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Simulation of Stress-Corrosion Cracking by the Cohesive Model

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Abstract. The effect of hydrogen on the mechanical behaviour is twofold: It affects the local yield stress and it accelerates material damage. On the other hand, the diffusion behaviour is influenced by the hydrostatic stress, the plastic deformation and the strain rate. This requires a coupled model of deformation, damage and diffusion. The deformation behaviour is described by von Mises plasticity with pure isotropic hardening, and crack extension is simulated by a cohesive zone model. The local hydrogen concentration, which is obtained from the diffusion analysis, causes a reduction of the cohesive strength. Crack extension in a C(T) specimen of a ferritic steel under hydrogen charging is simulated by fully coupled diffusion and mechanical finite element analyses with ABAQUS and the results are compared with test results.

Introduction

Hydrogen induced failure is mainly observed in steels with high yield strength. Elastic lattice expansion at notches and cracks and the high mobility of hydrogen promote the accumulation of hydrogen in these locations. It affects the local yield stress [1], [2] and it reduces the cohesive strength [3], [4]. The degradation of the material can be described by a reduction of crack resistance. Since the hydrogen diffusion is a transient process, the crack-extension rate depends on the deformation rate [5]. Conversely, hydrostatic stress, plastic deformation and strain rate affect diffusion. Advanced models distinguish between hydrogen, which diffuses freely in the lattice, and *trapped* hydrogen, which is not disposable in the lattice diffusion process [6].

Simulation of hydrogen-induced stress-corrosion cracking (HISCC) requires the modelling of diffusion kinetics, plastic deformation and ductile crack extension and their respective interaction. This is realised by fully coupled numerical diffusion and stress analyses, which are able to model the hydrogen transport as well as crack growth. The latter is described by a cohesive model [7], which is widely used for simulations of crack extension [8]. Cohesive zone models with inherent dependence on hydrogen concentration have also been used in [9], [10]. Transport equations are applied for diffusion modelling, accounting the effects mechanical field quantities.

A numerical study shows the influence of various parameters on hydrogen diffusion and crack-resistance.

The HISCC Model

Hydrogen Diffusion. Diffusion is described by the enhanced equation of Krom et al. [11], [12], which distinguishes between trapped and interstitial lattice hydrogen concentrations, C_T and C_L , and accounts for the affect of mechanical quantities on the diffusion.

$$\frac{C_L + C_T(1 - \theta_T)}{C_L} \frac{\partial C_L}{\partial t} - \nabla \cdot \left(\frac{D_L C_L V_H}{RT} \nabla \sigma_h \right) + \theta_T \frac{dN_T}{d\varepsilon_p} \frac{\partial \varepsilon_p}{\partial t} = 0, \quad (1)$$

where θ_T is the occupancy of the trap sites, D_L the lattice diffusivity, V_H the partial molar volume of hydrogen, R the universal gas constant, T the absolute temperature, σ_h the hydrostatic stress, N_T the trap density and ε_p the equivalent plastic strain.

The boundary condition for the adsorption of hydrogen into the specimen is applied at the crack tip according to the sorption model of Zheng and Zhang [13].

The Cohesive Law. Local material degradation and failure is described by a cohesive model [14] relating normal tractions, σ_n , at the element boundaries to the normal separation, δ_n ,

$$\sigma_n = \sigma_n^c \begin{cases} 2\left(\frac{\delta_n}{\delta_1}\right) - \left(\frac{\delta_n}{\delta_1}\right)^2 & \text{for } \delta_n \leq \delta_1 \\ 1 & \text{for } \delta_1 \leq \delta_n \leq \delta_2 \\ 1 - 3\left(\frac{\delta_n - \delta_2}{\delta_n^c - \delta_2}\right)^2 + 2\left(\frac{\delta_n - \delta_2}{\delta_n^c - \delta_2}\right)^3 & \text{for } \delta_2 \leq \delta_n \leq \delta_n^c \end{cases} \quad (2)$$

where the cohesive strength, σ_n^c , depends on the total (both lattice and trap) hydrogen occupancy θ [7],

$$\sigma_n^{c,H}(\theta) = \sigma_n^c (1 + a_1\theta + a_2\theta^2) \quad (3)$$

The quantities a_1 and a_2 are adjusting parameter. The critical separation, δ_n^c , is assumed as independent of the hydrogen concentration.

The Constitutive Law. The deformation behaviour is described by von Mises plasticity with pure isotropic hardening, where the yield strength, $\sigma_Y(\varepsilon_p)$, depends on the lattice hydrogen concentration [15], [16], [17],

$$\sigma_Y^H(\varepsilon_p, C_L) = \sigma_Y(\varepsilon_p) [(\xi - 1)\theta_L(C_L) + 1], \quad (4)$$

where θ_L is the occupancy of the interstitial lattice sites and $\xi < 1$ is an adjusting parameter.

Numerical Simulations of Crack Extension in a C(T) Specimen

Specimen. C(T) specimens of width $W = 40$ mm and thickness $B = 19$ mm made of FeE690T (17MnCrMo3-3) with a yield strength of $\sigma_Y = 693$ MPa have been tested. The specimens were electrolytically charged in situ with hydrogen via cathodic polarisation at -900 mV vs. Ag/AgCl electrode in substitute ocean water according to ASTM D 1141, and were loaded at various constant deformation rates. Crack extension has been simulated numerically by the model described above. The cohesive parameters of the material tested in laboratory air are $\sigma_n^c = 2440$ MPa and $\delta_n^c = 0.016$ mm. Diffusion coefficient $D_L = 7.5 \cdot 10^{-9}$ m²/s and trap densities N_T have been determined in a previous study. The factors in eqs. (3) and (4), a_1 , a_2 , and ξ , have been adjusted to the test results at the lowest deformation rate of 1 $\mu\text{m/h}$.

Boundary Condition for Hydrogen. The hydrogen charging occurred at the actual crack tip and was modelled as a time-dependent boundary condition according to Zhang and Zheng [13] based on test results on the sorption behaviour of hydrogen at metal surfaces as displayed in Fig 1.

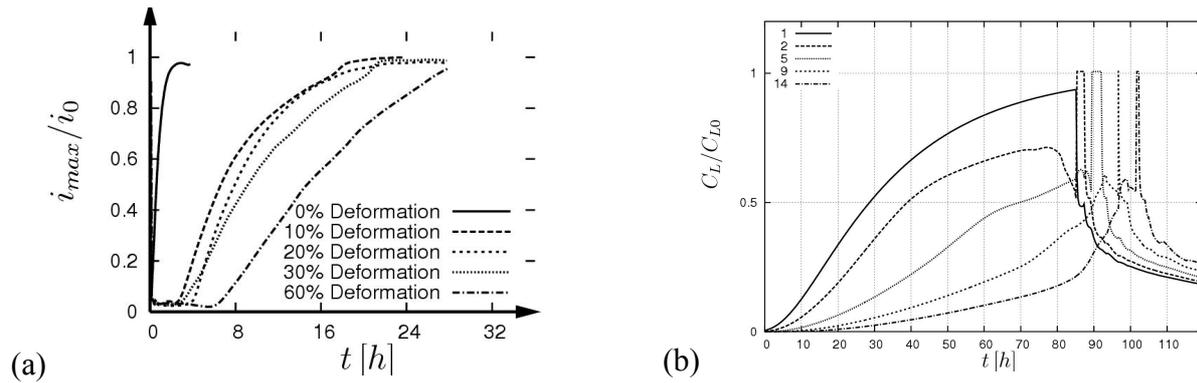


Figure 1: Boundary conditions for permeation of hydrogen; (a) Permeation flux density of hydrogen at a metal surfaces for varying deformation (test results), (b) Applied hydrogen concentration at the crack tip.

Hydrogen Concentration in the Specimen. The coupling between hydrogen diffusion and mechanical quantities can be seen in Figs. 2 and 3. The coordinate x denotes the distance to the crack tip. The lattice hydrogen concentration, C_L , is linked to the gradient of hydrostatic stresses, σ_h , and the concentration of trapped hydrogen, C_T , to the plastic deformation.

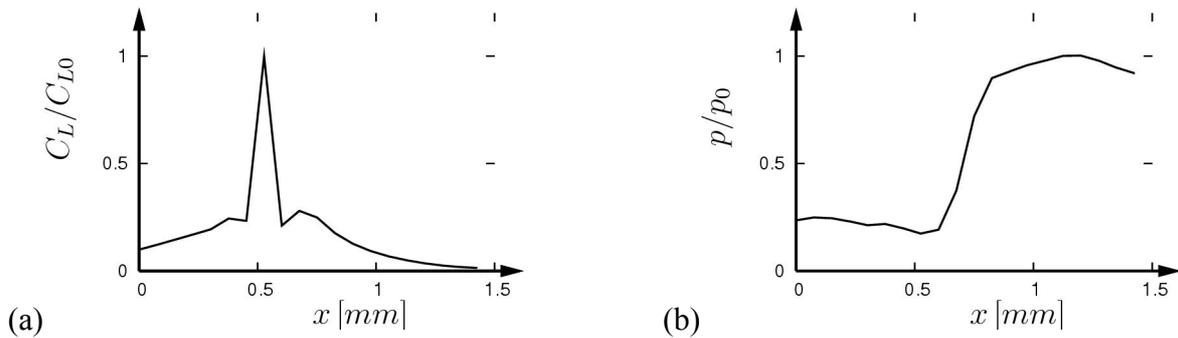


Figure 2: Coupling of hydrogen diffusion with mechanical quantities; (a) Concentration of lattice hydrogen, (b) Hydrostatic stresses.

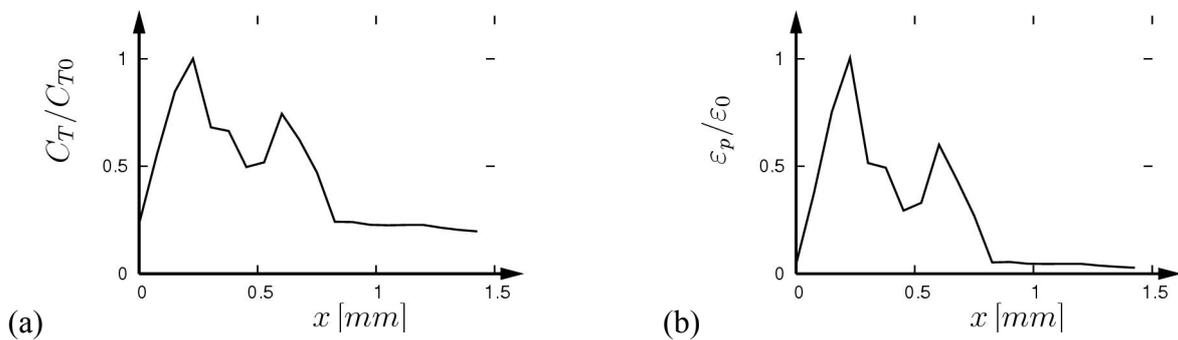


Figure 3: Coupling of hydrogen diffusion with mechanical quantities; (a) Concentration of trapped hydrogen, (b) Equivalent plastic strain..

Resistance curves. Crack-tip opening displacement (CTOD), δ_s , has been evaluated and plotted in dependence on crack extension, Δa , in Fig. 4. The model parameters have been identified from the tests “on air” and at a deformation rate of $1 \mu\text{m/h}$. The two other curves at $10 \mu\text{m/h}$ and $100 \mu\text{m/h}$ are predictions. The model captures the rate dependence of the R-curves due to the time dependent hydrogen diffusion quite well.

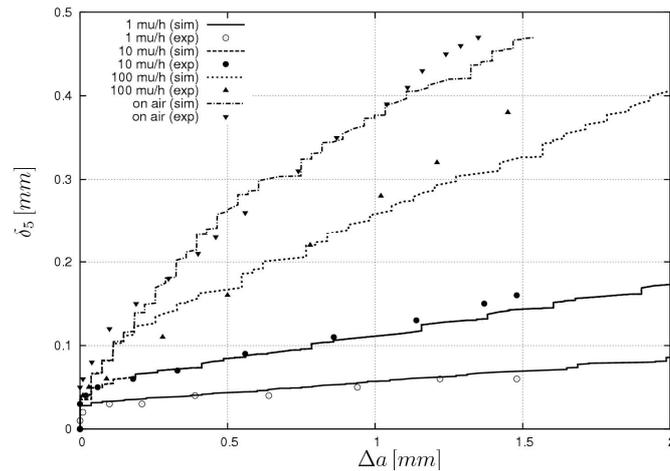


Figure 4: R-curves of C(T) specimens under hydrogen charging for varying deformation rates.

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