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

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Thesis defense
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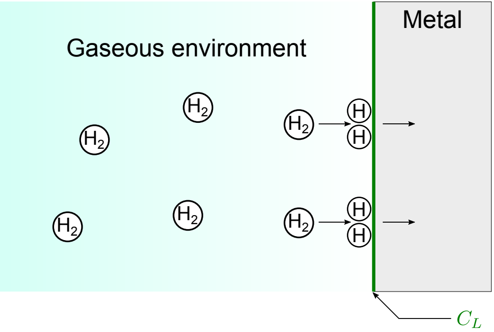
Outline

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

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

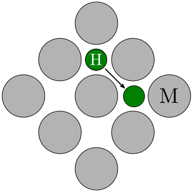
Hydrogen solubility (H at./ Iron at.)

H2 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: $C_T = N_T(\kappa)\theta_T$



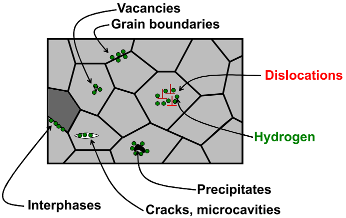
- **Hydrogen flux:**

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

- **Oriani's equilibrium:**

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

(Coupling terms)

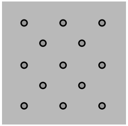


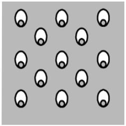
Damage

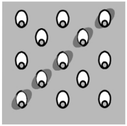
- The **ductile behavior** of the metal is described by the **GTN model** (Tvergaard *et al.* 1984):

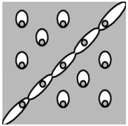
$$\frac{\sigma_{eq}^2}{\sigma_F^2} + 2q_1 f_* \cosh\left(\frac{q_2}{2}\frac{\sigma_{ii}}{\sigma_F}\right) - 1 - q_1^2 f_*^2 = 0$$

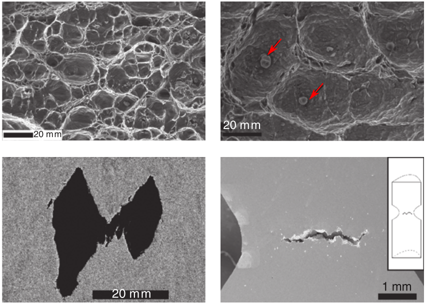
$$\dot{f} = \dot{f}_{nucleation} + \dot{f}_{growth}$$


Impurities or second phase particles


Void nucleation and growth


Strain localization


Void coalescence and fracture



Hydrogen embrittlement

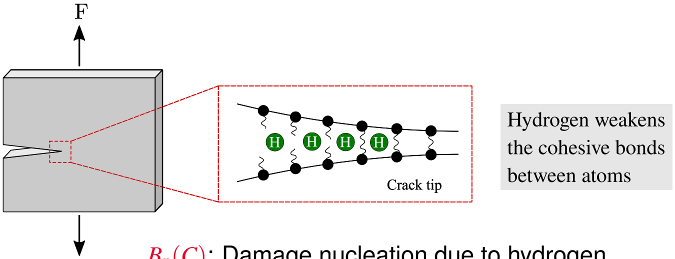
- **Void growth**: Unchanged due to mass conservation

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

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

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

(Coupling terms)



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

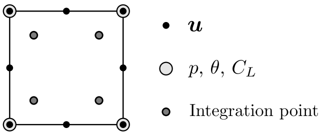
Mixed formulation

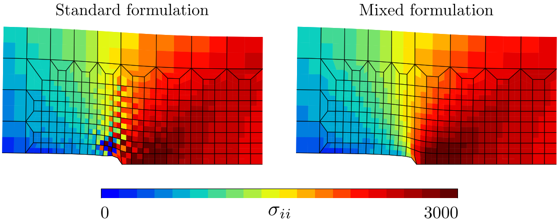
- Fully implicit finite strain framework
- Based on a mixed formulation: $\underline{u}, P, \theta$ (Zhang *et al.* 2017) and C_L
- Quadratic elements with reduced integration
- **Aim:** better pressure fields by avoiding volumetric locking

Advantage

∇p can be directly computed from nodal values

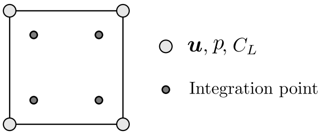
$$J = -D_L \nabla C_L + \frac{D_L C_L V_H}{RT} \nabla p$$

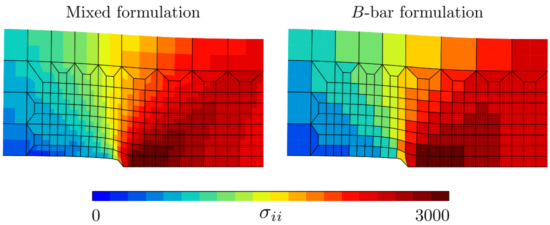




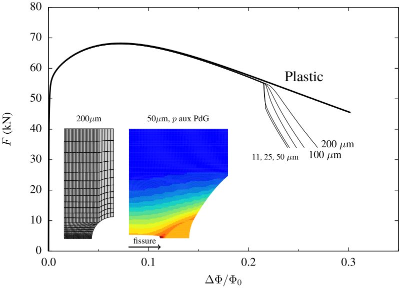
$\boldsymbol{B}$-bar formulation

- The use of quadratic elements with additional dofs lead to high simulation times
- $\boldsymbol{B}$-bar formulation (Hughes, 1980):
  - Linear elements with full integration
  - Solves volumetric locking by modifying the strain-displacement matrix $\boldsymbol{B}$
  - To avoid extrapolating p to the nodes for ∇p computation, it is considered as a dof

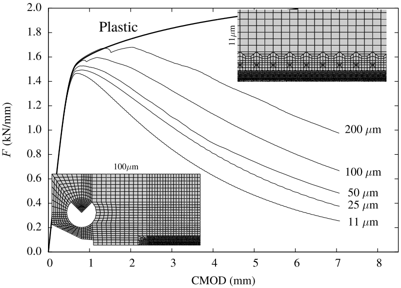




- Damage models such as the GTN model are known to induce **spurious mesh dependency** (element size, type and orientation)
- To solve this problem, it is proposed to use a **nonlocal damage model** based on the **implicit gradient** by Peerlings *et al.*, 1996



Notched tensile (NT) specimen

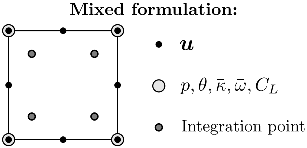


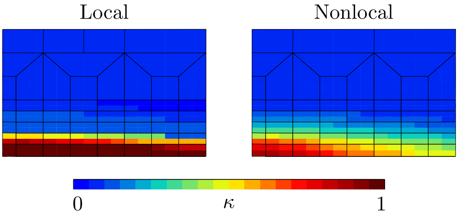
Compact tension (CT) specimen

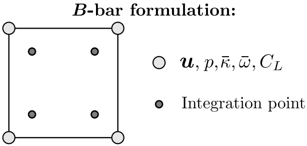
(Besson, 2021)

Nonlocal damage model

- Two variables are used (two associated internal lengths: $\bar{\omega}$ and $\bar{\kappa}$):
  - **Plastic volume variation:** $\bar{\omega} - \ell_\omega^2 \Delta\bar{\omega} = \omega$ where $\omega = \mathrm{trace}(\dot{\underline{\varepsilon}}_p)$
  - **Accumulated plastic strain:** $\bar{\kappa} - \ell_\kappa^2 \Delta\bar{\kappa} = \kappa$
- The modified evolution laws for the damage variables are now:
  - **Void growth:** $\dot{f}_g = (1 - f_g)\dot{\bar{\omega}}$
  - **Void nucleation:** $\dot{f}_n = A_n \dot{\bar{\kappa}} + B_n(C)\dot{\bar{\kappa}}$







Thank you for your attention

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