PHD thesis at Laboratoire des Sciences de l'Ingénieur pour l'Environnement, LaSIE, La Rochelle, France

Effect of grain boundary nature and connectivity on the hydrogen diffusion in heterogeneous materials: Modelling and experimental study

Description :

Hydrogen is very detrimental to the durability of materials. This problem affects the structural materials in various industries, from subsea pipelines to aircraft and nuclear reactors. This severe degradation can manifest itself in several ways such as a decrease in tensile elongation to cause fracture, or a decrease in the static load that can be supported by the metallic structure as an example. With hydrogen's small size, it can easily penetrate and segregate in most metals, leading to a degradation of materials' mechanical properties. The effects of hydrogen on the ductility, toughness, and tensile strength are known to be significant. The performance and lifetime of materials are reduced with the presence of hydrogen. This outcome is known as Hydrogen Embrittlement (HE). This phenomenon results from a combination of different parameters related to the material's characteristics, the source of hydrogen (internal or external) and to the mechanical solicitations.

Several studies have pointed out the determining role of grain boundaries in the hydrogen diffusion and trapping mechanisms. However, it is difficult to find diffusivity data associated to each category of GBs. In our previous work, we showed that the boundary nature remarkedly influences the hydrogen diffusion and segregation, by combining diffusion measurements and microstructure characterization of polycrystalline nickel [Oudriss 2012]. In addition to the boundary nature, we pointed out the importance of including the connectivity of boundaries with different characters to better describe the effects of grain boundaries on the overall diffusion. we investigated the effects of a heterogeneous grain boundary networks on the effective diffusivity in polycrystalline materials, using finite elements modeling. Hydrogen diffusion through heterogeneous materials was modeled by a ternary continuum composite media. By characterizing the grain-boundary connectivity, the strong correlations between the grain-boundary connectivity parameters and the effective diffusivity was proven [Osman Hoch 2015].

In regard to the GB diffusivity, this classification is still controversial because a direct relationship between this crystallographic property and the GB property has not been elucidated [Priester 2012]. Indeed, based on our recent study on a series of two-grains systems separated by a grain boundary classified as special with a greater or lesser free volume. Some of our case studies demonstrated that some boundaries labeled as special behaved as a "random" boundary [Li 2017].

However, the investigations on the correlations between the overall hydrogen diffusion and the grain-boundary character distribution remain rare, even-nonexistent and triple junction is set aside. This is mainly **due to the experimental difficulties to explore the grain boundary and triple junction diffusion in polycrystalline materials. Also, the analysis of HE is complex since all phenomena of all scales are linked altogether, and the numerous mechanisms intervene at the same time.**

Hence, this thesis will question the effects of various grain boundaries and triple junctions and their connectivity on hydrogen diffusion by coupling numerical and experimental technics.

Numerical tools : FEM : Comsol Multiphysics, Programming : Matlab, Statistics, Homogenization

Characterization : Electrochemical : Permeation, Thermal-Desorption Spectroscopy (TDS)

Imaging : TEM, SEM- EBSD, SEM-FIB

Mechanical : micro-tensile test bench, nano-indentation

Starting Date: October 1st 2019

Candidate'skills and background :

Master in Material Science and Engineering or similar
Programming skills are crucial with a good knowledge of finite element methods.
Proficiency in English is necessary as all the communications, publications and the thesis will be written in English.

Contact:
Please send your resume and application letter to both advisors:
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[Li 2017] J. Li, A. Metsue, A. Oudriss, J. Bouhattate, X. Feaugas: "Anisotropy of hydrogen diffusion in nickel single crystals: the effects of self-stress and hydrogen concentration on diffusion » Scientific report 7, 45041 (2017)

[Osman Hoch 2015] Osman Hoch, B., Metsue, A., Bouhattate, J., Feaugas, X. "Effects of grain-boundary networks on the macroscopic diffusivity of hydrogen in polycrystalline materials" Computational Materials Science, 97 (2015) 276-284.

[Oudriss 2012] A. Oudriss, J. Creus, J. Bouhattate, E. Conforto, C. Berziou, C. Savall, X. Feaugas, Grain size and grain-boundary effects on diffusion and trapping of hydrogen in pure nickel, Acta Materialia, Volume 60, Issue 19, November 2012, Pages 6814-6828

[Priester 2012] L. Priester, Grain boundaries: from theory to engineering. (Springer Science & Business Media, 2012).