Engineering Fracture Mechanics 185 (2017) 210–226

Contents lists available at ScienceDirect

Engineering Fracture Mechanics

journal homepage: www.elsevier.com/locate/engfracmech

A cohesive zone framework for environmentally assisted fatigue

Susana del Busto [a], Covadonga Betegón [a], Emilio Martínez-Pañeda [b,*]

[a] Department of Construction and Manufacturing Engineering, University of Oviedo, Gijón 33203, Spain
[b] Department of Mechanical Engineering, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark

ARTICLE INFO

Article history:
Received 6 February 2017
Received in revised form 14 May 2017
Accepted 16 May 2017
Available online 27 May 2017

Keywords:
Hydrogen embrittlement
Cohesive zone models
Hydrogen diffusion
Finite element analysis
Fatigue crack growth

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.

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

* Corresponding author.
E-mail address: mail@empaneda.com (E. Martínez-Pañeda).

http://dx.doi.org/10.1016/j.engfracmech.2017.05.021

Nomenclature

α	compression penalty factor
$\overline{V}_H$	partial molar volume of hydrogen
β	number of lattice sites per solvent atom
Δg_b^0	Gibbs free energy difference
Δ_n	normal cohesive separation
δ_n	characteristic normal cohesive length
δ_Σ	accumulated cohesive length
$\mathcal{C}, m$	Paris law coefficients
$\mathcal{D}, \mathcal{D}_e$	standard and effective diffusion coefficients
$\mathcal{N}$	strain hardening exponent
$\mathcal{R}$	universal gas constant
$\mathcal{T}$	absolute temperature
μ_L	lattice chemical potential
ϕ_n	normal cohesive energy
ρ	density
σ_f	cohesive endurance limit
σ_H	hydrostatic stress
σ_Y	initial yield stress
$\sigma_{\max}, \sigma_{\max,0}$	current and original cohesive strength
θ_H	hydrogen coverage
θ_L, θ_T	occupancy of lattice and trapping sites
ε_p	equivalent plastic strain
$\boldsymbol{\Delta}, \tilde{\boldsymbol{\Delta}}$	local field and nodal separation vectors
$\boldsymbol{\mathcal{L}}$	elastoplastic constitutive matrix
$\boldsymbol{\sigma}$	Cauchy stress tensor
$\boldsymbol{\varepsilon}$	Cauchy strain tensor
$\boldsymbol{B_c}$	global cohesive displacement-separation matrix
$\boldsymbol{B}$	standard strain-displacement matrix
$\boldsymbol{f_c}$	cohesive internal force vector
$\boldsymbol{J}$	hydrogen flux vector
$\boldsymbol{K_c}$	cohesive tangent stiffness matrix
$\boldsymbol{L}$	local displacement-separation matrix
$\boldsymbol{N}$	shape functions matrix
$\boldsymbol{R}$	rotational matrix
$\boldsymbol{t}$	external traction vector
$\boldsymbol{T}, \tilde{\boldsymbol{T}}$	standard and effective cohesive traction vectors
$\boldsymbol{U}$	global nodal displacement vector
$\boldsymbol{u}, \tilde{\boldsymbol{u}}$	field and local nodal displacement vectors
a	crack length
b, b_0	current and initial crack opening displacement
C	total hydrogen concentration
C_L, C_T	hydrogen concentration in lattice and trapping sites
c_q	specific heat capacity
D, D_c, D_m	damage variable: total, cyclic and monotonic
E	Young's modulus
f	load frequency
K, K_0	remote and reference stress intensity factor
K_T	trap equilibrium constant
N	number of cycles
N_A	Avogadro's number
N_L, N_T	number of lattice and trapping sites per unit volume
q	heat flux per unit area
R	load ratio
R_0	reference plastic length
T	elastic T-stress
T_n	normal cohesive traction
U	internal energy per unit mass
V_M	molar volume of the host lattice
W_B	trap binding energy