Available online at www.sciencedirect.com

ScienceDirect

Procedia Engineering 10 (2011) 2657–2662

Engineering Procedia

ICM11

Influence of hydrogen coverage on the parameters of a cohesive zone model dedicated to fatigue crack propagation

C. Moriconi[a]*, G. Henaff[a], D. Halm[a]

[a]*Institut P' (UPR 3346) – CNRS – ENSMA – Université de Poitiers, département Physique et Mécanique des Matériaux, ENSMA, 1 Avenue Clément Ader, BP40109, 86961 FUTUROSCOPE CHASSENEUIL, FRANCE*

Abstract

Experimental studies indicate a deleterious influence of a hydrogenous environment on the fatigue crack propagation resistance of metallic materials. In order to provide a predictive tool to assess fatigue lifetime of structures subjected to hydrogen, an ABAQUS finite element model of a compact tension (CT) specimen has been developed. A cohesive zone model (CZM) with a specific traction-separation law is used in conjunction with an elastic-plastic bulk material to model fatigue crack growth. The traction-separation law has been developed to take into account the influence of cyclic loading on crack propagation. A special attention has been paid to develop the model in the framework of thermodynamics, i.e. to ensure that the dissipation remains positive at any time. In addition, the parameters of the traction-separation law depend on local hydrogen concentration. This traction-separation law was implemented using ABAQUS user element subroutine UEL which is used to predict the influence of hydrogen on fatigue crack growth rates. Given the similarity between heat and mass diffusion equations, the coupling between hydrogen diffusion and the mechanical behaviour of the material has been implemented using ABAQUS coupled temperature-displacement procedure.

Keywords: Fatigue damage; hydrogen; simulation; cohesive zone model

1. Introduction

At a time where one of the world's greatest challenges is finding new sources of energy, scientists consider the idea of using hydrogen as an energy supply. With this respect, studying and understanding the complex interactions between hydrogen and deformation remains a critical point, so that gaseous hydrogen may be stored and transported at minimal risk. More particularly, experience shows that hydrogen has a deleterious influence on the fatigue crack propagation resistance of metallic materials. This paper presents a work under progress that aims at creating a numerical tool able to predict crack propagation in a structure exposed to gaseous hydrogen and submitted to fluctuating loads.

In literature, numerous possibilities to model damage at a crack tip are proposed. One can mention global approaches, such as J-integral and CTOD methods, micromechanical models such as Gurson's model [1], as well as

* Corresponding author. Tel.: +33 5 49 49 82 15; fax: +33 5 49 49 82 38.
E-mail address: clara.moriconi@ensma.fr.

Selection and peer-review under responsibility of ICM11 doi:10.1016/j.proeng.2011.04.443

more recent phenomenological numerical approaches, such as the eXtended Finite Element Method (X-FEM), developed by Belytschko et al [2], and cohesive zone models (CZM), originally introduced by Dugdale [3] and Barenblatt [4]. The latter represents the area near the crack tip by a relation between cohesive stress and crack opening, called traction-separation law. Cohesive zone models have the advantage of being flexible, considering that the traction-separation law shape is a matter for phenomenological issues; however, they usually require a predefined crack path. Literature indicates that the traction-separation laws that are the most used are linear [5], multi-linear [6], polynomial [7] or exponential [8]. However, these traction-separation laws suffer from the absence of stiffness degradation under cyclic loading.

In this study, a specific law has been developed in order to model the progressive degradation of stiffness during cyclic loading, thus enabling fatigue crack propagation. This paper is focused on the principles of the model construction. Much attention has been given to develop a traction-separation law in the framework of the Thermodynamics of Irreversible Processes. Furthermore, the harmful influence of hydrogen on fatigue crack growth [9] has been taken into account by making the traction-separation law's parameters depend on hydrogen coverage [10]. This will be further detailed in Section 2. The cohesive zone model has been implemented in the finite element program ABAQUS, using user element subroutine UEL. The user element supports hydrogen diffusion.

Given the similarity between heat and mass diffusion equations, the coupling between hydrogen diffusion and the mechanical behavior of the material has been implemented using the coupled temperature-displacement procedure available in ABAQUS. This will be further detailed in Section 3.

2. 2D hydrogen-influenced "fatigue" traction-separation law

The more recent versions of ABAQUS offer a vast library of elements, which includes cohesive elements. However, they only allow linear or exponential damage evolution and are not adapted to cyclic loadings. Therefore, a specific "fatigue" (*i.e.*, accounting for damage accumulation under cyclic loading) traction-separation law has been developed and implemented in finite element software ABAQUS using user element subroutine UEL.

Cohesive zone models describe the area near the crack tip – called "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. 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:

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

where <…> stands for the positive part. The scalar D is the damage parameter, ranging from 0 to 1. Constants k, k_{comp} and k_t are, respectively, the initial normal tension stiffness, the compression stiffness (high value penalization coefficient to avoid material interpenetration) and the tangent stiffness (as only mode I propagations are here considered, we assume that there is no damage under shear loading). The cohesive traction vector $\vec{T}(T_n, T_t)$ is derived from the potential φ by the following relations:

$$T_n = \frac{\partial\varphi}{\partial\delta_n} = k(1-D)\langle\delta_n\rangle + k_{comp}\langle-\delta_n\rangle \qquad (2)$$

$$T_t = \frac{\partial\varphi}{\partial\delta_t} = k_t\delta_t \qquad (3)$$

The damage threshold f=0, involving the loading history, is chosen as follows:

$$f = \int_0^t \langle\dot{Y}\rangle(1-D)d\tau - (c+mD) \qquad (4)$$

where c is a constant. The constant m influences the evolution of the damage variable D. The thermodynamic force Y associated with the damage variable D is defined as follows:

$$Y = -\frac{\partial \varphi}{\partial D} = \frac{1}{2} k \langle \delta_n \rangle^2 \tag{5}$$

The expression of the evolution of D is obtained from the consistency equation $\dot{f} = 0$, stating that, while the damage criterion f=0 is satisfied, the damage loading process is pursued:

$$\dot{D} = \frac{k}{m}(1 - D)\langle \delta_n \rangle \langle \dot{\delta}_n \rangle \tag{6}$$

Eq. 6 shows that the value of the damage variable D increases when the normal opening displacement δ_n and its time derivative are both strictly positive. However D is not allowed to decrease. This means that damage increases during loading phases – if the damage threshold is reached – and remains constant during unloading. Fig. 1 represents the normal cohesive traction T_n versus the normal opening displacement δ_n under monotonous and cyclic loading (prescribed displacement amplitude $\Delta\delta_{pre}$). Note the progressive decrease of the traction cycle after cycle. In Fig. 1, the values of the parameters are k=10^8 MPa/mm, m=300 N, and c=5 N. These values were chosen as a first approximation; in the future, an identification method will allow to determine more precise values.

In order to take into account the influence of hydrogen on fatigue crack growth, the parameters k and m of the traction-separation law are supposed to depend on hydrogen coverage θ [10], ranging from 0 to 1, which is defined as a function of local hydrogen concentration in the material C_H and the Gibbs free energy difference between the interface and the bulk material Δg^0_b:

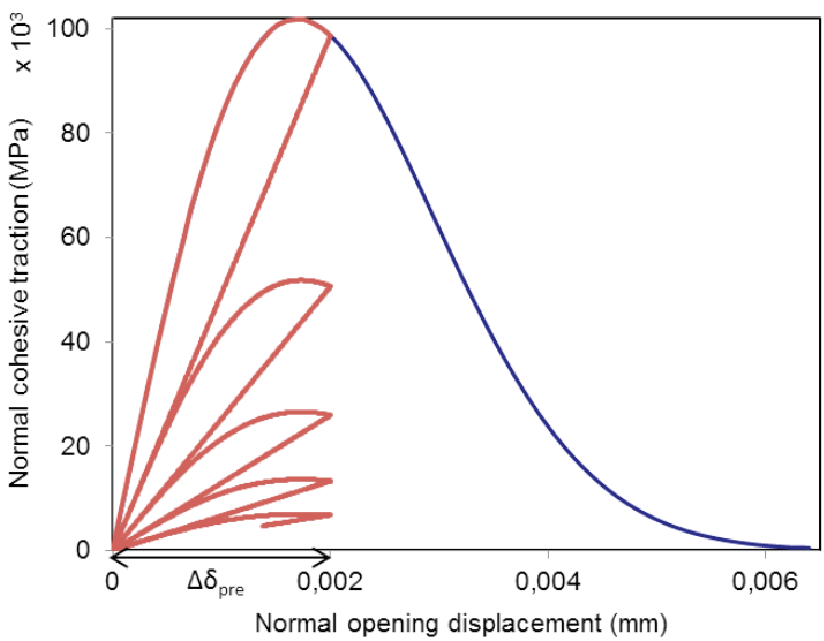

Fig. 1. Normal traction-separation law under monotonous (blue curve) and cyclic (red curve) loadings, for k=10^8 MPa/mm, m=300 N and c=5 N.

$$\theta = \frac{C_H}{C_H + \exp\left(-\Delta g_b^0 / RT\right)} \tag{7}$$

An increase in hydrogen coverage leads to a lower stiffness and a quicker failure of the interface, *i.e.* a smaller number of cycles is needed for the element to break. Therefore, it is assumed that increasing hydrogen coverage leads to a decrease of traction-separation parameters k and m. In first approach, the hydrogen coverage θ is supposed to influence differently the parameters k and m and the following expressions are chosen:

$$k(\theta) = (1-\theta)k(0) \tag{8}$$

$$m(\theta) = (1-\theta)^2 m(0) \tag{9}$$

where k(0) and m(0) are the values of k and m without hydrogen. Fig. 2 shows the normalized traction-separation law for various values of hydrogen coverage. As hydrogen coverage increases, the traction-separation law starts to soften sooner; furthermore, the maximum value of normal stress traction decreases, and failure occurs for a smaller normal opening displacement.

3. Implementation of the hydrogen diffusion equation

In ABAQUS, no coupled mechanics – mass diffusion procedure is available. Hopefully, the equation of hydrogen diffusion shares many similarities with the heat equation. As shown in Table 1, a parallel can be drawn between nodal temperature and nodal hydrogen concentration, as well as heat flux and mass diffusion flux.

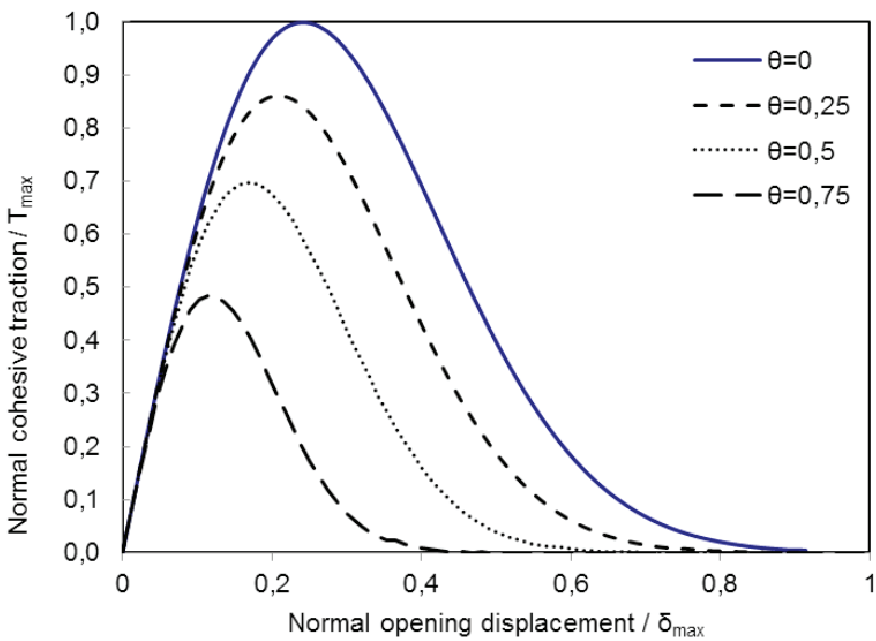

Fig. 2. Normalized traction-separation law under monotonous loading for different values of hydrogen coverage.

Table 1. Parallel between heat equation and mass diffusion equation

	Heat equation	Mass diffusion equation
	$\rho C_P \frac{\partial T}{\partial t} + div\vec{J}_q + r_q = 0$	$\frac{\partial C}{\partial t} + div\vec{J}_m + r_m = 0$
Nodal quantity (unit)	Temperature T (K)	Hydrogen concentration C (g/mol)
Heat/mass flux (unit)	$\vec{J}_q$ (W/m^2)	$\vec{J}_m$ (g.m/mol/s)
Heat/mass source (unit)	r_q (W/m^3)	r_m (g/mol/s)

Therefore, the coupling between mechanics and hydrogen diffusion can be modeled using the coupled temperature-displacement step, which is available in ABAQUS. A user-defined mass diffusion equation can be implemented in ABAQUS using subroutine UMATHT, which defines user thermal behavior. In the present study, the diffusion of hydrogen in the bulk material is governed by the equation proposed by Liang and Sofronis [11], which is detailed below. Let the hydrogen concentration at lattice sites be written as C_L, and the hydrogen concentration at trap sites be written as C_T. The hydrogen conservation equation gives:

$$\frac{\partial}{\partial t}\int_V \{C_L + C_T\}dV + \int_S \vec{J}.\vec{n}dS = 0. \quad (10)$$

$\vec{J}$ is the hydrogen flux and is defined by a modified Fick's law with respect to the hydrostatic stress σ_h:

$$\vec{J} = -D_L\vec{\nabla}C_L + \frac{D_L C_L V_H}{RT}\vec{\nabla}\sigma_h \quad (11)$$

In Eq. 11, D_L is the hydrogen lattice diffusion coefficient, V_H is the partial molar volume of hydrogen, σ_h is the hydrostatic stress, R is the gas constant, and T is the absolute temperature.

As shown in Eq. 11, hydrogen diffusion is driven by the gradient of hydrogen concentration, and the gradient of hydrostatic stress. The former is available in subroutine UMATHT, while the latter is estimated using ABAQUS subroutine USDFLD. The hydrostatic stress gradient at the integration points of the element is calculated by interpolating hydrostatic stress between the integration points of the bulk elements.

Finally, the hydrogen diffusion equation – with Fick's law – is also implemented in the subroutine UEL to allow hydrogen diffusion in the process zone.

4. Conclusion

A model of hydrogen-assisted crack propagation in metals was developed in the commercial software ABAQUS. A cohesive user element with a specific traction-separation law adapted to cyclic loadings was implemented via a subroutine UEL. The parameters of the traction-separation law depend on hydrogen concentration. In the bulk material, the coupling between hydrogen diffusion and mechanical behavior was taken into account via a coupled temperature-displacement procedure.

The continuation of the present study will be to simulate the influence of hydrogen on the fatigue crack growth in metals and to confront the results with experimental crack propagation [12].

References

[1] Gurson A. Continuum theory of ductile rupture by void nucleation and growth: part I. Yield criteria and flow rules for porous ductile media. *Journal of Engineering Materials and Technology* 1977;**99**:2–15.

[2] Belytschko T, Dolbow J, Moes N. A finite element method for crack growth without remeshing. *International Journal for Numerical Methods in Engineering* 1999;**46**:131–150.

[3] Dugdale D. Yielding of steel sheets containing slits. *Journal of the Mechanics and Physics of Solids* 1960;**8**:100–104.

[4] Barenblatt G. The mathematical theory of equilibrium cracks in brittle fracture. *Advances in Applied Mechanics* 1962;20.

[5] Camacho G T, Ortiz M. Computational modelling of impact damage in brittle materials. *International Journal of Solids and Structures* 1996;**33**:2899–2938.

[6] Tvergaard V, Hutchinson J. The relation between crack growth resistance and fracture process parameters in elastic-plastic solids. *J Mech Phys Solids* 1992;**40**:1377–1397.

[7] Tvergaard V. Effect of fiber debonding in a whisker-reinforced metal. *Advances Engineering Materials* 1990;**125**:203–213.

[8] Xu X, Needleman A. Void nucleation by inclusion debonding in a crystal matrix. *Modelling and Simulation in Materials Science and Engineering* 1993;**1**:111–132.

[9] Cialone HJ, Holbrook JH. Effects of gaseous hydrogen on fatigue crack growth in pipeline steel. *Metallurgical Transactions A* 1985;**16A**:115-122.

[10] Olden V, Thaulow C, Johnsen R. Modelling of hydrogen diffusion and hydrogen induced cracking in supermartensitic and duplex stainless steels. *Materials and Design* 2008;**29**:1934–1948.

[11] Liang Y, Sofronis P. Toward a phenomenological description of hydrogen-induced decohesion at particle/matrix interfaces. *J Mech Phys Solids* 2003;**51**:1509–31.

[12] Sun Z, Moriconi C, Hamon F, Benoit G, Henaff G. Fatigue crack propagation under gaseous hydrogen in a precipitation-hardened martensitic stainless steel*, to be published.*