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

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Thesis defense

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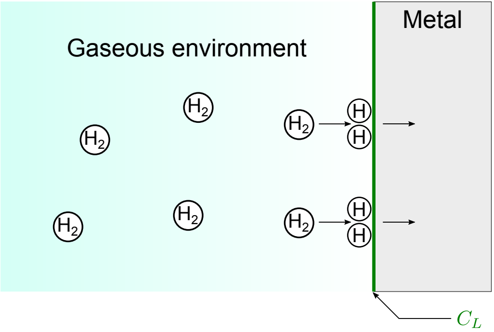
Outline

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



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

Thermally activated term

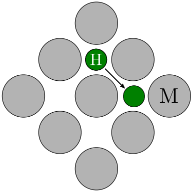
Hydrogen solubility (H at./ Iron at.)

H_2 pressure (MPa)

Hydrogen diffusion and trapping

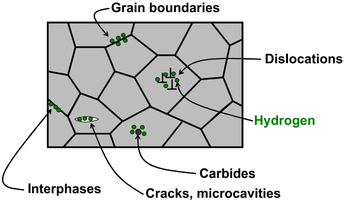
- Model from Sofronis and McMeeking (1989) and corrected by Krom *et al.* (1999)

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



- **Hydrogen flux:**

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



- **Oriani's equilibrium:**

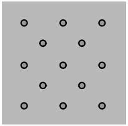
$$\frac{1-\theta_L}{\theta_L} \frac{\theta_T^i}{1-\theta_T^i} = K$$

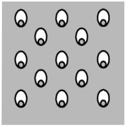
(Coupling terms)

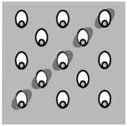
- The **ductile behavior** of the metal is described by the **GTN model** (Tvergaard *et al.* 1984):

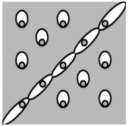
$$\frac{\sigma_{eq}^2}{\sigma_F^2} + 2q_1 f_* \cosh\left(\frac{q_2}{2}\frac{\sigma_{ii}}{\sigma_F}\right) - 1 - q_1^2 f_*^2 = 0$$

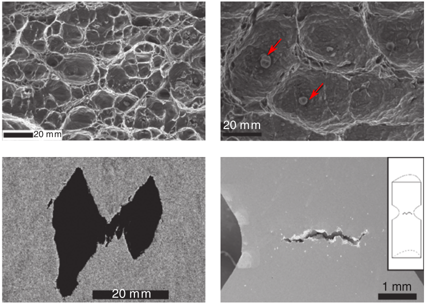
$$\dot{f} = \dot{f}_{nucleation} + \dot{f}_{growth}$$


Impurities or second phase particles


Void nucleation and growth


Strain localization


Void coalescence and fracture



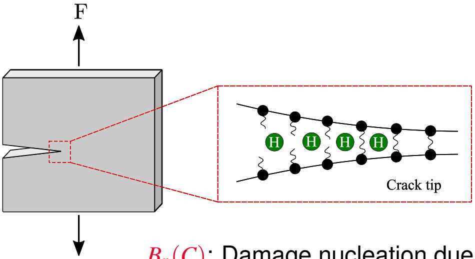
- **Void growth**: Unchanged due to mass conservation

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

- **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

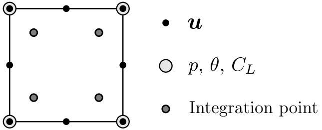
$B_n(C)$: Damage nucleation due to hydrogen
HEDE (Hydrogen Enhanced Decohesion)

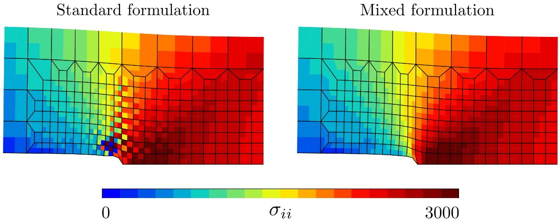
- Fully implicit finite strain framework
- Based on a mixed formulation: $\underline{u}, P, \theta$ (Zhang *et al.* 2017) and C_L
- Quadratic elements with reduced integration
- **Aim:** better pressure fields by avoiding volumetric locking

Advantage

∇p can be directly computed from nodal values

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



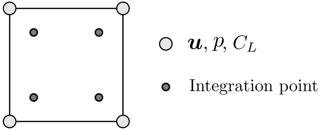


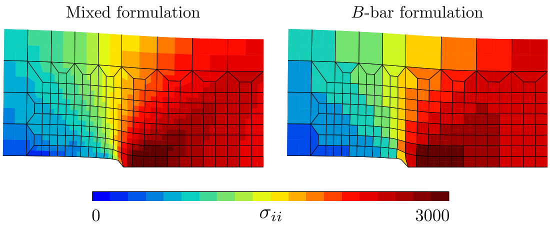
$\boldsymbol{B}$-bar formulation

- The use of **quadratic elements** with additional dofs lead to **high simulation times**
- $\boldsymbol{B}$-bar (or $\bar{\boldsymbol{B}}$) formulation (Hughes, 1980):
  - Linear elements with full integration
  - Solves volumetric locking by modifying the strain-displacement matrix:

$$\bar{\boldsymbol{B}} = \boldsymbol{B}_d + \bar{\boldsymbol{B}}_h$$

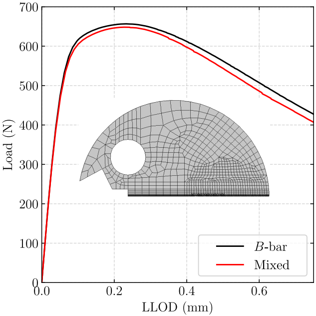
  - To avoid extrapolating p to the nodes for ∇p computation, it is considered as a dof

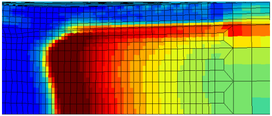




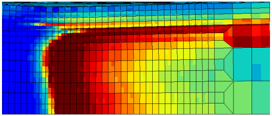
- Test on a Disk Compact Tension (DCT) specimen with 5200 elements:
  - **Mixed formulation**: 103,762 dofs, 1h 40 minutes to complete
  - ***B*-bar formulation**: 33,974 dofs, 18 minutes to complete

- Slightly higher force for the *B*-bar formulation → Linear elements are inherently stiffer since they have less nodes

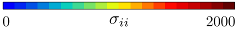




Mixed formulation

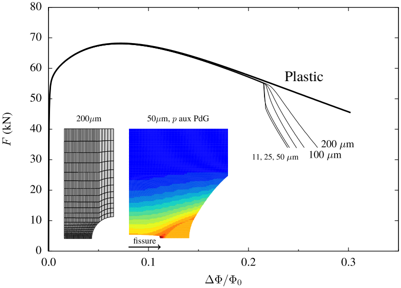


B-bar formulation

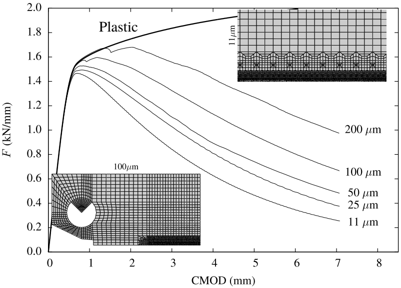


Nonlocal damage model

- 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

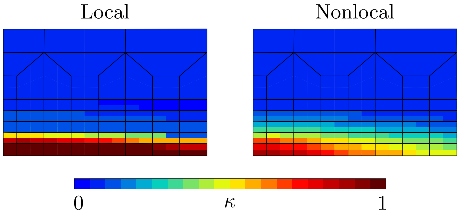


Compact tension (CT) specimen

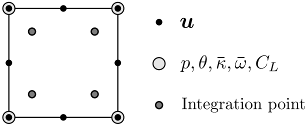
(Besson, 2021)

- Two variables are used (two associated internal lengths: $\bar{\omega}$ and $\bar{\kappa}$):
  - **Plastic volume variation:** $\bar{\omega} - \ell_{\omega}^2 \Delta \bar{\omega} = \omega \quad \text{where} \quad \omega = \mathrm{trace}(\dot{\underset{\sim}{\varepsilon}}_p)$
  - **Accumulated plastic strain:** $\bar{\kappa} - \ell_{\kappa}^2 \Delta \bar{\kappa} = \kappa$

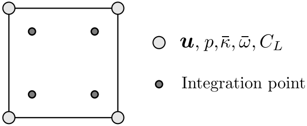
- The modified evolution laws for the damage variables are now:
  - **Void growth:** $\dot{f}_g = (1 - f_g)\dot{\bar{\omega}}$
  - **Void nucleation:** $\dot{f}_n = A_n \dot{\bar{\kappa}} + B_n(C)\dot{\bar{\kappa}}$



Mixed formulation:



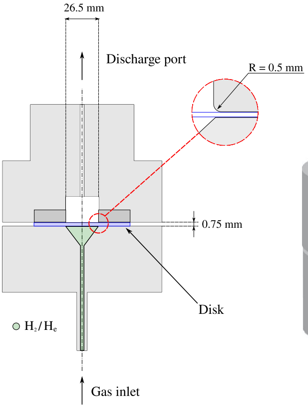
B-bar formulation:



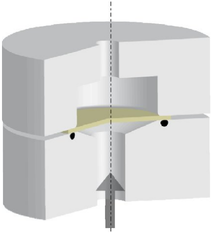
Outline

Context

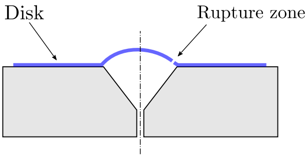
- **ISO 11114-4 standard:** uses pressurized disk tests for selecting metallic materials resistant to hydrogen embrittlement
- Disk often fails in the clamping zone → **Hard analysis**
- **First step:** redesigning the disk geometry to control failure location



$$\mathrm{HEI} = \frac{P_r(\mathrm{He})}{P_r(\mathrm{H_2})}$$

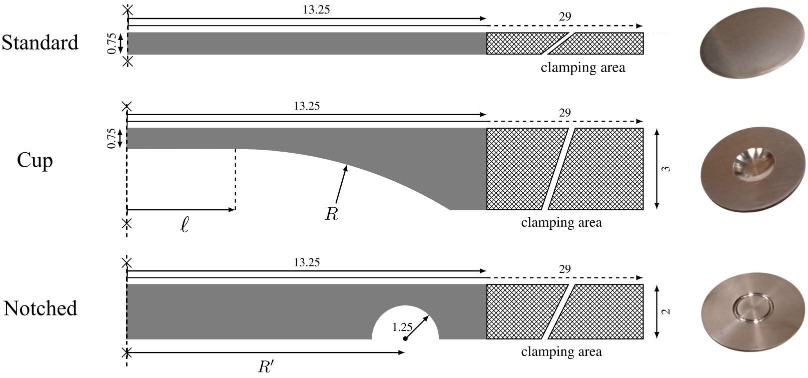


Disk specimen:



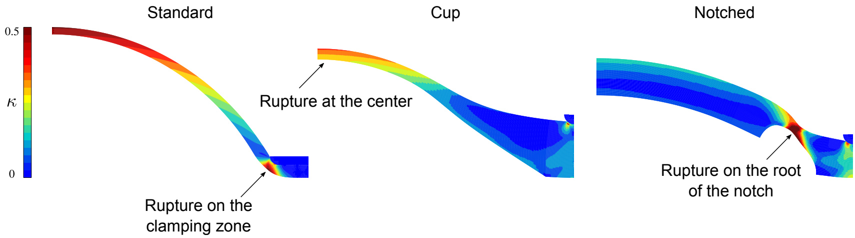
Redesign of the disk geometry

- New proposed geometries:
  - No need to modify the test setup
  - Keep the same minimum thickness of the standard (0.75 mm)
- Optimization with respect to ℓ, R and R' with FE simulations considering an elasto-plastic behavior



Redesign of the disk geometry

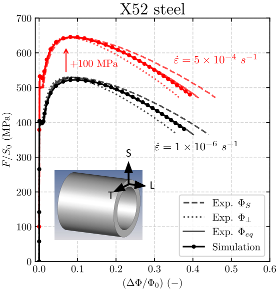
- The location of the maximum accumulated plastic strain (κ) corresponds to the failure location

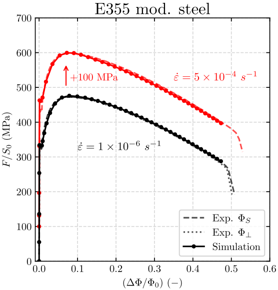


Materials

- **X52 vintage steel:**
  - Yield strength: 400 MPa
  - Different elongation at rupture in T and L directions
- **E355 mod. steel:**
  - Yield strength: 330 MPa
  - Higher elongation at rupture and lower Ultimate Tensile Strength in relation with the vintage material
  - Similar elongation at rupture in both directions
- Elasto(visco)-plastic model coefficients' identified through optimization:

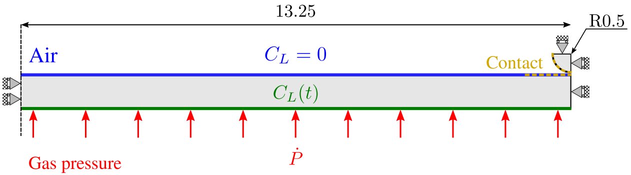
$$\sigma_F(p) = \max(\sigma_L, \sigma_0 + Q_1(1 - \exp(-b_1 p)) + Q_2(1 - \exp(-b_2 p)) + Hp)$$





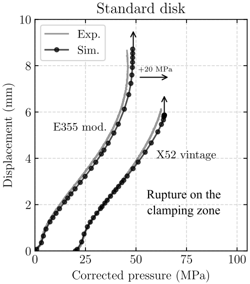
Simulation of pressurized disks

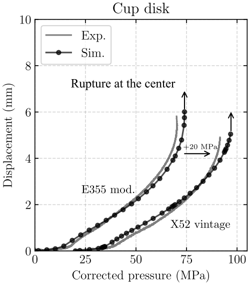
- Axisymmetric model, quadratic elements with reduced integration (mixed formulation)
- Hydrogen diffusion parameters taken from the literature
- Since damage is not considered into the numerical model, the simulations were stopped once they reached experimentally observed rupture pressure (P_r)
- Model's boundary conditions:

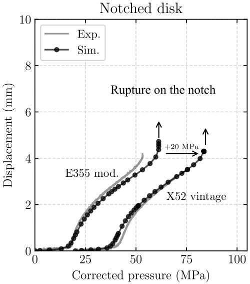


Geometry effect (under helium)

- Good agreement between experimental and numerical results
- Successfully modification of fracture location
- Failure is primarily driven by plasticity and occurs under a limit load scenario







- Considers only dislocations as traps

Thank you for your attention

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