

Cohesive zone modeling of hydrogen-induced stress cracking in 25% Cr duplex stainless steel

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Received 7 May 2007; accepted 4 June 2007

Available online 6 July 2007

Hydrogen-influenced cohesive zone elements are implemented in finite element models of rectangular notched tensile specimens of 25% Cr stainless steel. A three-step procedure consisting of stress analysis, diffusion analysis and cohesive zone fracture initiation analysis was performed. A linear traction separation law gives a good fit with experimental results for stress levels just below the material yield stress. Hydrogen concentrations of 40 ppm at the surface and 1 ppm in bulk always produces crack initiation at the surface. © 2007 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.

Keywords: Stainless steels; Cohesive zone modeling; Environmentally assisted cracking; Structural assessment; Pipelines

The occurrence of cracks in offshore structures and pipelines can cause catastrophic failures. In recent years several incidents of hydrogen-induced failure have been reported in subsea oil and gas pipelines and installations in the North Sea. There is a need of establishing reliable and practical test methods and implementing robust requirements in standards and guidelines for materials under hydrogen influence in oil and gas industry. An extra challenge in testing of hydrogen-induced stress cracking (HISC) is the time aspect. Due to very slow hydrogen diffusion rates in stainless steel, laboratory testing aimed at material qualification can be a demanding task.

The present work describes how hydrogen diffusion modeling and cohesive zone modeling (CZM) can offer a supplement to laboratory material qualification.

Two of the most established micromechanical models of hydrogen-assisted fracture are the hydrogen-enhanced decohesion model (HEDE) and the hydrogen-enhanced local plasticity model (HELP). In both models hydrogen fracture is regarded as a result of a critical combination of stress, strain and hydrogen concentration, but the proposed mechanisms for crack initiation and growth are basically different.

The HEDE mechanism was first proposed by Troiano in 1960 [1] and further developed by Oriani [2]

and Gerberich et al. [3]. HEDE is based on the hypothesis that interstitial hydrogen lowers the cohesive strength by dilatation of the atomic lattice and hence lowers the fracture energy. This implies that hydrogen decreases the energy barrier for either grain boundary or cleavage plane decohesion.

HELP is characterized by atomic hydrogen that enhances the mobility of dislocations through an elastic shielding effect in preferred crystallographic planes at the crack tip causing locally reduced shear strength. This “local softening” results in cracking by microvoid coalescence along these planes. The mechanism was first introduced by Birnbaum and co-workers in 1990 [4].

The cohesive element can be pictured as two faces separated by a thickness, which is close to zero. The relative motion of the top and bottom faces in the thickness direction represents opening or closing of the interface. The relevant constitutive “material” response is a traction–separation description; an evaluation which gives the amount of energy required to create new surfaces. A traction–separation law (TSL) is a function described by the cohesive stress (σ) and separation (δ). The area below the curve represents the separation energy, Γ_c . A variety of shapes of the TSL have been reported by different authors [5]. Hydrogen influence can be built into the TSL represented by a gradual decrease in the separation energy with increasing hydrogen content.

Recent approaches in cohesive modeling of hydrogen-assisted fracture are represented by Serebrinsky et al. [6], who have implemented the HEDE approach

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with a brittle TSL response. In the present work the approach as described by Serebrinsky et al. has been applied for the prediction of hydrogen-induced crack initiation in a 25% Cr stainless steel. A linear law for separation of the atomic lattice is applied [9].

$$\sigma(\delta) = \sigma_c \left(1 - \frac{\delta}{\delta_c}\right) \quad \text{for } \delta < \delta_c, \quad \text{otherwise } 0 \quad (1)$$

This implies that the TSL (on an atomic level) is rigid up to a critical stress σ_c and subsequently drops linearly down to zero upon the attainment of a critical δ_c . Serebrinsky et al. [6] suggest the following relation for the coupling between hydrogen coverage, θ , and the critical hydrogen dependent cohesive stress, $\sigma_c(\theta)$:

$$\frac{\sigma_c(\theta)}{\sigma_c(0)} = 1 - 1.0467\theta + 0.1687\theta^2 \quad (2)$$

The relation is based on a fitting of surface energy values calculated by Jiang and Carter [8]. $\sigma_c(0)$ is the critical cohesive stress without hydrogen influence. Hydrogen coverage is defined as a function of the hydrogen concentration and the Gibbs free energy difference between the interface and the surrounding material as expressed in the Langmuir–McLean isotherm [8]:

$$\theta = \frac{C}{C + \exp(-\Delta g_b^0/RT)} \quad (3)$$

where C is the hydrogen concentration (ppm), Δg_b^0 is the Gibbs free energy difference between the surface and the bulk (kJ mol^{-1}), R is the gas constant ($8.3142 \text{ J mol}^{-1} \text{ K}$) and T is the temperature (K).

The hydrogen-influenced TSL is implemented as a two-dimensional user-defined cohesive element and described in a FORTRAN subroutine. A modification of the cohesive element developed by Scheider [9] is applied. The element definition requires a non-zero value for the opening at the critical traction stress, hence a very small value δ_1 of $1.0 \times 10^{-7} \text{ mm}$ is set (see Fig. 2). Crack initiation is defined as the achievement of zero stress and critical opening (δ_c) in the first cohesive element.

The ruling equation for stress driven diffusion given in ABAQUS [10] is

$$J = -sD \left(\frac{\partial \phi}{\partial x} + \frac{\kappa_p \partial p}{\partial x} \right) \quad (4)$$

where J is the hydrogen flux, s is the solubility of hydrogen in Fe, D is the hydrogen diffusion coefficient, ϕ is the normalized hydrogen concentration C/s and x is the position in the body. κ_p is the stress factor linked to gradients in equivalent stress ($\partial p/\partial x$). The mass conservation equation requires:

$$-\frac{\partial}{\partial x} \cdot J = \frac{\partial C}{\partial t} \quad (5)$$

Inserting Eq. (4) into Eq. (5) and using $\phi = C/s$ gives a modified Fick's law with respect to hydrostatic stress:

$$\frac{\partial C}{\partial t} = D \cdot \left[\frac{\partial^2 C}{\partial x^2} + \kappa_p \cdot \frac{\partial C}{\partial x} \cdot \frac{\partial p}{\partial x} + \kappa_p \cdot C \cdot \frac{\partial^2 p}{\partial x^2} \right] \quad (6)$$

As far as possible, material and diffusion data representative of 25% Cr duplex stainless steel are used in the FE model. Supplementary input data for other types of steel are used when no data for 25% Cr duplex steel are available.

The cohesive model is calibrated using data from laboratory testing of 25% Cr duplex steel [11]. A comparison between the predicted time to fracture and the time to fracture observed in the laboratory specimens is the main objective.

The simulations are performed in three steps: (1) stress analysis without hydrogen influence to generate stress fields to be read by diffusion model; (2) transient diffusion analysis with stress driven diffusion. The analyses give the hydrogen distribution to be read into the cohesive elements; and (3) stress analysis using hydrogen dependent user-defined cohesive elements in the crack path.

The material model represents a 25% Cr duplex stainless steel. Young's modulus is taken as 200,000 MPa and Poisson's ratio ν is 0.3. The yield stress is 600 MPa defined at 0.5% total strain.

The samples thickness is 12 mm, the width 9 mm and the length 120 mm. The notch depth is 1.5 mm for the *V*-notch and 2.0 mm for the *U*-notch. In the cohesive model, four-node linear cohesive elements with a length of $\Delta = 10 \mu\text{m}$ are defined at a path along the *x*-axis starting from the bottom of the notch through the cross-section of model. The element mesh in the notch area is presented in Figure 1.

In the elastic plastic stress analysis and the cohesive analyses a constant uniaxial tension stress of 485, 510, 540 and 570 MPa are used, which represents from 80% to 95% of the yield stress. As a reference also zero stress level cases are investigated in the diffusion analyses.

Selected input parameters for the diffusion analyses are presented in Table 1. Note that solubility of hydrogen in ferritic steel is chosen. This is based on the assumption that cracking initiates in ferrite. The diffusion coefficient is calculated from regression equations for lattice diffusion in a 25% Cr steel published by Turnbull et al. [12].

A bulk hydrogen concentration of 1 ppm is chosen. A constant hydrogen concentration of 40 ppm is applied on all outer surfaces. The temperature of 4 °C is representative of the pipes outer surface in subsea conditions. The value of κ_p refers to Eq. (6). The maximum diffusion time is 10,000 h (~416 days). The diffusion time is chosen based on the maximum duration of the laboratory tests.

The laboratory samples were submerged in 4 °C 3.5 wt.% NaCl solution with a cathodic potential (CP) of $-1050 \text{ mV}_{\text{SCE}}$.

The applied linear cohesive law described by Eqs. (1)–(3) requires values for critical traction stress, critical separation and knowledge of the hydrogen distribution in the prescribed crack path. With reference to Serebrinsky et al. [6] and Tvergaard and Hutchinson [13], the

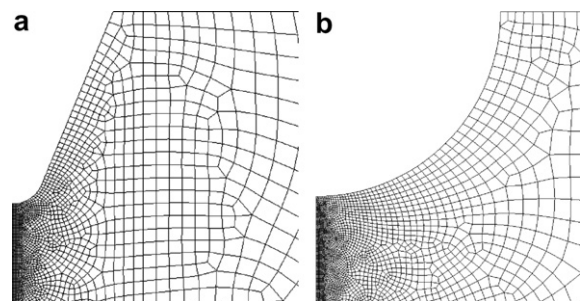


Figure 1. Element mesh in notch area. (a) *V*-notch; (b) *U*-notch.

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