Proposition of PhD thesis subject

Design and characterisation of nickel alloys
with an improved resistance to hydrogen embrittlement

Context and aims

As many metals, nickel alloys can become brittle in the presence of hydrogen, which can have severe economical, human and environmental consequences, for instance in the nuclear industry or in the oil & gas sector. Therefore, there is a need for new alloys with an improved resistance to hydrogen embrittlement (RHE) as well as good mechanical properties and corrosion resistance, a low cost… Instead of alloy selection from available grades, the trend is now the design of made-to-measure alloys to reach a given set of properties. Recently, computer-aided alloy design has been implemented, notably using thermodynamics as well as artificial intelligence including data mining / machine learning and multi-objective optimisation by genetic algorithms. The aim of this project is the computational design of nickel alloys with, among others, an optimised RHE.

Description of subject

The first issue that will be dealt with is a better understanding and description of some material-hydrogen interaction mechanisms. For this, model alloys will be designed with specific structural features or with simple microstructures, i.e. containing precipitates with a controlled nature, volume fraction and solubility. This will be made using a combination of existing genetic algorithm optimisation, physical models, data mining models and computational thermodynamics. Such alloys will then be elaborated by vacuum melting and hot working, and investigated for mechanical properties and microstructure (SEM, EDS, WDS, EBSD…). They will also be studied in the presence of hydrogen: permeation, TDS, tensile testing on hydrogen-precharged specimens or under in-situ cathodic charging to assess the RHE. Based on the gained knowledge, “industrial” alloys with an improved RHE will be designed, produced and experimentally studied, using the same set of tools as in the first part of the project.

Locations and other details

The PhD will start Fall 2019. The first part (approximately 1 year) will take place at the University of Nantes / Institut des Matériaux Jean Rouxel (IMN), France, and the second part (approximately 2 years) at Ecole des Mines de Saint-Etienne / Laboratoire Georges Friedel (LGF), France. The PhD student will be registered at the University of Nantes. The PhD is funded for 3 years by the French Research Agency (ANR) in the Frame of the "Cadohrs" project. This project involves researchers in Physical Metallurgy, Hydrogen Embrittlement, Atomistic Simulations and Computer Science.
IMN and LGF are two of the most active institutes in Materials in France, each of them consisting of approximately 50 academic permanent staff and about 100 PhD students and post-docs. PhD students have access to a wide range of modern and well-equipped facilities to conduct their research. Researchers involved in the Cadohrs project are very active in different communities (computational alloy design, hydrogen embrittlement, ab initio simulation of metals) at the French and European scale.

Skills needed

- Master's degree in Materials
- Good knowledge of metallurgy
- Basic skills in computer programming
- Interest in both experimental work and modelling
- Ability for team working
- Self-motivated, independent, enthusiast
- Good command of English
- Good level in scientific writing and presenting
- Willing to publish research findings in international journals

Contacts

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