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Hydrogen diffusion under the effect of stress and temperature gradients

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Abstract. In this paper, a finite element (FE) model is developed to investigate lattice hydrogen diffusion in a solid metal under the influence of stress and temperature gradients. This model is applied to a plate with a circular hole which is subjected to temperature and hydrogen concentration gradients. It is demonstrated that temperature gradients significantly influence hydrogen diffusion and hence susceptibility to hydrogen embrittlement when utilizing hydrogen for gas turbines.

1. Introduction

Hydrogen can be used to store renewable energy, and then converted back to electricity using gas turbines [1, 2, 3]. Currently, the utilisation of hydrogen is limited due to the high costs and difficulties in storage and transportation, which have been investigated previously [4]. However, hydrogen embrittlement, a commonly observed adverse effect on metals and alloys, has rarely been studied in relation to gas turbines.

Hydrogen embrittlement is the reduction of ductility and toughness in a metal when a small amount of hydrogen is present, which induces sudden failure [5]. Consequently, the distribution of hydrogen concentration is of paramount importance. Hydrogen transport in the material takes place via either lattice diffusion or dislocation movement [6]. Thus, some hydrogen atoms move to normal interstitial lattice sites which are the majority, whilst the others stay in defect-traps which are the minor fraction of sites [7]. Nevertheless, most studies on hydrogen embrittlement have not considered high temperature conditions, especially where a temperature gradient exists, which is the typical working environment for major metallic components in gas turbines and fuel cells.

Therefore, this paper aims to investigate hydrogen diffusion in lattice sites under the influence of both stress and temperature gradients by a finite element (FE) model.

2. Methodology

An FE model is developed using Abaqus 6.14 in order to solve the transport equations for hydrogen and heat, which is subsequently validated by literature data [7].



2.1. Hydrogen transport equation

The conservation of hydrogen concentration can be written as:

$$\frac{\partial C}{\partial t} + \nabla \cdot \mathbf{J} = 0 \quad (1)$$

where C is the hydrogen concentration (mol/m^3), $\mathbf{J}$ is the concentration flux ($\text{mol}/(\text{m}^2\text{s})$), and t is time (s). Next, the mass flux $\mathbf{J}$ here is obtained as:

$$\mathbf{J} = -\frac{DC}{RT} \nabla \mu = -DS \left\{ \nabla \phi + \frac{\phi \ln \phi}{T} \nabla T - \frac{\phi V_H}{RT} \nabla \sigma_H \right\} \quad (2)$$

Here D is diffusivity (m^2/s), R is the gas constant ($8.31 \text{ J}/(\text{mol K})$), T is temperature (K), μ is the chemical potential (J/mol), σ_H is the hydrostatic stress (Pa), V_H is the partial molar volume of hydrogen, $\phi = C/S$ is the normalized concentration and S is the hydrogen solubility.

2.2. FE model and validation

The FE model is validated for a square plate with a hole under plane strain conditions. Making use of the symmetry conditions, a quarter of the geometry illustrated in Figure 1 is modelled.

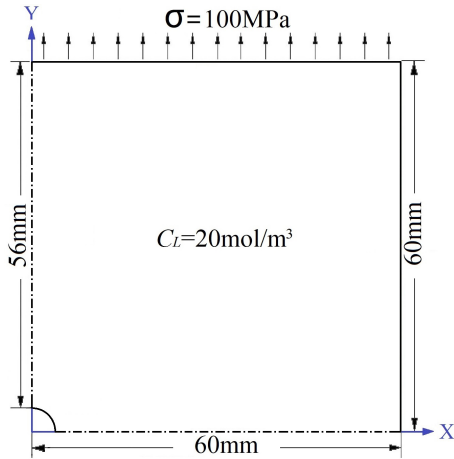


Table 1: Material properties representative of Alloy 690.

Parameter	Value
ρ (kg/m^3)	8.19×10^3
N_L ($/\text{m}^3$)	9.24×10^{28}
D (m^2/s)	3.8×10^{-11}
E (GPa)	200
ν	0.3
V_H (m^3/mol)	2×10^{-6}

Figure 1: Geometry and boundary conditions.

The plate is maintained in a constant temperature environment, and has an initial uniform hydrogen concentration of $20 \text{ mol}/\text{m}^3$. Hydrogen flux at all boundaries are zero. An evenly distributed tensile load of 100 MPa is on the top surface. An FE mesh with an element size of 1 mm is generated away from the hole, and the near-hole mesh is refined to 0.1 mm . Material properties representative of a Nickel based Alloy 690 are listed in Table 1. Figure 2 (a) shows that the hydrostatic stress σ_H is concentrated near the hole. Consequently, steady state hydrogen concentration at points A and C changes accordingly, whilst hydrogen at point B remains constant. Comparing hydrogen concentration at locations A, B and C to the literature results [7], we find a discrepancy of less than 0.85% .

3. Results and discussion

Since the FE model developed can accurately predict stress mediated hydrogen diffusion, it is now employed to investigate the combined influence of temperature and stress gradients on hydrogen concentration at steady state. Table 2 lists boundary conditions for two new case studies A and B. The difference between the two cases is the temperature distribution, which is shown in Figure 3.

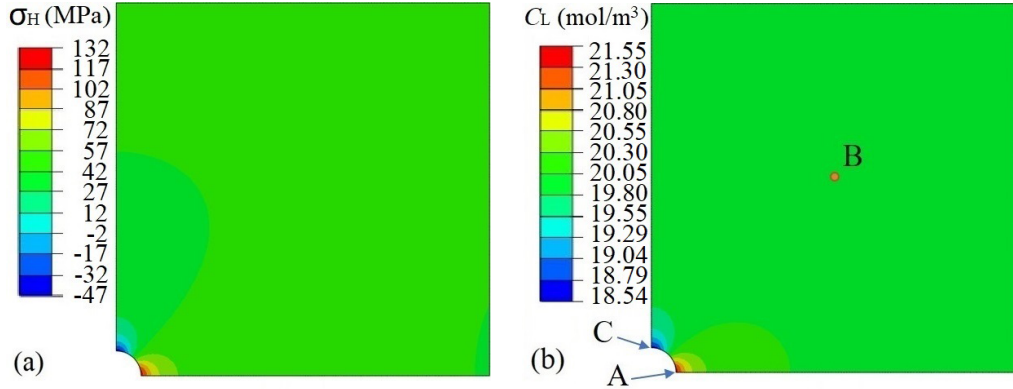


Figure 2: Distribution of hydrostatic stress (a) and lattice hydrogen concentration (b).

Table 2: Boundary conditions of Case A and B.

Boundary	Traction (MPa)	Displacement	Temperature (K)		Concentration (mol/m ³)
Top	$t_1 = 0, t_2 = 200$		$T_A = 300$	$T_B = 1000$	$C_L = 0$
Bottom	$t_1 = 0$	$U_2 = 0$	$\nabla T_A = 0$	$\nabla T_B = 0$	$\nabla C_L = 0$
Left	$t_2 = 0$	$U_1 = 0$	$\nabla T_A = 0$	$\nabla T_B = 0$	$\nabla C_L = 0$
Right	$t_1 = 0, t_2 = 0$		$T_A = 300$	$T_B = 1000$	$C_L = 0$
Hole	$t_1 = 0, t_2 = 0$		$T_A = 1000$	$T_B = 300$	$C_L = 100$

*The subscripts A and B here refer to the temperature in Case A and B respectively.

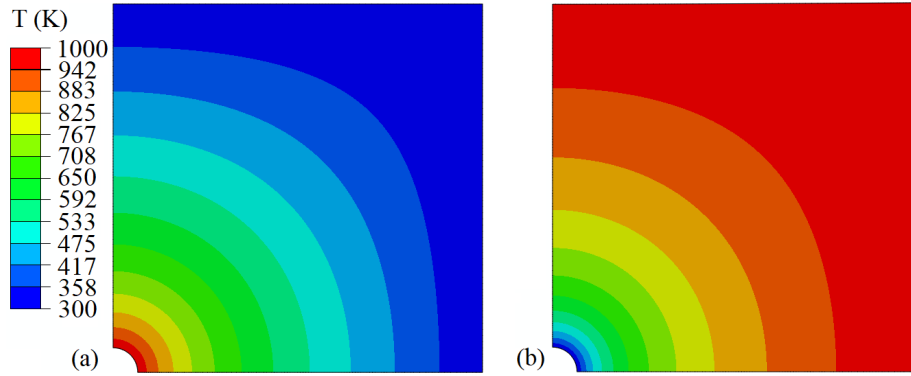


Figure 3: Temperature distribution in Case A (a) and B (b).

Figure 4 illustrates steady state lattice hydrogen concentration profiles (C_L). According to Figure 4 (a), C_L decreases nearly linearly away from the hole, where the temperature is high. However, in the low-temperature zone in Case A, there is a convex in the concentration profile. This feature is a direct result of $\frac{\phi \ln \phi}{T} \nabla T$ in Equation (2), which shows that a temperature gradient is a driving force for the transport of lattice hydrogen.

The effect of the temperature gradient is more clearly illustrated along the line ($y = 0$) by plotting C_L and $\phi \ln \phi$ against the X coordinate in Figure 5. Here $\phi \ln \phi$ is the coefficient in front of $T^{-1} \nabla T$ in Equation (2) and is termed the Soret effect factor. In Figure 5 (a), $\phi \ln \phi$ peaks in the low-temperature zone, which ultimately results a bump in the C_L profile. In contrast, Figure 4 (b) demonstrates that hydrogen diffusion is negligible due to the combined effects of the

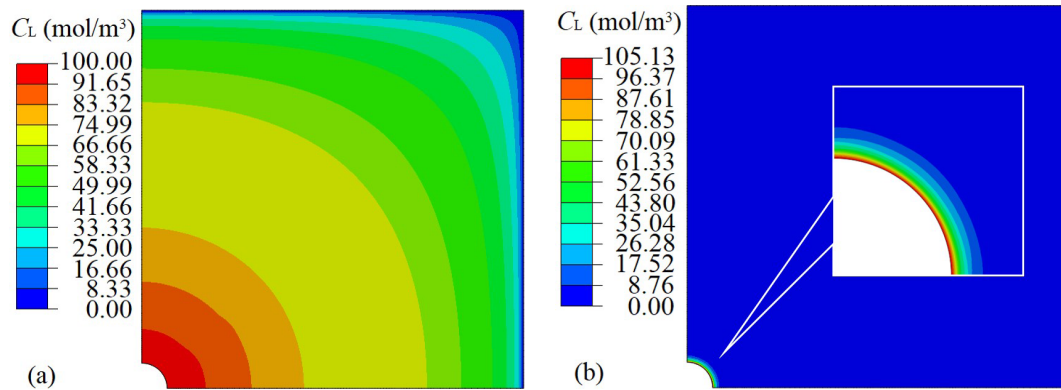


Figure 4: Effect of $\nabla\sigma_H$ and ∇T on hydrogen diffusion in Case A (a) and B (b)

temperature gradient and the fact that the mass diffusivity decays exponentially with decreasing temperature. Consequently, the majority of hydrogen atoms stay very close to the hole. This is potentially very beneficial to the mechanical reliability of materials in contact with hydrogen gas.

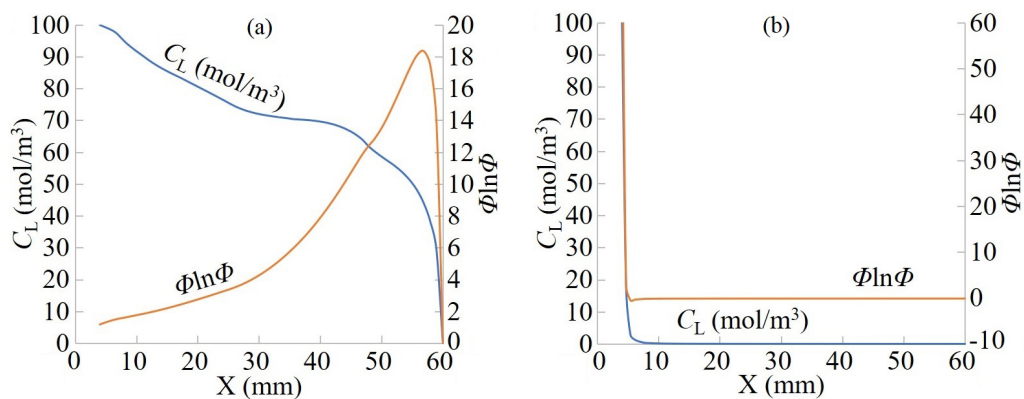


Figure 5: C_L and $\phi \ln \phi$ along the line ($Y = 0$) at Case A (a) and B (b).

4. Conclusions

The findings demonstrate the temperature gradient effect on steady state hydrogen distribution. Depending on the direction of the thermal gradient, this effect can either enhance mass diffusion and even cause a local increase in hydrogen concentration profiles, or severely hinder hydrogen diffusion. Consequently, the temperature gradient is an important factor which should be accounted for the assessment of hydrogen embrittlement in gas turbines.

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