Simulation of hydrogen fatigue crack propagation in heterogeneous media

General context

The use of hydrogen as an energy carrier is one of the ways to reduce the carbon impact. High pressure is currently one of the most mature means of transporting and storing this gas efficiently. The improvement of tanks and transport systems requires an understanding and control of the phenomenon of hydrogen embrittlement in the steel grades used. For example, there is a significant increase in fatigue crack growth rate in metals when subjected to certain hydrogen pressure and cyclic loading conditions.

In order to respond to this problem, the "HyperStock" Priority Research Programme (www.celluleenergie.cnrs.fr/pepr/hyperstock/), funded by the French National Research Agency, brings together the knowledge and resources of several French laboratories that are experts in hydrogen storage materials in order to accelerate the mass deployment of these technological solutions, to respond to the economic and societal imperatives of this change of scale, and to envisage an ecological transition that includes the use of decarbonised hydrogen in order to significantly reduce the carbon impact. The Pprime Institute (CNRS, ISAE-ENSMA and the University of Poitiers) and the LSPM (CNRS and the University of Sorbonne Paris Nord) wish to develop tools to model these degradation phenomena.

The Pprime Institute has test facilities for characterising material properties under H2 pressure under different stress conditions [1] and is developing routines for simulating hydrogen-assisted cracking [2]. The LSPM, for its part, has numerical simulation tools using finite elements that allow coupled chemo-thermo-elastoplastic calculations to be carried out on different scales on metallic structures [3,4], integrating in particular crystalline plasticity, transient (multi)trapping, and the effect of temperature and mechanical fields on these processes.

Work programme

Numerical simulation of hydrogen gas assisted crack initiation and propagation processes still faces many challenges due to the complexity and multiplicity of the phenomena involved at different scales, especially in the case of cyclic loading. As a result, it remains difficult to predict quantitatively the effects of pressure and parameters such as frequency in the case of cyclic loading.

The modelling work will aim to set up a tool capable of predicting the effects of hydrogen on the cracking kinetics of metallic materials, for different exposure conditions (H2 pressure, frequency) and loading conditions (stress intensity factor). It will benefit from the collaborative environment of the HyperStock project, some of whose tasks are dedicated to the interactions between hydrogen and metal on the surface, and hydrogen and plasticity in volume. This knowledge will feed the modelling approach and help identify parameters. The phase field method will be used to represent localized interfaces in a diffuse way, coupled with cohesive zones [5,6]. The study will be carried out at the aggregate level. At this level, the geometric variations (such as grain size, orientation and distribution) are represented by stress field distributions. The aim is to develop a damage model coupling hydrogen diffusion, plasticity and degradation within the framework of the finite element method, taking into account the specific aspects of accumulation inherent to cyclic loading. Thanks to this numerical tool, it will be possible to evaluate different embrittlement criteria based either on the local hydrogen concentration or on its gradient, and more generally, the parameters controlling the propagation of fatigue cracks. The partnership between the two laboratories will also allow an evaluation of the robustness and performance of different finite element softwares, whether commercial (Abaqus, for LSPM) or developed in-house (FoXTRoT, for Pprime). The modelling approach will be validated in terms of its ability to reproduce and therefore predict crack propagation velocities in pre-cracked samples in a hydrogen atmosphere.

Required profile:

A Master's student or engineer, with a solid knowledge in mechanics of materials, finite elements and an aptitude in software development. An interest for multiphysics approaches and experimental-digital dialogue is a plus. The PhD student will register at ISAE-ENSMA in Poitiers at the start of the 2023 academic year. Occasional stays at the LSPM are to be expected. The supervisory team will consist of Damien HALM (Pprime), Yann CHARLES (LSPM) and Azdine NAIT-ALI (Pprime). The gross monthly salary will be 2045€. Applications should be sent to damien.halm@ensma.fr, yann.charles@univ-paris13.fr and azdine.nait-ali@ensma.fr.

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[6] Golahmar, A., Kristensen, PK., Niordson, CF., Martínez-Pañeda, E., A phase field model for hydrogen-assisted fatigue, Int J Fatigue, 2022, 154, pp 106521.