EU-DOCS for SmUCS

CO-SUPERVISED SUBJECT PROPOSAL FOR A DOCTORAL CONTRACT

Title of the thesis project Influence of grain boundaries in high-pressure **HY**drogen **COAST**al storage materials for green hydrogen	
La Rochelle University Research Unit LaSIE Laboratoire des Sciences de l'Ingénieur pour l'Environnement	**Partner university** FAU Erlangen-Nuremberg, Germany **Cotutelle research** Department of Materials Science
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Main research field: Corrosion **Secondary research fields:** Material Science, Mechanical Engineering, Green Hydrogen	
Keywords: Corrosion, hydrogen embrittlement, grain boundaries	

Hydrogen is seen as a clean, mobile energy carrier and source of fuel, as it has the great advantage of being present on the planet in an abundant amount. A genuine 'hydrogen economy' is henceforth envisioned. Much of the technology is established from the chemical industry using high-value materials, but cost pressure from investment and maintenance is becoming significant now that these technologies are rolled out at the gigawatt scale [1-3]. One of the main challenges consists of the development of suitable, cost-effective, and durable materials for the transportation of hydrogen. Indeed, a major concern with hydrogen is that it 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 [4-6]. 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, for example. The effects of hydrogen on the ductility, toughness, and tensile strength are known to be significant, as the performance and lifetime of materials are drastically reduced in the presence of hydrogen. This outcome, known as Hydrogen Embrittlement (HE), was first described in 1875 by Johnson [7]. This phenomenon results from a combination of different parameters related to the material's characteristics, the source of hydrogen (internal or external), and the mechanical solicitations.

Nowadays, coastal areas are quickly becoming one of the main sources of green hydrogen due to their favorable potential for wind, tidal/wave, and solar power to drive water electrolysis. While complementary, these green power sources do show some intermittence, making buffering of the produced gaseous hydrogen in e.g. high-pressure tanks, necessary. These tanks and auxiliary equipment already exist; however, they are currently made from non-optimized materials, due to a lack of understanding in detail of the underlying failure mechanisms. Especially, the most important role of crystal interfaces, such as grain and grain boundaries, is not fundamentally understood.

In this project, the applicants will leverage their complementary expertise in model material synthesis, characterization, and simulation (LaSIE), as well as high-pressure materials testing and atomic-scale analysis (FAU), to gain fundamental insights into the role of grain boundaries (GBs) as critical failure points in hydrogen-facing materials under pressure. Nickel (Ni) is selected as the model material due to its well-characterized behavior and suitability for fundamental studies. The applicants will synthesize Ni single crystals (SX) and bicrystals (BX) at the macroscale, enabling the isolation and analysis of individual grain boundaries and the comparison to boundary-free systems. **The central objective of the proposal is to assess and predict grain boundary networks and microstructures that exhibit reduced sensitivity to hydrogen embrittlement through grain boundary engineering**.

Programme

SO1: Fabricate the samples with zero or one grain boundaries.

To fill an important gap concerning the effect of GB, it is necessary to have access to experimental knowledge on samples of different, well-defined single GBs.

SO2: Develop a database of material characterization testing on representative grain boundaries in nickel.

There is a strong need to document the effect of GB on the diffusion of hydrogen in metals, using a harmonized building protocol which will be established in the framework of this project. These will be exposed to electrochemical (LaSIE) and high-pressure (FAU) hydrogen in the form of protium and deuterium.

SO3: Develop an atomistic numerical modelling approach for simulating and predicting hydrogen diffusion and trapping at the GB.

In this Sub-objective, the atomistic level investigation will be done to understand the fundamentals of hydrogen embrittlement of GBs and TJs.

SO4: To facilitate the uptake and exploitation of the project results by the academic community, technology developers, and end-users.

Communication is a key lever to ensure that the project effectively reaches specific audiences, promoting the project and its results, generating awareness and interest, and encouraging engagement with the project activities and results. The main strategic objective of the communication plan is to ensure that the project results are widely communicated to the target communities via appropriate means and translated into meaningful and tangible action.

<u>Description of the Doctoral Candidate's tasks:</u>

Technical program

In La Rochelle:
Crystal growth of a bi-crystal and a tri-crystal
Characterization (XRD, EBSD, TEM) of each grain and grain boundary (a minimum of 4 GBs) and a triple junction
Hydrogen charging (electrochemical), TDS
Mechanical testing with and without H
Modelling application in FEM

In FAU Erlangen:
Gaseous hydrogen charging (cylindrical samples), TDS
Atom Probe
HRTEM at least one bi-crystal and one tri-crystal
Mechanical testing on cylindrical samples with and without H

Secondment in HEREON:
Synchrotron nano-tomography and diffraction imaging to capture 3D defect distributions.

Communication program
Participation in one domestic conference/year and one international conference
Writing of at least 2 journal papers as first author
3 outreach activities (ma these en 180s, et fête de la science, Long night of science at FAU)

Training Program
In agreement with both doctoral schools, La Rochelle and FAU Erlangen.

PhD student profile and skills required

The PhD student applicant should have a master's degree in Mechanical/Materials Science Engineering with an appetite for both experimental and numerical research. A high proficiency in English is expected, along with a strong capacity for teamwork, adaptability, and autonomy.

Scientific alignment with EU-DOCs for SmUCS objectives

Nowadays, coastal areas are quickly becoming one of the main sources of green hydrogen due to their favorable potential for wind, tidal/wave, and solar power to drive water electrolysis. While complementary, these green power sources exhibit some intermittency, necessitating the buffering of the produced gaseous hydrogen, e.g., in high-pressure tanks. These tanks and auxiliary equipment already exist; however, they are currently made from non-optimized materials due to a lack of detailed understanding of the underlying failure mechanisms. Especially, the role of crystal interfaces, such as grain and grain boundaries, is not fundamentally understood.

In marine environments, hydrogen can contribute to corrosion through various mechanisms. Corrosion reactions, particularly in seawater, produce hydrogen as a byproduct, which is then absorbed by metals.

Furthermore, cathodic protection, while intended to prevent corrosion, also generates hydrogen at the cathode, potentially leading to hydrogen embrittlement. Hydrogen sulfide, microbial activity, and other sources also create hydrogen-rich conditions in the marine environment.

Societal and economic challenges and contributions

Economic impact: From an economic perspective, the project will provide solutions to the problems of stress corrosion and, more specifically, to hydrogen embrittlement. In particular, it will offer the opportunity to begin the development of new microstructural states less sensitive to the effects of hydrogen and thus leaner and more sustainable alloys. As the hydrogen-based fuel consumption will increase, the economic losses due to the hydrogen embrittlement can be countered. The discoveries associated with this project will lead us to the development of so-called "intelligent" and more "resistant" metallurgical states, considering the microstructural elements rather than alloying elements, which will increase the durability and safety of metal structures and thus reduce the costs associated with the maintenance of certain systems and structures. Thus, the project carefully designed the impact logic to ensure that the project results directly and indirectly contribute to the increase of knowledge about the microstructure-H interaction. Indeed, the project will have a significant impact due to the direct link with the growth of the hydrogen sector, which is planned to continue its ascension in the following years. The demand for hydrogen is projected to increase exponentially, with the potential for the market to reach $2.5 trillion annually by 2050, according to a report by the Hydrogen Council. Additionally, the EC has set a goal for hydrogen to represent up to 14% of the EU's energy mix by 2050. As the market demand for hydrogen and hydrogen-related technologies continues to grow, the project is well-positioned to contribute to the development of a hydrogen-based energy system in Europe and beyond.

Societal and environmental benefits

From a societal point of view, the use of hydrogen as a "clean" energy vector will reduce carbon emissions, which in turn improves the air quality. Consequently, the results of this project will provide answers in the choice of alloys necessary for the safe transportation and storage of hydrogen with better management of the risk of hydrogen embrittlement. The success of this project will pave the way towards a hydrogen-based economy beneficial for the environment.

Partnership context

Peter Felfer and Jamaa Bouhattate have been following each other's work for the past decade. They met repeatedly during RFCS evaluations for European funding. They decided to start a collaboration as their 2 groups possess complementary and highly synergistic knowledge and equipment. Since it is a beginning collaboration, their work has not yet been published, as the work is ongoing.

A precious addition to the great HyCOAST project is the secondment that will be led by Florian Pyczak at Helmholtz-Zentrum Hereon, where the student will have access to a synchrotron to shed light on the effects of anisotropy on hydrogen diffusion.

Peter Felfer and Florian Pyczak have cooperated since 2016 in the field of advanced characterization of metallic and intermetallic materials, resulting in joint publications, the most current of which was published in 2024.

This project has the potential to impel a fruitful and long-term collaboration on several levels through research and PHD training activities.