Finite element models for the study of hydrogen embrittlement of steel structures

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Thesis defense

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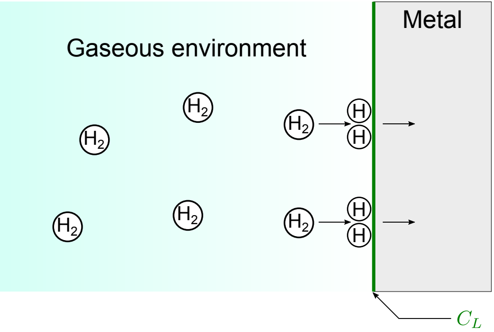
Outline

Hydrogen inside metals

Finite element formulation

Hydrogen uptake

- **Sieverts' law:** The solubility of a diatomic gas in a metal is proportional to the square root of the gas pressure



Thermally activated term

$$C_L = \gamma\sqrt{P}$$

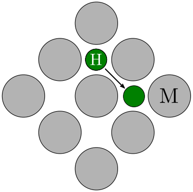
Hydrogen solubility (H at./ Iron at.)

H_2 pressure (MPa)

Hydrogen diffusion and trapping

- Model from Sofronis and McMeeking (1989) and corrected by Krom *et al.* (1999)

- **Hydrogen concentration:** $C = C_L + C_T$
  - Lattice concentration: $C_L = \beta N_L \theta_L$
  - Trapped concentration: $C_T = N_T(\kappa)\theta_T$



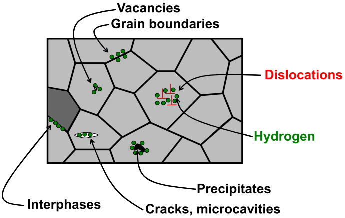
- **Hydrogen flux:**

$$J = -D_L \nabla C_L + \frac{D_L C_L V_H}{RT} \nabla P$$

- **Oriani's equilibrium:**

$$\frac{1-\theta_L}{\theta_L} \frac{\theta_T}{1-\theta_T} = K$$

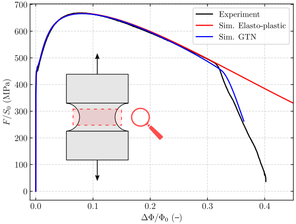
(Coupling terms)

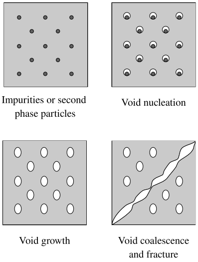


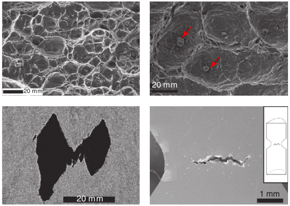
- The **ductile behavior** of the metal is described by the **GTN model** (Tvergaard *et al.* 1984):

$$\frac{\sigma_{eq}^2}{\sigma_F^2} + 2q_1 f_* \cosh\left(\frac{q_2}{2}\frac{\sigma_{ii}}{\sigma_F}\right) - 1 - q_1^2 f_*^2 = 0$$

$$\dot{f} = \dot{f}_{nucleation} + \dot{f}_{growth}$$







Hydrogen embrittlement

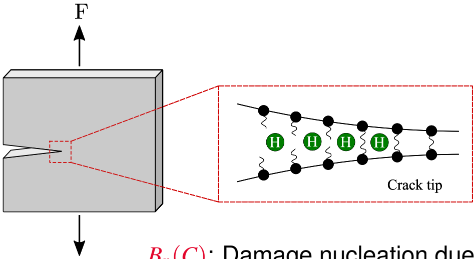
- **Void growth**: Unchanged due to mass conservation

$$\dot{f}_g = (1 - f_g)\,\mathrm{trace}(\dot{\varepsilon}_p)$$

- **Void nucleation**: Proposed dependance on hydrogen concentration

$$\dot{f}_n = A_n(\kappa)\dot{\kappa} + B_n(C)\dot{\kappa}$$

(Coupling terms)



Hydrogen weakens the cohesive bonds between atoms

$B_n(C)$: Damage nucleation due to hydrogen
HEDE (Hydrogen Enhanced Decohesion)

Outline

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Finite element formulation

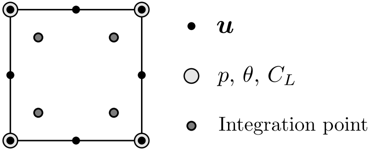
Mixed formulation

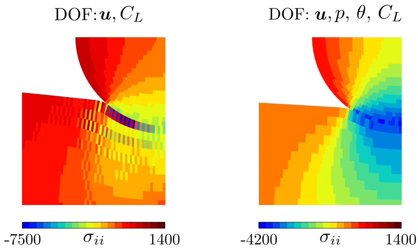
- Fully implicit finite strain framework
- Based on a mixed formulation: $\underline{u}, P, \theta$ (Zhang *et al.* 2017) and C_L
- Quadratic elements with reduced integration
- **Aim:** better pressure fields by avoiding volumetric locking

Advantage

∇P can be directly computed from nodal values

$$J = -D_L \nabla C_L + \frac{D_L C_L V_H}{RT} \nabla P$$





B-bar formulation

- The use of quadratic element lead to high simulation times
- B-bar formulation:

Thank you for your attention

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