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Cohesive zone modeling of fatigue crack propagation assisted by gaseous hydrogen in metals

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ABSTRACT

Experimental studies in a hydrogenous environment indicate that hydrogen leads to a modification of deformation and damage mechanisms at the fatigue crack tip in metals, resulting in a significant decrease of crack propagation resistance. This study aims at building a model of these complex phenomena in the framework of damage mechanics, and to confront it with the results of fatigue crack propagation tests in high pressure hydrogen on a 15-5PH martensitic stainless steel. A cohesive zone model is implemented in the finite element code ABAQUS. A specific traction-separation law is developed, which is suitable for cyclic loadings, and whose parameters depend on local hydrogen concentration. Furthermore, hydrogen diffusion in the bulk material takes into account the influence of hydrostatic stress and trapping. Simulated fatigue crack propagation rates in hydrogen are compared to experimental measurements. The model ability to assess the respective contributions of the different damage mechanisms in the degradation of the crack resistance of the 15-5PH steel is discussed.

1. Introduction

The role of hydrogen in deformation and damage processes taking place at the crack tip has been commonly evoked to account for environmentally-assisted fatigue crack growth in metals exposed to an hydrogenous environment [1], although the mechanisms responsible for the observed loss of crack growth resistance, which can be tremendous in some cases, were not fully elucidated. This issue meets a renewed interest due to the forthcoming shortage of fossil energy sources and environmental concerns which motivate the development of hydrogen-based energy infrastructure. Indeed, the materials which would be used in such infrastructures and that may contain crack-like defects would have to withstand a direct exposure to high pressure of gaseous hydrogen in conjunction with the application of a cyclic mechanical loading. This question is generally tackled from the point of view of the compatibility of a given metal with gaseous hydrogen [2]. However the question of compatibility of a given material is not straightforward and one has to define the boundary of safe operation conditions. Therefore, the integrity of the hydrogen transport and storage structures cannot be guaranteed without a sound understanding of the damage mechanisms prevailing at a crack tip in a gaseous hydrogen environment and an identification of the controlling factors. From a more fundamental point of view, an improved understanding of hydrogen interactions with deformation and damage mechanisms at the tip of a fatigue crack is needed.

With this perspective, the Pprime Institute has undertaken, a couple of years ago, the development of a new test bench named Hycomat in order to investigate the mechanical behavior of structural materials under high pressure of gaseous environments [3,4]. Hycomat is composed of a specially designed autoclave assembled to a servohydraulic loadframe. The maximum operating pressure is 40 MPa, and the highest temperature in the autoclave is 150 °C. Cyclic loadings can be applied with different frequencies on Compact Tension specimens. A computerized system is associated to control the testing process by monitoring the crack length by means of a potential drop technique. However, such experiments are costly and the results are extremely complex to analyze, for instance when considering different pressure/load frequency conditions as [4]. This is the reason why it was decided at the same time to develop a model based on coupled effects between mechanical cyclic loading and hydrogen diffusion. A specifically designed cohesive zone approach, in which hydrogen directly affects the traction-separation law, is investigated. The objective is not only to simulate the experimental results or provide accurate fatigue life predictions, but also to provide a numerical tool that can be used to analyze and understand the different pressure and/or frequency effects on fatigue crack growth rates. This paper

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Nomenclature

ΔK	stress intensity factor amplitude (MPa $\times$ m$^{1/2}$)
R	load ratio
δ_n	normal component of the displacement in the cohesive zone
$\delta_{n,max}$	maximum value of δ_n
δ_t	tangential component of the displacement in the cohesive zone
φ	thermodynamic potential of the traction-separation law
D	damage variable, ranging from 0 to 1
D_m	monotonic part of the damage variable
D_c	cyclic part of the damage variable
k	initial normal tension stiffness,
k_{comp}	compression stiffness
k_t	tangent stiffness
δ_0	dimensionless parameter
$\vec{T}(T_n, T_t)$	cohesive traction vector
$T_{n,in}$	value of the normal cohesive traction component at damage initiation
f_c	threshold function for the onset of the cyclic damage
f_m	threshold function for the onset of the monotonic damage
c_c	constant related to the cyclic damage initiation
c_m	constant related to the monotonic damage initiation
m_c	constant controlling the cyclic damage progressivity
n_c	cyclic exponent
N_L	density of hydrogen lattice sites
N_T	density of hydrogen trap sites
m_m	constant controlling the monotonic damage progressivity
n_m	monotonic exponent
$r_{p,cyc}$	size of the cyclic plastic zone
Y	thermodynamic force associated with the damage parameter D
F_{sta}	mean value of the applied cyclic loading
ΔF	amplitude of the applied cyclic loading
Δg_b^0	Gibbs free energy difference between a microstructural interface (crystallographic planes, grain boundary,...) and the bulk material
C_H	hydrogen concentration
θ	hydrogen coverage rate
C_L	hydrogen concentration in lattice
C_T	hydrogen concentration in traps,
D_L	the lattice diffusivity coefficient,
$\overline{V}_h$	mean molar volume of hydrogen
σ_h	hydrostatic stress

presents the principles of the model considered and preliminary results from numerical computations.

2. A cohesive zone model for cyclic loading

2.1. Selection of the type of model

Literature offers various possibilities to model damage at a crack tip at different scales. Thermodynamic approaches [5] can indicate if hydrogen embrittlement is likely to occur but they do not explicitly address the damage process, especially at the crack scale. Meanwhile hydrogen-assisted fracture can be envisaged from an atomistic point of view [6]. Some attempts have been made to fill the gap between these two types of envision [7]. On the opposite, global approaches, based on continuum mechanics, such as J-integral and CTOD methods, micromechanical models such as the Gurson model [8], as well as more recent phenomenological numerical approaches, such as the eXtended Finite Element Method (X-FEM), developed by Belytschko et al. [9,10], have been successfully applied to address fracture problems without most generally considering a specific role of hydrogen. Among these approaches, the cohesive zone models (CZM), based on the original work of Dugdale [11] and Barenblatt [12], deserve attention. Indeed the cohesive zone represents the area near the crack tip (the so-called process zone) by a relation between cohesive stress and crack opening displacement, called the Traction-Separation Law (TSL). Moreover the cohesive zone models have the advantage of being flexible, considering that the TSL shape is a matter for phenomenological issues. One main limitation in this kind of approach resides in the fact that it usually requires a predefined crack path. The usual traction-separation laws include linear [13] , multilinear [14,15], polynomial [16] or exponential [17] laws. Furthermore it has to be noticed that they have been applied with a certain success to account for hydrogen-assisted cracking under monotonic or static loading [18–21]. However, the traction-separation laws suffer from the absence of stiffness degradation under cyclic loading, with the noticeable exceptions in [22–24].

As mentioned in the previous section, the main goal of this study is to develop a simulation tool that can predict the fatigue crack growth under different hydrogen exposure conditions, that is to say different pressures, loading frequencies and possibly various temperatures, but not, at this stage, to predict the crack path within a component submitted to a complex loading. Therefore the limitation related to a predefined crack path is not really an issue. Meanwhile the capability of CZM to describe hydrogen-assisted fracture under static and monotonic loading is attractive. Therefore a CZM approach was selected in this study, with the development of a specific TSL, established within the framework of the Thermodynamics of Irreversible Processes and that could address the various issues listed here above. Indeed this TSL has firstly to describe fatigue crack propagation. Furthermore, the parameters of this TSL are dependent on hydrogen coverage in an attempt to account for the detrimental influence of hydrogen on fatigue crack growth [4]. The basic idea is that the damage process is localized within the cohesive zone, which means that the bulk material surrounding this zone is not damaged despite the elasto-plastic cyclic deformation endured. The TSL is described by 2 vectors, namely a crack opening displacement vector and a cohesive stress vector. At this first stage, the model will be developed in a 2D framework.

The mechanical behavior of the bulk will be described by conventional elasto-plastic constitutive laws while the local hydrogen concentrations will be determined from constitutive equations for hydrogen and trapping, including the effects of traps.

2.2. Development of a specific traction-separation law

2.2.1. Monotonic and cyclic damage

Cohesive zone models describe the area near the crack tip – called the "process zone" – by a local relation between the cohesive traction vector and the opening displacement, which is the difference between the top and bottom crack lip displacements [17,25–27]. In a 2D framework, the opening displacement is defined by its normal (δ_n) and tangential (δ_t) components. The cohesive law is introduced via the thermodynamic potential φ:

$$\varphi = \frac{1}{2}k(1-D)\frac{\langle\delta_n\rangle^2}{\delta_0} + \frac{1}{2}k_{comp}\frac{\langle-\delta_n\rangle^2}{\delta_0} + \frac{1}{2}k_t\frac{\delta_t{}^2}{\delta_0} \quad (1)$$

where $\langle\ldots\rangle$ stands for the positive part.