MESOSCALE MODELING OF HYDROGEN ASSISTED CRACK GROWTH IN HETEROGENEOUS MATERIALS

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ABSTRACT

Results of fracture mechanics SCC tests performed on pre-cracked specimens of a low alloy structural steel are analysed in terms of a mesoscale crack growth model. The specimens had been subjected to various constant load-line displacement rates while being charged with hydrogen, and a clear correlation was found between the deformation rate and the crack front shape regarding both the crack opening angle as well as the crack front roughness. To rationalise these findings, a mesoscale bundle-of-bars model was developed in which the crack growth process is treated as a sequence of single random fracture events. In this model, the heterogeneity of the material is taken into account by assuming a site dependent critical strain, and failure caused by stress transfer to neighbouring sites from a site which had just failed is quantified by introducing a failure probability. When relating this probability of failure and the failure strain to the local density of atomic hydrogen diffusing into the material from the interface between the crack tip and the environment the model predictions were found to be in good agreement with the experimental data.

1 INTRODUCTION

Stress corrosion cracking (SCC) is a major cause for failure of engineering components and structures. One of the mechanisms leading to this failure is the embrittlement of the material due to the uptake of atomic hydrogen from the environment (Gao [1]). To further investigate this phenomenon, in the past fracture mechanics tests had been performed on pre-cracked C(T) specimens of a low alloy structural steel (FeE 690 T) in ASTM substitute ocean water under hydrogen charging conditions, and data thus obtained were compared with results derived from a simplified model of crack growth due to hydrogen embrittlement (Dietzel [2], Pfuff [3]). In this model, the hydrogen induced contribution to the crack propagation was related to the hydrogen concentration in front of the growing crack, and this concentration was calculated using an effective diffusion coefficient characterising the hydrogen transport from the crack edges through the plastic zone. The total crack extension was calculated by superimposing two contributions caused by ductile failure and by hydrogen embrittlement, respectively, and was found to be in good agreement with the experimental data.

No much insight into the mechanism of hydrogen embrittlement, however, is obtained from this phenomenalistic approach. Therefore, a mesoscale model of hydrogen assisted crack growth was developed which takes into account some of the mechanisms underlying the hydrogen embrittlement. The striking feature of the model is the observation that a technical material is heterogeneous on a mesoscale, i.e., that the mechanical properties are no longer constant in space on a micrometer scale. This heterogeneity is taken into consideration by assuming that the local strain to failure is randomly distributed in the material. A pre-existing crack grows by random local failure in the area of highest strain near the crack tip. Hydrogen increases the rate of failure events at a fixed deformation rate by reducing the strain to failure, i.e., it enhances the crack growth velocity. Moreover, by stress transfer the failure can extend to sites which surround the site just failed. Since the material is heterogeneous, this propagation of failure is not deterministic, but has to be treated in terms of probability. Therefore, a probability of the failure transfer is introduced into the model, and it is assumed that this probability depends on the ductility of the material. By reducing this ductility, hydrogen raises the probability of failure transfer from a fractured site to neighbouring sites.

2 MODEL OF HYDROGEN ASSISTED CRACK GROWTH

The model used to treat the influence of hydrogen on the cracking process is essentially a planar model in which statistical aspects due to the heterogeneity of the material are incorporated. Details of the model can be found elsewhere (Pfuff [4]), and only the main ideas and basic assumptions are presented here.

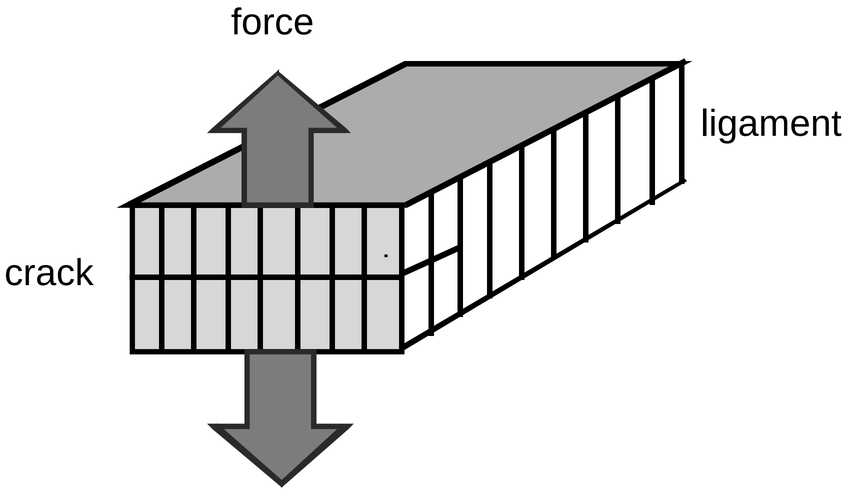

Figure 1: Bundle of bars modelling the area around the plane of a growing crack; a force acting in the direction of the arrows opens the crack at a constant deformation rate.

The area around the crack plane is represented by a bundle of parallel bars which are arranged perpendicularly to this plane, as is indicated in Figure 1. The crack advances by straining to failure the bars at the crack tip. The heterogeneity of the material is taken into account by assuming that the critical strain of the bars is distributed at random. This model is well established in the literature as the "fiber bundle model" (Rosen [5], Phoenix [6]). It has in the past successfully been applied to investigate the consequences of local mesoscale disorder with respect to the fracture behaviour of heterogeneous materials (Curtin [7], Wittkowsky [8], Herrmann [9], Schlangen [10]).

Hydrogen diffuses from the tip of the randomly growing crack into the bulk. The diffusion process is mathematically treated as a two-dimensional phenomenon and by solving a non-linear diffusion equation which takes trapping effects due to plastic deformation into account (Krom [11], Dietzel [12]). This hydrogen embrittles the material by reducing the local fracture strain, ε_f. For simplicity, it is assumed that ε_f linearly decreases with the local concentration of hydrogen atoms dissolved in the lattice,

$$\varepsilon_f = \varepsilon_{f0}\left(1 - \alpha_H c_H\right), \qquad (1)$$

where α_H is a material constant, c_H is the concentration of lattice hydrogen, and ε_{f0}, ε_f are the critical strains for a material deformed in air and under hydrogen charging, respectively.

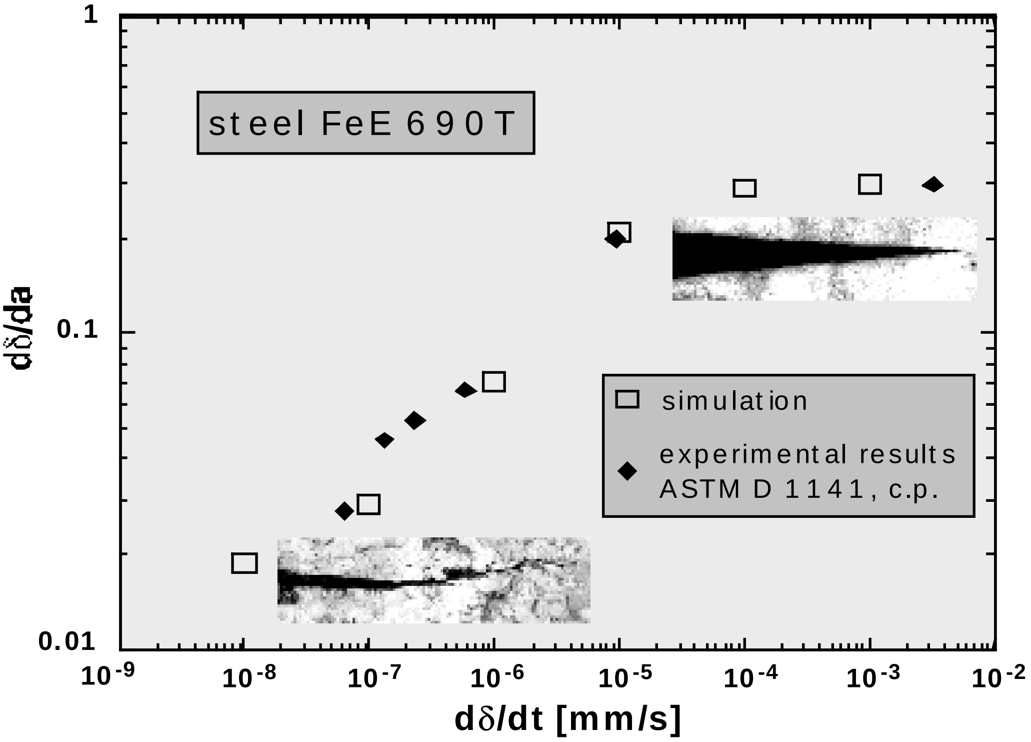

Figure 2: Relationship between deformation rate and crack opening angle.

By reducing the local strain to failure, hydrogen lowers the amount of plastic deformation and, at the same time, enhances the probability of failure occurring due to stress transfer in the neighbourhood of a breaking site. For sites surrounding the breaking site, this probability, p_f, is assumed to depend on the hydrogen concentration at these sites as

$$p_f = 1 - \exp\left(-\beta_H c_H\right), \tag{2}$$

where the constant β_H depends on the material properties. At low rates of crack propagation, the hydrogen concentration ahead of the crack tip can attain fairly large values. According to eqn (2), the failure transfer is in this case significantly enhanced, and the crack propagates by single discrete fracture events of irregular form and size. As will be confirmed by the results of simulations presented in the following section, this mechanism can explain the irregular crack front shape observed in the experiments at low rates of displacement.

2 RESULTS

To verify the model introduced in the preceding section, it was applied to results which had been obtained in rising displacement tests performed on pre-cracked specimens of a low alloy structural steel (FeE 690T) in ASTM substitute ocean water (Dietzel [2], Pfuff [3]). The use of eqns (1) and

(2) requires values to be assigned to the material constants α_H and β_H and to fix the unknown boundary conditions for the concentration of lattice hydrogen at the crack tip.

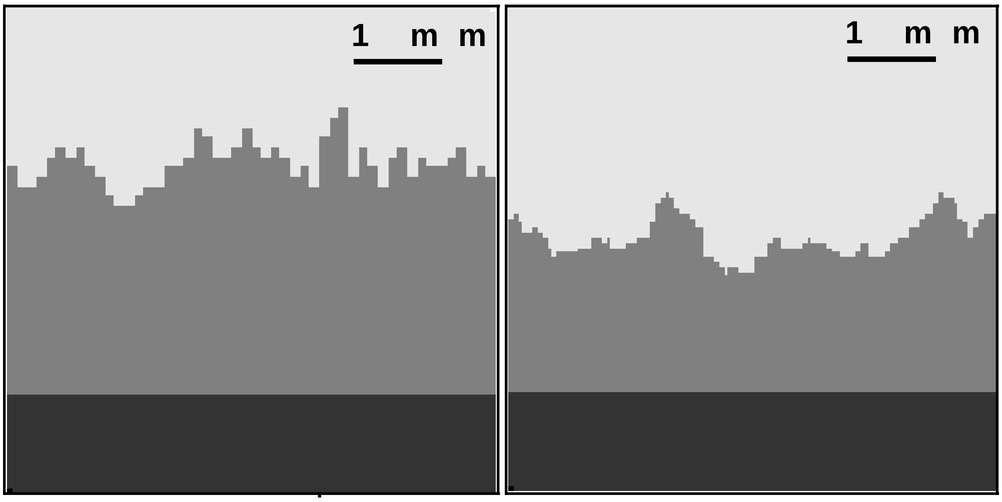

Figure 3: Crack fronts observed in rising displacement experiments (left) and calculated using the bundle-of-bars model (right). The cracks grow from the bottom to the top, and the upper shape (grey) is obtained at a deformation rate of 1 μm/h, the lower (black) at 1 mm/h.

Since the right hand side of these equations depends only on the products of the constants and on the hydrogen concentration, the boundary values of these products were chosen to yield good agreement of the model predictions with the experimental data. This was achieved by setting

$$\alpha_H\, c_{Hboundary} = 0.9 \text{ and } \beta_H\, c_{Hboundary} = 1.0.$$

In Figure 2, the values of the crack tip opening angle obtained from both the experiments and the model calculations for conditions of constant crack growth velocity are shown as a function of the deformation rates applied. Since the model does not allow for calculating crack growth in materials tested in air, the good agreement between the calculated and the experimental results was obtained by adjusting the value of the opening angle at the highest deformation rate applied to the experimental value. The mean critical strain at the crack tip for hydrogen free material was set to be 0.8 (Heerens [13]). Its dependence on the hydrogen concentration was calculated using eqn (1), and it was assumed that the unknown strain rate at the crack tip linearly depends on the measured displacement rate. As can be seen from Figure 2, the results of this simulation are in good agreement with the experimental data.

The shapes of crack fronts observed in the experiments as a function of the applied deformation rates were simulated by assuming a random scatter of the local critical strain in hydrogen free material around the mean value of up to ±0.004 and by using eqn (2) to account for failure due to stress transfer. In Figure 3, fracture surfaces which had been obtained in tests at two different displacement rates, differing by three orders of magnitude, are compared with corresponding crack fronts derived from the simulations. The experimental results shown were taken from photographs of the fracture surfaces which had been marked by fatigue after testing, and at a resolution of 100 μm. The simulations were performed using bar elements with a cross-section size of 50 μm times 50 μm, to represent the model specimen. The results shown in Figure 3 suggest that the roughness of the crack front observed at low rate of deformation can be explained by the embrittling effect of the hydrogen in combination with the heterogeneity of the material.

4 CONCLUSIONS

Results obtained from rising displacement tests on pre-cracked compact tension specimens under hydrogen charging conditions are interpreted in terms of a mesoscale model. In this model, the heterogeneity of the material is taken into account by treating crack growth as a sequence of individual, randomly distributed rupture events. The frequency and size of these events are related to the hydrogen content at the front of the growing crack. The hydrogen concentration in the material is calculated by numerically solving a non-linear diffusion equation which takes into account the effect of trapping caused by plastic deformation on the diffusion rates.

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