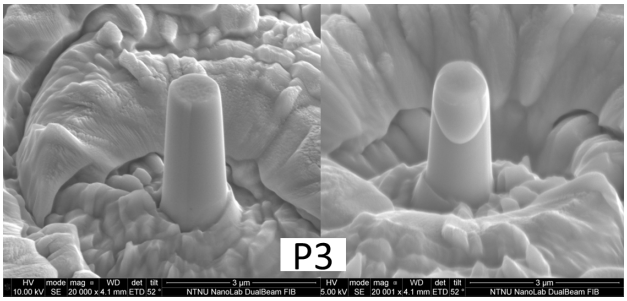
Experimental evaluation of H diffusion and trapping parameters using electrochemical permeation tests and thermal desorption spectroscopy (TDS) is well underway. A new electrochemical permeation cell has been developed that will enable more precise determination of H diffusion and trapping parameters. H permeation tests have so-far been performed for all VAS-concept steels in CS2. Tests have also been carried out for the TKSE concept steels in CS2 as well as the model materials in CS1 and CS3 in order to determine the optimum test conditions. Preliminary TDS measurements have also been performed for the materials in CS2 and CS3. Procedures to resolve H diffusion and trapping parameters from the permeation and TDS measurements based on the numerical models have also been developed, with some results already being used in FE simulations.



Thermal desorption spectra for one of the AHSS steel grades in CS2 at difference heating rates.

Experimental work is also underway to determine the macroscopic thresholds for H-assisted fracture. Based on analysis of in-service failures, testing in CS1 will focus on evaluating the influence of H on fracture toughness. Fracture mechanics samples for the materials are near completion and will be tested shortly. In CS2, in-situ tensile tests of the model steels are being performed under conditions similar to those used in H permeation testing. Combined with detailed fractography, these tests will elucidate the distribution of H amongst the various phases and crystal defects at the time of fracture. Preliminary rolling contact fatigue tests in CS3 have also been performed with the aim of establishing test conditions.

Micromechanical tests are being performed in order to evaluate the influences of H on the mechanical behaviour of the model materials at a scale as close



An FIB-prepared nanopillar in one of the AHSS grades before and after compression using a nanoindentor.

as possible to the atomistic models. A procedure for machining of micropillars from the model materials using focused ion beam (FIB) for nanoindentation with in-situ electrochemical H charging has been developed. Tests so far have focused on testing micropillars in ferrite grains in dual-phase steels in CS2. Due to the small grain size of these materials, a procedure to identify similarly-oriented grains in which the pillars are machined has been developed and tested.

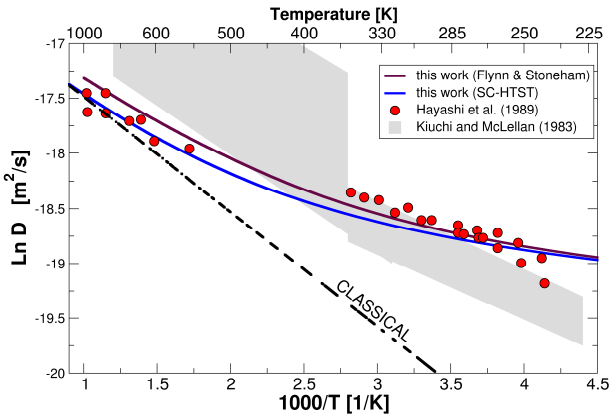
The initial and boundary conditions for the numerical models in MultiHy will be furnished by data collected from in-service observations and measurements. To this end, critical data related to H-assisted failures in the three case studies has been collected and analysed. The data includes analysis of H uptake by materials and components during manufacture and operation as well as the phenomenology and morphology of H-related failures.

The atomistic studies have so-far focused mainly on calculations of H diffusion barriers in strained bulk phases of Fe and Ni. The influences of various modes of strain on the binding energies and diffusion barriers in bcc Fe and fcc Ni were evaluated using first-principles density functional theory (DFT) calculations and parameterized by analytical functional forms. A key outcome is that calculations for H in bcc Fe must be corrected for quantum tunnelling between interstitial sites. Atomistic calculations for the interaction of H with crystal defects are also underway. Preliminary DFT simulations for H segregation at grain boundaries have been performed. Validation tests have been performed using tight binding models for H in Fe; the results indicate that the models are sufficiently reliable to simulate H segregation at extended defects. Tight binding models have also been used to evaluate H binding with vacancies in bcc Fe. Several large-scale molecular dynamics simulations for H in Ni have been performed to test the massively parallel LAMMPS code using classical interatomic potentials based on the embedded-atom method (EAM).

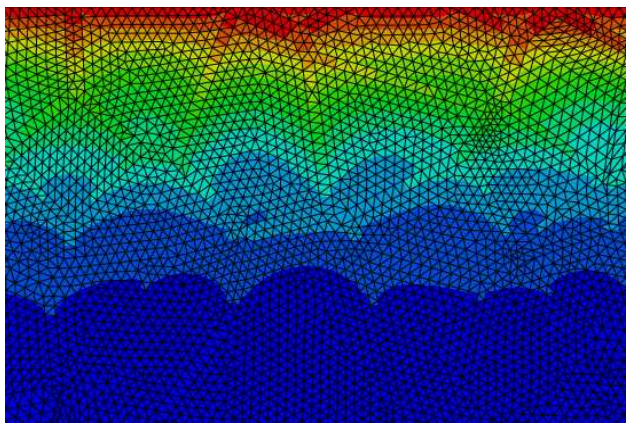
Results of atomistic calculations have already been used in KMC calculations of H diffusion in the presence of crystal defects. KMC simulations have been used to evaluate the influence of vacancies on the diffusion of H in bcc-Fe. Simulations have also been performed for coupled diffusion of H and vacancies in order to evaluate the conditions corresponding to immobilisation of vacancies by trapped H atoms and formation of vacancy clusters.

A key achievement of macroscopic modelling work to date has been the use of a common modelling approach based on generalised constitutive equations for H diffusion and trapping. These constitutive equations have been implemented in a variety of platforms by the project participants, either as bespoke FE codes or as user-defined subroutines in commercial FE packages. Most importantly, we have developed and tested subroutines within the commercial software package Abaqus. The Abaqus subroutines have already been applied to continuum modelling of H diffusion in simulated polycrystalline microstructures in order to determine the conditions for grain boundary, bulk and mixed mode H diffusion in Ni. They have also been applied in simulations of H diffusion and trapping in test specimens in CS2 using preliminary results of electrochemical permeation tests. Further developments of the constitutive equations are expected as the results of atomistic and KMC models for H interactions with crystal defects become available.

So-far, the project has focused on gathering the information necessary for the development of the theoretical models, e.g. details of the material microstructures and phenomenology of H-related failures in service, as well as on developing experimental methods and modeling tools. During the next phase of the project, we will focus our efforts on the correlation of results of experimental and theoretical evaluations of H-microstructure interactions and on linking simulations at difference length scales. We will begin to develop libraries of binding energies and energy barriers for H near extended crystallographic defects using atomistic simulations. These libraries will then be used in KMC simulations, the results of which can be



Comparison of theoretically predicted temperature dependence of diffusion coefficient with available experimental data in bcc Fe-H system.



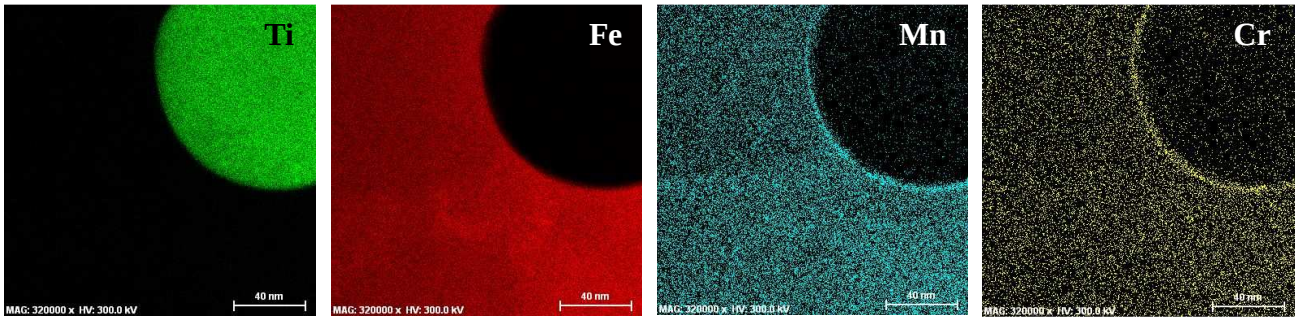
Finite element simulation of hydrogen diffusion in a polycrystal environment

compared with those of electrochemical permeation and TDS measurements and directly incorporated into FE models. We will also begin to scale-up our FE models to simulate of H diffusion and trapping in full components using data collected through in-service observations and measurements. This will no doubt lead to more interesting results in the upcoming months.

Best wishes

Nick Winzer

MultiHy Coordinator



STEM images showing the segregation of Cr and Mn at the interface of TiC particles.

Fraunhofer IWM

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BMW Group

NTNU Norwegian University of Science and Technology

voestalpine ONE STEP AHEAD.

The University of Salamanca

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