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

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**Thesis defense**
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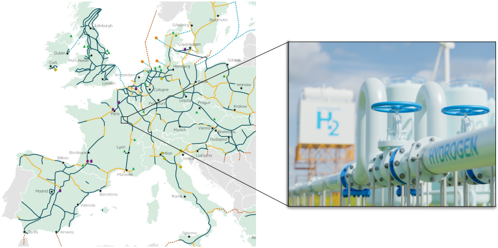
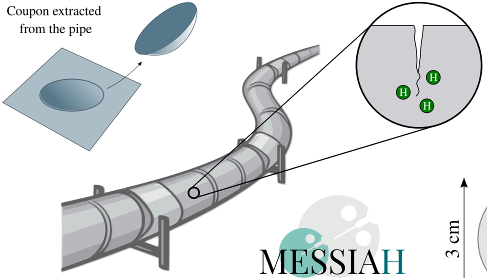
# Background and challenges

- In the context of **energy transition**, **hydrogen** plays an important role as an **energy vector**
- Hydrogen can be produced from other **renewable sources**, such as wind and solar
- Hydrogen transport using **existing natural gas pipelines** (40,000 km in France, 50 billion in assets, up to 80 years old) is a proposal for hydrogen transport

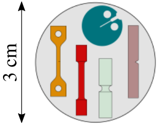
# Background and challenges

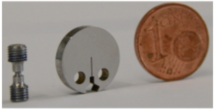
- **Hydrogen embrittlement:** ductility and toughness reduction, premature failure




**Measure material properties from small samples without service interruption**

MESSIAH
Chaire ANR industrielle



## Objectives:

- Develop a model coupling plasticity, damage and hydrogen diffusion
- Validate this model on experimental results
- Simulate size and thickness effect on toughness with sub-size specimens

Introduction

Hydrogen inside metals

Finite element formulation

Numerical simulations
- Pressurized disks tests
- Hydrogen uptake during a tensile test
- Hydrogen embrittlement modeling
- Simulation of fracture toughness tests

Conclusions

Perspectives

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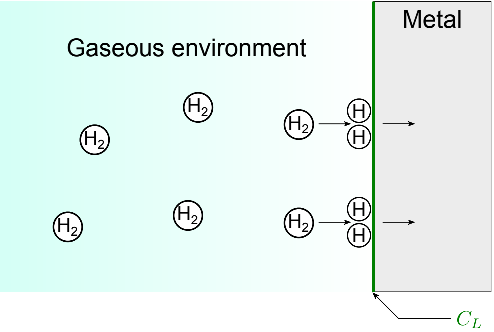
- **Sieverts' law:** The solubility of a diatomic gas in a metal is proportional to the square root of the gas pressure

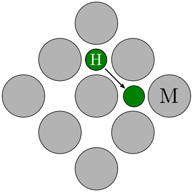



$$\underbrace{C_L}_{\text{Hydrogen solubility (H at./ Iron at.)}} = \underbrace{\gamma}_{\text{Thermally activated term}} \sqrt{\underbrace{P_a}_{H_2 \text{ pressure (MPa)}}}$$

# Hydrogen diffusion and trapping

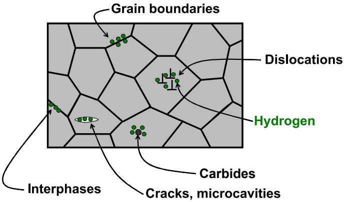
- Model from Sofronis and McMeeking (1989) and corrected by Krom *et al.* (1999)

- **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:**

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

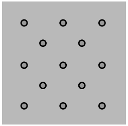
(Coupling terms)

# Material damage

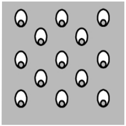
- The **ductile behavior** of the metal is described by the **GTN model** (Tvergaard *et al.* 1984):

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

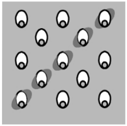
$$\dot{f} = \dot{f}_{nucleation} + \dot{f}_{growth}$$



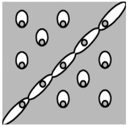
Impurities or second phase particles



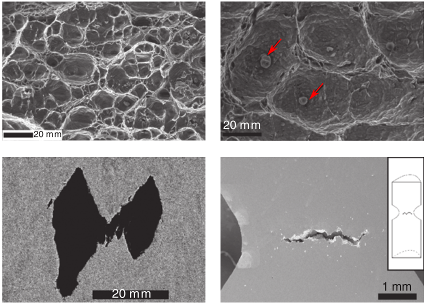
Void nucleation and growth



Strain localization



Void coalescence and fracture



# Hydrogen embrittlement

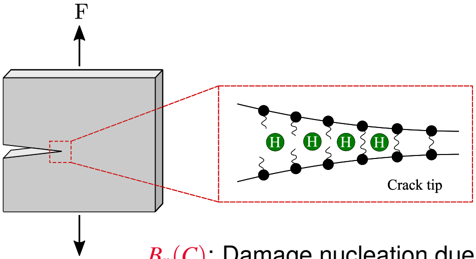
- **Void growth**: Unchanged due to mass conservation

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

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

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

(Coupling terms)




Hydrogen weakens the cohesive bonds between atoms

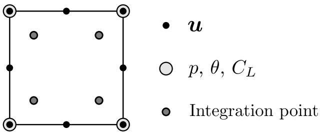
$B_n(C)$: Damage nucleation due to hydrogen
**HEDE** (Hydrogen Enhanced Decohesion)

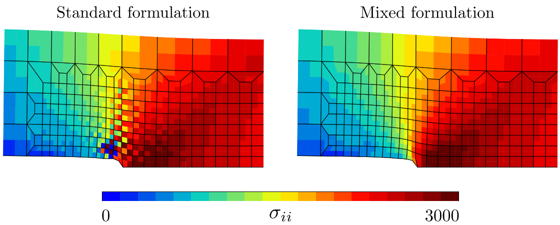
- Fully implicit finite strain framework
- Based on a mixed formulation: $\underline{u}, P, \theta$ (Zhang *et al.* 2017) and $C_L$
- Quadratic elements with reduced integration
- **Aim:** better pressure fields by avoiding volumetric locking

## Advantage

$\nabla p$ can be directly computed from nodal values

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

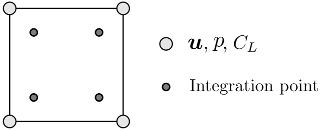


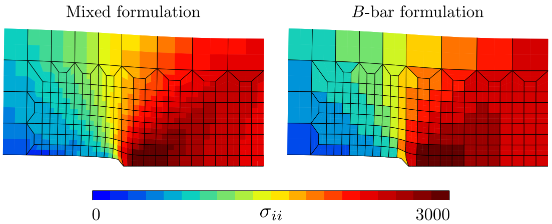



- The use of **quadratic elements** with additional dofs lead to **high simulation times**
- $\boldsymbol{B}$-bar (or $\bar{\boldsymbol{B}}$) formulation (Hughes, 1980):
  - Linear elements with full integration
  - Solves volumetric locking by modifying the strain-displacement matrix:

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

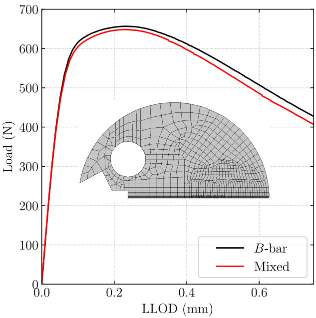
  - To avoid extrapolating $p$ to the nodes for $\nabla p$ computation, it is considered as a dof

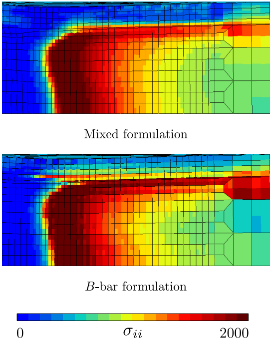


# $B$-bar formulation

- 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 $\rightarrow$ Linear elements are inherently stiffer since they have less nodes

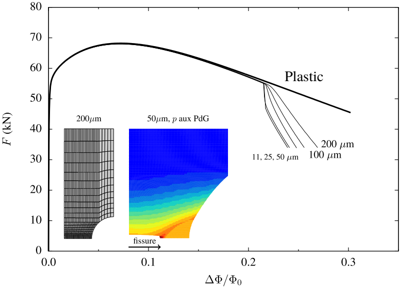


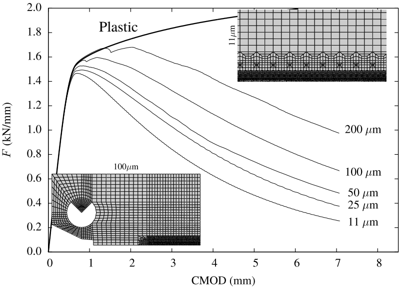

Mixed formulation

$B$-bar formulation

- 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

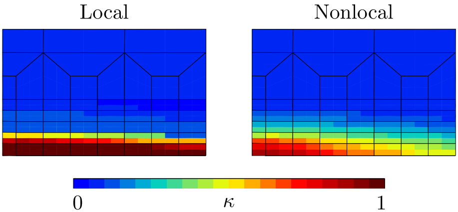



Compact tension (CT) specimen

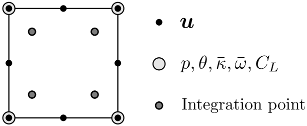
(Besson, 2021)

# Nonlocal damage model

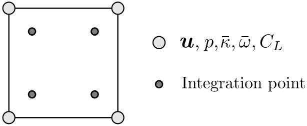
- Two variables are used (two associated internal lengths: $\bar{\omega}$ and $\bar{\kappa}$):
  - **Plastic volume variation:** $\bar{\omega} - \ell_\omega^2 \Delta\bar{\omega} = \omega \quad \text{where} \quad \omega = \text{trace}(\dot{\underset{\sim}{\varepsilon}}_p)$
  - **Accumulated plastic strain:**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



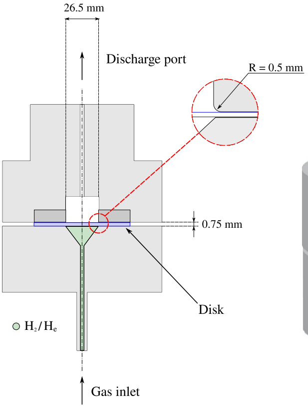

**$B$-bar formulation:**



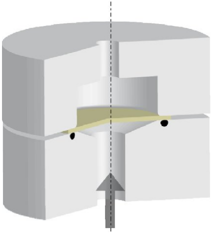
# Outline

# Context

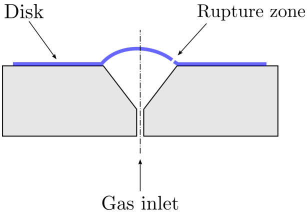
- **ISO 11114-4 standard:** uses pressurized disk tests for selecting metallic materials resistant to hydrogen embrittlement
- Disk often fails in the clamping zone
- **First step:** redesigning the disk geometry to control failure location




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

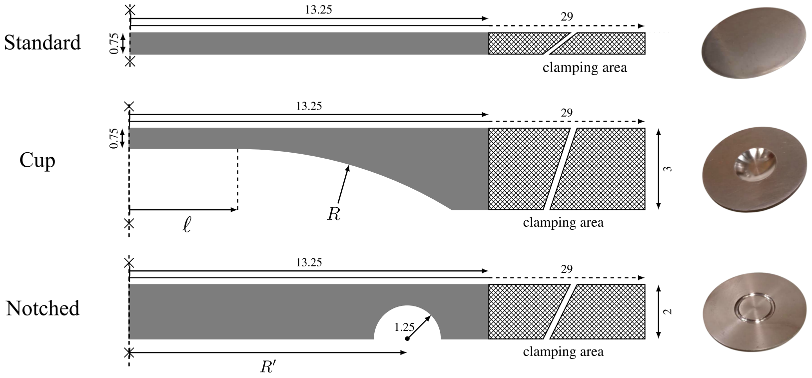


Disk specimen:



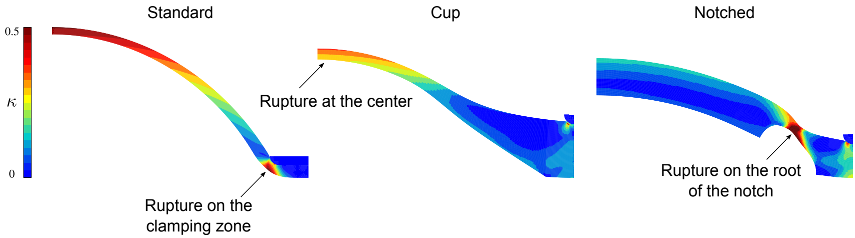
# Redesign of the disk geometry

- 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 $\ell$, $R$ and $R'$ with FE simulations considering an elasto-plastic behavior



# Redesign of the disk geometry

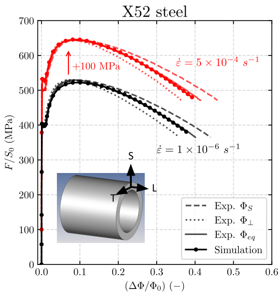
- The location of the maximum accumulated plastic strain ($\kappa$) corresponds to the failure location

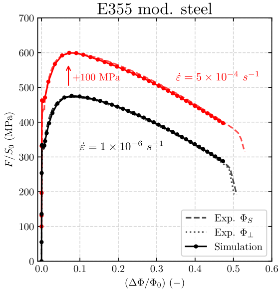


# Materials

- **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:

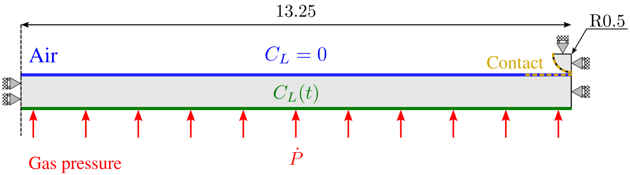
$$\sigma_F(p) = \max(\sigma_L, \sigma_0 + Q_1(1 - \exp(-b_1 p)) + Q_2(1 - \exp(-b_2 p)) + Hp)$$



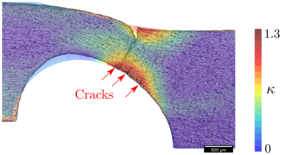
# Simulation of pressurized disks

- 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:

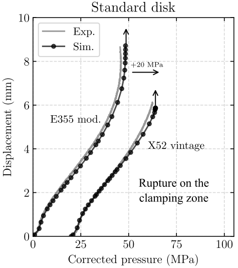


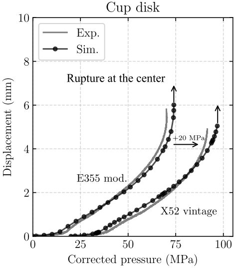
# Results under helium

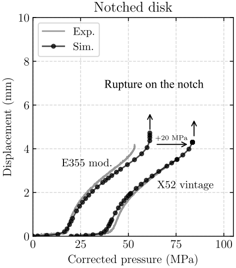
- Experiments carried out by Luciano Santana
- Successfully modification of fracture location
- Failure is primarily driven by plasticity and occurs under a limit load scenario



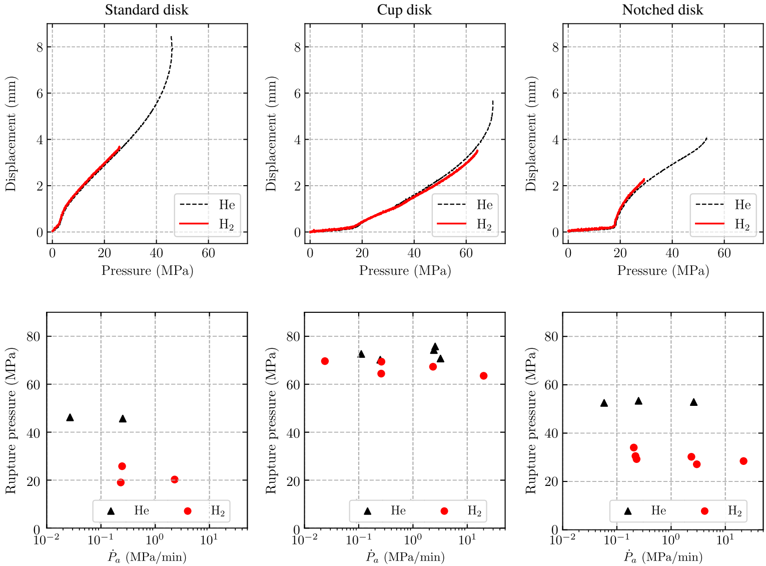




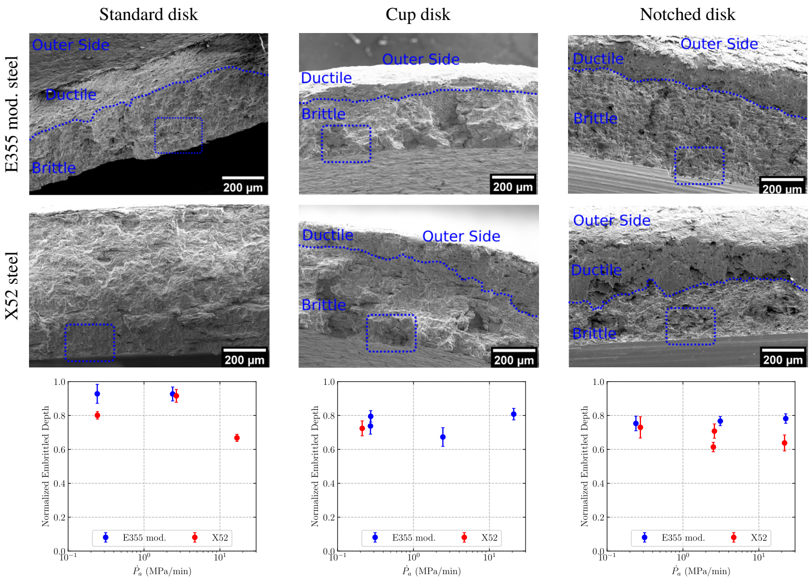



# Results under hydrogen (E355 mod. steel)



# Hydrogen embrittled depth

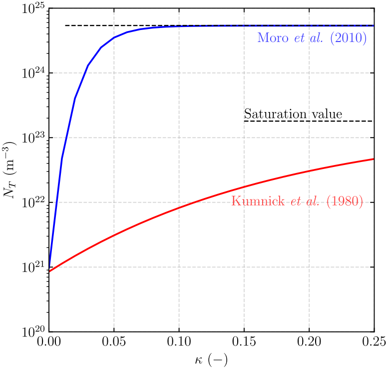


# Hydrogen trapping model

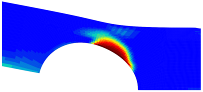
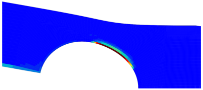
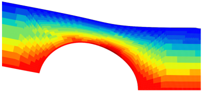
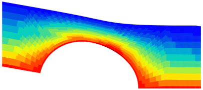
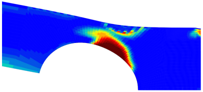
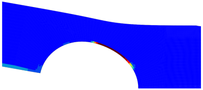
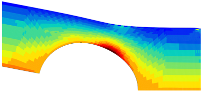
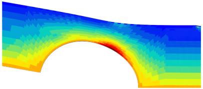
- Considers only one kind of trap: dislocations
- Trap binding energies ($W_B$) and trap densities ($N_T$) were taken from the literature and analyzed based on the experimental observations
- Based on the models proposed by Moro *et al.* (2010) and Kumnick *et al.* (1980), four cases emerge

$$W_B = \begin{cases} 40\ \mathrm{kJ/mol} \\ 60\ \mathrm{kJ/mol} \end{cases}$$

$$N_T = \begin{cases} \log_{10} N_T = 24.73 - 3.74\exp(-60.17\kappa) \\ \log_{10} N_T = 23.26 - 2.33\exp(-5.5\kappa) \end{cases}$$

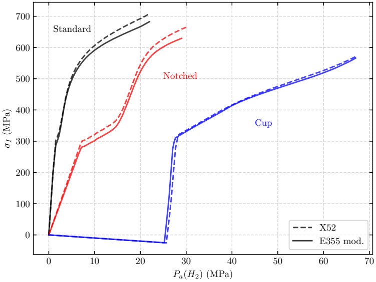


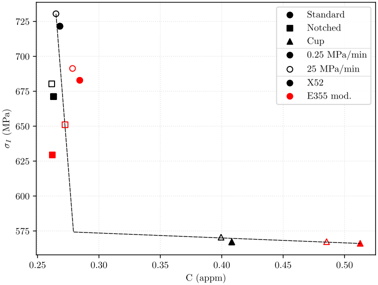
# Hydrogen embrittled depth

| | $\dot{P} = 0.25$ MPa/min | $\dot{P} = 25$ MPa/min | $C_{max}$ (appm) |
| --- | --- | --- | --- |
| $W_B = 40$ kJ/mol<br>$N_T$ from Moro *et al.* |  |  | 16 |
| $W_B = 40$ kJ/mol<br>$N_T$ from Kumnick *et al.* |  |  | 0.3 |
| $W_B = 60$ kJ/mol<br>$N_T$ from Moro *et al.* |  |  | 60 |
| $W_B = 60$ kJ/mol<br>$N_T$ from Kumnick *et al.* |  |  | 0.4 |

# Principal stress evolution

- Specimens that develop higher principal stress ($\sigma_I$) in the fracture zone fail at a lower hydrogen pressure ($P_a(H_2)$)
- The total hydrogen concentration reduces the maximum principal stress that that triggers fracture



# Outline

# Thank you for your attention

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