



Coupled hydrogen diffusion simulation using a heat transfer analogy



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ABSTRACT

Simulations of Hydrogen Assisted Cracking (HAC) in metals and alloys include hydrogen concentration as a crucial variable. With this objective, phenomenological diffusion models that consider chemical potential gradients as the driving force for diffusion are described. Equations are then modified to include the influence of the stress-strain state and trapping.

A crack tip, whose field of stresses and displacements is described by fracture mechanics, is modelled while diffusion equations are implemented through subroutines in the commercial program ABAQUS by means of the analogy between diffusion equations and heat transfer. Effects of trapping on hydrogen transport are then discussed. Moreover, hydrogen induces a lattice dilatation and a modification of the local plastic flow; this coupled behaviour is also modelled through the heat transfer analogy. Finally, stress-dependent boundary conditions are implemented, representing hydrogen entry in a more realistic way.

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1. Introduction

Metals and alloys are degraded in the presence of hydrogen. One of these phenomena is known as hydrogen embrittlement, and mechanisms that operate at the microscopic and atomic levels are still not entirely clear. Modelling the interaction between hydrogen and the material in a crack tip is essential, because hydrogen drastically affects fracture behaviour. So damage models, both continuous damage models and cohesive models, must incorporate a new variable: hydrogen concentration. This paper aims to contribute to this first step in the hydrogen embrittlement modelling, i.e. to predict accurate hydrogen distributions near a crack tip.

With this objective, diffusion equations are derived from Fick's laws which describe the hydrogen flux due to a concentration gradient. Trapping is considered within this model in an explicit form in such a way that diffusion variables (concentration, occupancy, chemical potential and flux) are distinguished depending on whether hydrogen is in a lattice or a trapping site. These equations are also modified by the stress-strain field.

In order to properly include hydrogen trapping, there is currently no commercial Finite Element software in which these equations are implemented by default. It has been necessary, therefore, to develop a subroutine based on the analogy between diffusion and heat transfer. This procedure has been verified by

simulating hydrogen diffusion near a crack tip with a boundary layer approach, using the same geometry and parameters as those first proposed by Sofronis and McMeeking [1] for hydrogen in iron. This simulation has been repeatedly revisited in literature for the sake of comparison, and some improvements have been made: the inclusion of a plastic strain rate [2], the consideration of coupled diffusion [3,4] and stress-state dependent boundary conditions [5]. All of these improvements are discussed in the present paper and are implemented in Finite Element simulations following the analogy between diffusion and heat transfer. Emphasis is also put on the range of validity of the simplification usually assumed in diffusion models.

2. Hydrogen diffusion phenomenological model

Hydrogen Assisted Cracking must be modelled in a continuous scale in order to handle the stress-strain fields. For this reason, diffusion equations describing hydrogen transport are usually based on a phenomenological approach in which vector fluxes and mass balances are defined over the material domain [6].

Hydrogen atoms promote decohesion, modify dislocation motion and alter material properties in many different ways. In addition, the stress-strain field influences hydrogen transport by means of two phenomena: hydrostatic stress, which produces lattice dilatation so hydrogen will tend to reach expanded sites, and plastic strain, which increases the amount of crystal defects creating trapping sites.

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The latter phenomenon is crucial in a crack tip where plastic strain is highly localized. This is why hydrogen diffusion models consider a two-level approach as if there were two different chemical components. That is to say hydrogen might be localized in lattice sites (L subscript) or trapping sites (T subscript).

2.1. Fluxes

As it was noted, hydrogen diffusion models in metals usually consider two types of sites. Within the framework of non-equilibrium thermodynamics, mass fluxes derived from Onsager relationships are taken into account [7,8]. Even though mass concentration is the sought variable, chemical potential gradients $\nabla\mu_j$ represent the thermodynamic driving force which produces diffusion. Onsager coefficients L_{ij} denote the action of force j on component i ; negative sign indicates that the net movement of i -type hydrogen atoms, i.e. hydrogen flux J_i , occurs from high to low chemical potential regions:

$$J_i = - \sum_{j=1}^n L_{ij} \nabla\mu_j \quad (1)$$

Particularly, for the two-level diffusion model accounting for lattice and trapping sites, fluxes might be expressed in a matrix form:

$$\begin{bmatrix} J_L \\ J_T \end{bmatrix} = \begin{bmatrix} L_{LL} & L_{LT} \\ L_{TL} & L_{TT} \end{bmatrix} \begin{bmatrix} \nabla\mu_L \\ \nabla\mu_T \end{bmatrix} \quad (2)$$

However, it is usually assumed that the gradient of μ_L does not affect the flux between trapping sites and the gradient of μ_T does not affect the flux between lattice sites. Cross-terms are thus neglected, $L_{LT}=L_{TL}=0$, so:

$$J_L = - L_{LL} \nabla\mu_L \quad (3)$$

$$J_T = - L_{TT} \nabla\mu_T \quad (4)$$

Onsager coefficients are related to the Einstein equation of diffusion,

$$L_{LL} = \frac{D_{LL}}{RT} C_L \quad (5)$$

$$L_{TT} = \frac{D_{TT}}{RT} C_T \quad (6)$$

where D_{LL} is the lattice diffusivity, D_{TT} is the diffusivity between trapping sites, C_L and C_T are the hydrogen concentrations in lattice and trapping sites respectively, R is the universal constant of gases and T is the absolute temperature.

Additionally, chemical potential can be expressed in terms of hydrogen concentration. More precisely, it is related to occupancy of i -sites $\theta_i=C_i/N_i$, where N_i is the concentration of i -sites. From interstitial solid solutions thermodynamic theory, chemical potential usually comprises a term depending on configurational entropy, thus on occupancy, and another term μ_i^0 which express the chemical potential in the standard state. Influence of stress state is considered by means of a purely dilatational term, therefore a term is added consisting of hydrostatic stress $\sigma_h=\frac{1}{3}\text{trace}(\sigma)$ multiplied by the partial molar volume of hydrogen inside the metal \bar{V}_H . In the present work, it has been assumed, as it was by Di Leo et al. [5], that the chemical expansion is the same for lattice sites and trapping sites:

$$\mu_L = \mu_L^0 + RT \ln \frac{\theta_L}{1 - \theta_L} - \bar{V}_H \sigma_h \quad (7)$$

$$\mu_T = \mu_T^0 + RT \ln \frac{\theta_T}{1 - \theta_T} - \bar{V}_H \sigma_h \quad (8)$$

Substituting (5)–(8) into (3)–(4) gives:

$$J_L = - D_{LL} \frac{C_L}{(1 - \theta_L)} \left(\frac{\nabla C_L}{C_L} - \frac{\nabla N_L}{N_L} \right) + \frac{D_{LL}}{RT} C_L \bar{V}_H \nabla \sigma_h \quad (9)$$

$$J_T = - D_{TT} \frac{C_T}{(1 - \theta_T)} \left(\frac{\nabla C_T}{C_T} - \frac{\nabla N_T}{N_T} \right) + \frac{D_{TT}}{RT} C_T \bar{V}_H \nabla \sigma_h \quad (10)$$

2.2. Mass balance

In order to relate fluxes, which are established due to the chemical potential gradient, with concentration variation, a mass balance is required. Assuming no internal sources of hydrogen, the variation of total hydrogen concentration in a volume V must be equal to the flux through the surrounding surface S of such a volume:

$$\frac{d}{dt} \int_V (C_L + C_T) dV = - \int_S (J_L + J_T) \cdot n dS \quad (11)$$

Surface is orientated outwards, so negative sign means that positive fluxes represent hydrogen exit from the volume.

2.3. Simplified model

These expressions are usually simplified considering the following facts:

- Interstitial sites concentration is assumed constant: $\nabla N_L=0$. This is arguably because as traps are created the number of interstitial sites could be modified.
- In many alloys, especially in bcc lattices, it is expected low occupancy $\theta_L \ll 1$ because $N_L \gg C_L$. However, θ_L may not be small in FCC metals [9].
- Mobility between trapping sites, or equivalently diffusion coefficient, is considered near zero: $D_{TT} \approx 0$, because traps are not connected or because their deep potential energy well prevents hydrogen from diffusing, i.e. $\Delta E_{TT} \gg 1$. This will be discussed in detail in Section 5.

Assuming these simplifications, fluxes might be expressed as follows:

$$J_L = - D_{LL} \nabla C_L + \frac{D_{LL}}{RT} C_L \bar{V}_H \nabla \sigma_h \quad (12)$$

$$J_T = 0 \quad (13)$$

According to divergence theorem, Eq. (11) can be expressed:

$$\int_V \frac{d}{dt} (C_L + C_T) dV = - \int_V \nabla \cdot J_L dV \quad (14)$$

The balance equation to be solved is then:

$$\frac{dC_L}{dt} + \frac{dC_T}{dt} + \nabla \cdot J_L = 0 \quad (15)$$

2.4. Equilibrium

Having two unknowns (C_L and C_T), both variables should be connected using kinetic or thermodynamic assumptions. In this paper, equilibrium between the traps and interstitial sites is considered, i.e. $\mu_L = \mu_T$, which leads to the so-called Oriani's equilibrium [10]:

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