COMPUTATIONAL PREDICTIONS OF HYDROGEN ASSISTED FRACTURES

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Abstract
Hydrogen significantly reduces the ductility, toughness and fatigue crack growth resistance of metals, which leads to premature failures across many industrial sectors and compromises the role of hydrogen as energy carrier in the transition to a low carbon economy. This paper provides an overview of the efforts by the author and his collaborators in developing a computational framework capable of predicting hydrogen-assisted failures by providing a mechanistic description of hydrogen uptake, transport and embrittlement. The ability of the computational models developed to deliver predictions in agreement with laboratory experiments and over scales relevant to engineering practice is showcased.

1. Introduction

The ingress of hydrogen into a metal is known to cause a dramatic reduction in material strength, ductility, toughness and fatigue resistance, which has led to numerous catastrophic failures across the transport, defence, energy and construction sectors [1]. This phenomenon, referred to as *hydrogen embrittlement*, has attracted the attention of the material science and solid mechanics communities for decades due to its important technological implications and the scientific challenges inherent to its complex chemo-micromechanical nature. Moreover, the problem has come very much to the fore in recent years as a consequence of the higher susceptibility of new, high-strength alloys, and because of the promise that hydrogen holds as a future energy carrier, requiring the development of suitable structures for hydrogen storage and transport. As a result, there is significant interest in the development of computational tools that can enable simulation-based assessment of components exposed to hydrogen, so as to map safe regimes of operation, prevent catastrophic failures and enable a safe deployment of a hydrogen energy infrastructure. This paper describes how phase field and multi-physics (electro-chemo-mechanics) modelling can be combined to resolve the physical processes at play and predict hydrogen uptake, transport and subsequent fracture.

2. Results

A finite element-based computational framework is developed to capture the three stages involved in hydrogen-assisted fracture:

1) Hydrogen uptake: an electro-chemo-mechanical framework is presented that explicitly resolves the electrochemical behaviour of the electrolyte, the hydrogen and corrosion reactions, the kinetics of surface adsorption, and hydrogen uptake, diffusion and trapping in mechanically-deforming solids [2]. The model uses as degrees-of-freedom (DOFs) the electrolyte potential, the concentration of ionic species in the electrolyte, the surface coverage, the displacement of the metal and the hydrogen concentration in the metallic lattice. By resolving the reaction and adsorption kinetics, the uptake of hydrogen can be predicted for arbitrary choices of applied potential, defect geometry, fluid velocity and environment. For gaseous environments, the formulation is greatly simplified but still accounts for surface kinetics and the role of the hydrostatic stress in enhancing the material solubility.

2) Hydrogen transport in the metallic lattice: formulations are developed, considering both Oriani's equilibrium [3] and the more general case of McNabb-Foster [4], to describe lattice hydrogen diffusion and trapping. The presence of multiple trap types, with different densities and binding energies is accounted for.

3) Hydrogen-assisted fracture: the role of hydrogen in reducing the fracture and fatigue resistance of metals is incorporated by means of a novel phase field fracture formulation [5]. Hydrogen-toughness interactions are quantitatively incorporated by considering an implicitly multi-scale approach by which the degradation

of the fracture energy with surface coverage is connected to the hydrogen occupancy at critical interfaces through first-principles calculations. In addition, the modelling framework is extended to fatigue by means of a fatigue degradation function [6].

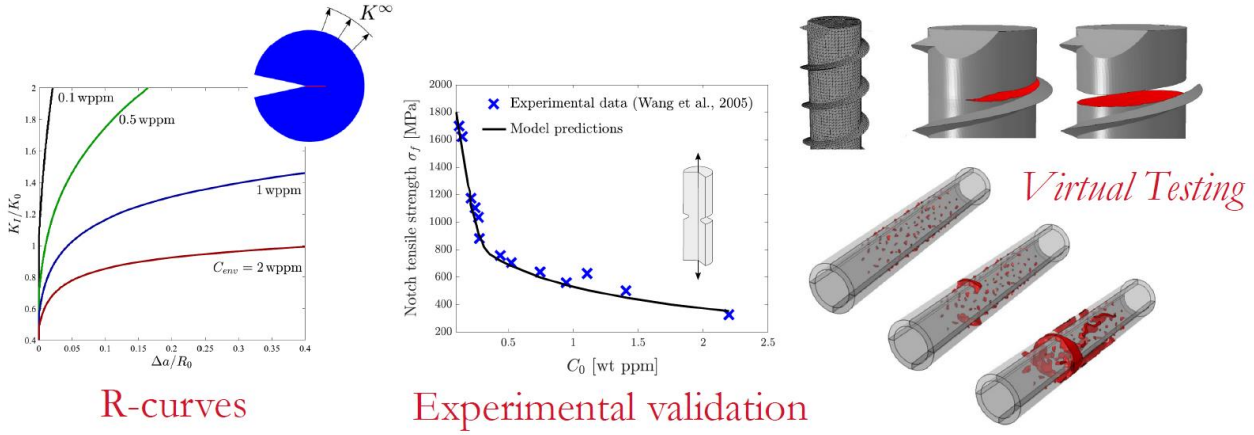

Fig.1 – Overview of the predictive capabilities of electro-chemo-mechanical phase field models for hydrogen embrittlement: from virtual laboratory experiments to technologically-relevant predictions [7].

3. Conclusions

Representative results are shown in Fig. 1. It can be seen that the multi-physics phase field-based framework developed can capture the qualitative effect that hydrogen has on crack growth resistance curves (R-curves) but can also quantitatively predict experimental measurements for a wide range of hydrogen contents. Moreover, the framework can simulate the nucleation and growth of cracks in hydrogen-containing environments over time and length scales relevant to engineering practice [8].

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