MODELING OF HYDROGEN EMBRITLLEMENT USING MIXED NONLOCAL FINITE ELEMENTS

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Abstract

Industrial power generation and transmission structures are designed to have a service life of 40 years. Knowledge of the evolution of material behavior over long periods of time is therefore crucial to ensure the safety and reliability of these facilities. Due to the continuously increasing power demand, new energy sources are needed. As part of the decarbonization of these sources, hydrogen will play an important role as an energy vector. However, hydrogen can easily diffuse in materials, inducing premature failure with reduced ductility and toughness. This phenomenon, called hydrogen embrittlement (HE), is a complex mechanism which combines mechanical and chemical loadings. Therefore, this work presents a strategy to simulate HE by the finite element method integrating plasticity and damage coupled to hydrogen diffusion. Since damage is highly dependent on local stresses and hydrostatic pressure mixed formulations in displacement, pressure and volume variation have been proposed to control volumetric locking. To represent ductile rupture, the Gurson-Tvergaard-Needleman (GTN) model based on an implicit gradient nonlocal formulation with two internal lengths is considered, which allows regularizing void growth and strain-controlled nucleation. All the implementations and simulations have been carried out using the Z-set software.

1. Introduction

Dissolved hydrogen atoms in metals degrade the material's mechanical properties, such as strength, ductility and toughness. Simulations of hydrogen embrittlement (HE) should characterize the detrimental effect that is associated to the presence of hydrogen in the material. Such simulations require the implementation of both hydrogen diffusion and hydrogen assisted material degradation. This study presents a framework for finite elements simulations combining plasticity, damage and hydrogen diffusion in a fully coupled way, with diffusion driven by hydrogen concentration and pressure gradient. To model ductile damage, the Gurson-Tvergaard-Needleman (GTN) [1] model, based on an implicit gradient nonlocal formulation with two internal lengths [2] is considered, which allows regularizing void growth and strain-controlled nucleation.

2. Results

Methodology: the model used in this study to represent the coupling between mechanical loading and hydrogen diffusion was proposed by Sofronis & McMeeking [3] and corrected by Krom *et al.* [4]. The hydrogen flux depends on the pressure gradient, so that hydrogen diffuses towards highly stressed areas. An alternative procedure to solve the coupled diffusion/mechanical behavior problem is presented. It is based on the use of mixed finite elements employed to solve problems in which volumetric locking is observed [5]. In this case, the nodal unknowns of the problem are the displacement, the pressure, volume variation and hydrogen concentration in the lattice. Using these elements, the hydrostatic stress is a nodal variable, so that it becomes straightforward to compute its gradient, which strongly influences hydrogen diffusion. The Gurson-Tvergaard-Needleman (GTN) is considered to model the ductile rupture. Such a model leads to spurious damage and strain localization (and mesh dependence). To solve this problem and to account for interactions between neighboring material points, a nonlocal FE formulation is used to regularize strain/damage localization. It is based on an implicit gradient nonlocal model with two internal lengths (applied to plastic volume variation and accumulated plastic strain). The model allows regularizing void growth, strain-controlled nucleation. Mesh size and orientation independence is achieved for sufficiently fine meshes.

Simulations: Figure 1 shows the pressure field under the contact zone for a disk test considering the regular and the mixed formulation, respectively. It is possible to observe that pressure becomes more continuous using the proposed formulation. The hydrogen diffusion can also be observed for the same disk test (see Figure 2). It is possible to observe that hydrogen diffuses towards the center of the disk, which is the mostly stressed area. Figure 3 shows that lower pressurization rates present a stronger softening since hydrogen has a longer time to diffuse in the material. However, failure corresponds to the limit load being reached since this case does not consider damage. The simulation of damage with a nonlocal GTN model coupled to hydrogen allows observing that damage is higher in the region where necking takes place (see Figure 4).

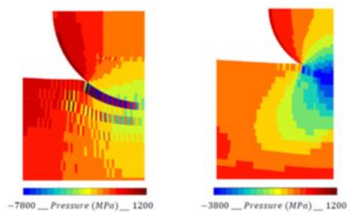

Figure 1 - Pressure fields obtained with the regular and the mixed element, respectively.

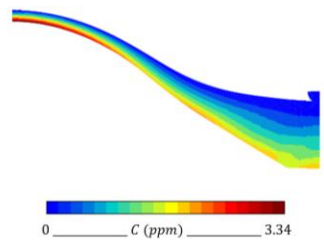

Figure 2 – Hydrogen distribution inside the disk.

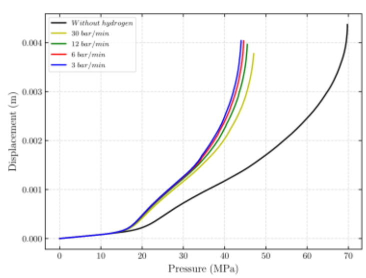

Figure 3 – Effect of hydrogen and loading rate.

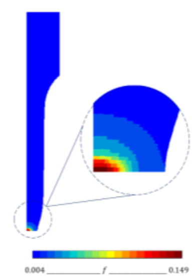

Figure 4 – Damage localization for a tensile test.

4. Conclusions

This study presented a strategy that is capable of simulating hydrogen embrittlement by the finite element method integrating plasticity and damage, coupled to hydrogen diffusion. The mixed formulations in displacement, pressure, volume variation and hydrogen lattice concentration proved to be efficient in controlling volumetric locking. The nonlocal FE formulation with two internal lengths allows regularizing strain/damage localization. Experiments will allow a better fit of the material parameters.

Acknowledgments

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