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## A cohesive zone framework for environmentally assisted fatigue

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#### ABSTRACT

We present a compelling finite element framework to model hydrogen assisted fatigue by means of a hydrogen- and cycle-dependent cohesive zone formulation. The model builds upon: (i) appropriate environmental boundary conditions, (ii) a coupled mechanical and hydrogen diffusion response, driven by chemical potential gradients, (iii) a mechanical behavior characterized by finite deformation J2 plasticity, (iv) a phenomenological trapping model, (v) an irreversible cohesive zone formulation for fatigue, grounded on continuum damage mechanics, and (vi) a traction-separation law dependent on hydrogen coverage calculated from first principles. The computations show that the present scheme appropriately captures the main experimental trends; namely, the sensitivity of fatigue crack growth rates to the loading frequency and the environment. The role of yield strength, work hardening, and constraint conditions in enhancing crack growth rates as a function of the frequency is thoroughly investigated. The results reveal the need to incorporate additional sources of stress elevation, such as gradient-enhanced dislocation hardening, to attain a quantitative agreement with the experiments.

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#### 1. Introduction

Metallic materials play a predominant role in structures and industrial components because of their strength, stiffness, toughness and tolerance of high temperatures. However, hydrogen has been known for over a hundred years to severely degrade the fracture resistance of advanced alloys, with cracking being observed in modern steels at one-tenth of the expected fracture toughness. With current engineering approaches being mainly empirical and highly conservative, there is a strong need to understand the mechanisms of such hydrogen-induced degradation and to develop mechanistic-based models able to reproduce the microstructure-dependent mechanical response at scales relevant to engineering practice.

Models based on the hydrogen enhanced decohesion (HEDE) mechanism have proven to capture the main experimental trends depicted by high-strength steels in aqueous solutions and hydrogen-containing gaseous environments [1]. The use of cohesive zone formulations is particularly appealing in this regard, as they constitute a suitable tool to characterize the sensitivity of the fracture energy to hydrogen coverage. The cohesive traction separation law can be derived from first principles quantum mechanics [2] or calibrated with experiments [3,4]. The statistical distribution of relevant microstructural features has also fostered the use of weakest-link approaches [5,6]. Very recently, Martínez-Pañeda et al. [7] integrated strain gradient plasticity simulations and electrochemical assessment of hydrogen solubility in Gerberich [8] model. The investigation of a Ni-Cu superalloy and a modern ultra-high-strength steel revealed an encouraging quantitative agreement with

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$\alpha$ compression penalty factor $\overline{V}_H$ partial molar volume of hydrogen $\beta_{B}$ number of lattice sites per solvent atom $\beta_{B}^{0}$ Gibbs free energy difference $A_n$ normal cohesive separation $\delta_n$ characteristic normal cohesive length $\delta_{\Sigma}$ accumulated cohesive length $\delta_{\Sigma}$ accumulated cohesive length $C, m$ Paris law coefficients $N, \mathcal{D}_{r}$ standard and effective diffusion coefficients $N$ strain hardening exponent $\mathcal{R}$ universal gas constant $\mathcal{T}$ absolute temperature $\mu_{L}$ lattice chemical potential $\phi_n$ normal cohesive energy $\rho$ density $\sigma_{IL}$ cohesive endurance limit $\sigma_{IL}$ normal cohesive energy $\rho$ density $\sigma_{IL}$ cohesive endurance limit $\sigma_{IL}$ normal cohesive and rapping sites $\delta_{T}$ equivalent plastic strain $\sigma_{IL}$ local field and nodal separation vectors $\mathcal{L}$ elastoplastic constitutive matrix $\sigma$ Cauchy strain tensor $\mathcal{L}$ cohesive displacement-separation matrix $\mathcal{R}$ rotation displacement separation matrix $\mathcal{R}$ rotational matrix $\mathcal{L}$ local displacement separation vectors $\mathcal{L}$ local displacement vector $\mathcal{L}$ local displacement vector $\mathcal{L}$ local displacement vector $\mathcal{L}$ local displacement vector $\mathcal{L}$ global nodal displacem	Nomenclature		
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