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Virtual Testing of materials and structures undergoing corrosion and/or hydrogen embrittlement

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https://www.imperial.ac.uk/mechanics-materials/

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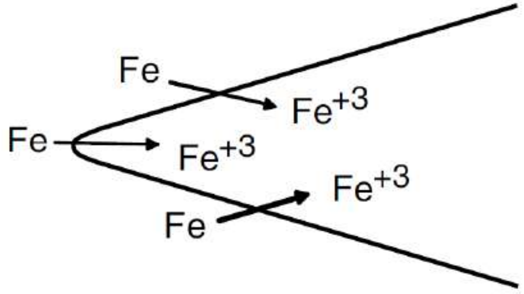
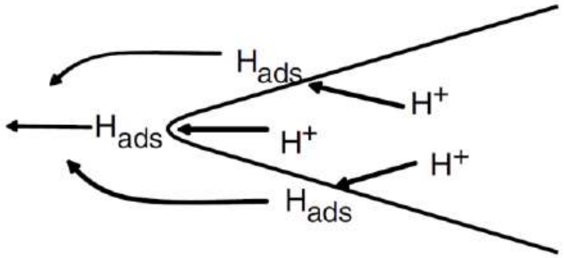
Environmentally assisted cracking

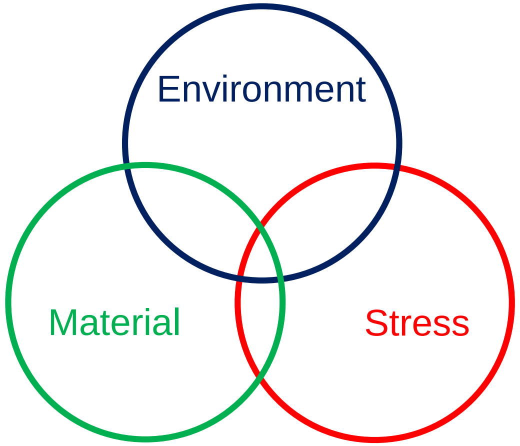
- ❑ Stress Corrosion Cracking (SCC)
  - ❑ Anodic-dissolution cracking



  - ❑ Hydrogen embrittlement



- ❑ Hydrogen embrittlement
- ❑ Liquid Metal Embrittlement
- ❑ Oxidation fatigue, *etc*.



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Environmentally assisted cracking

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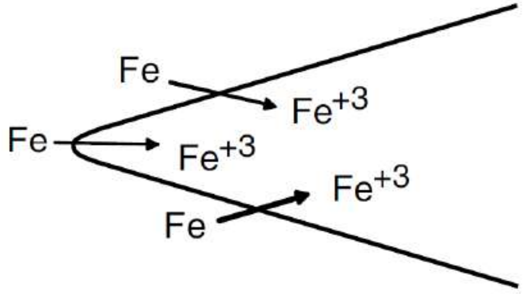
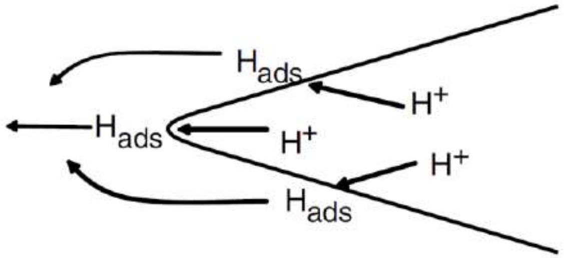


  - Hydrogen embrittlement



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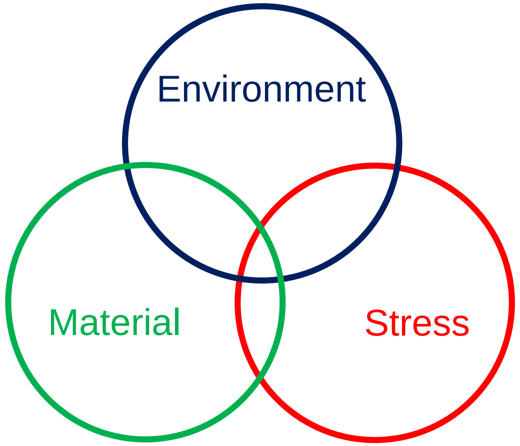

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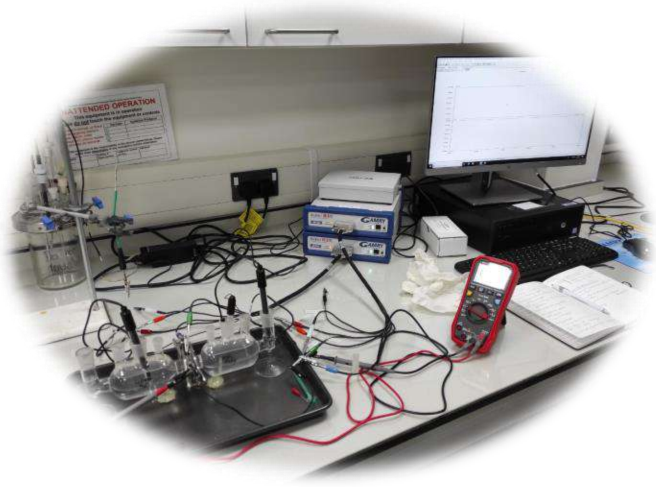
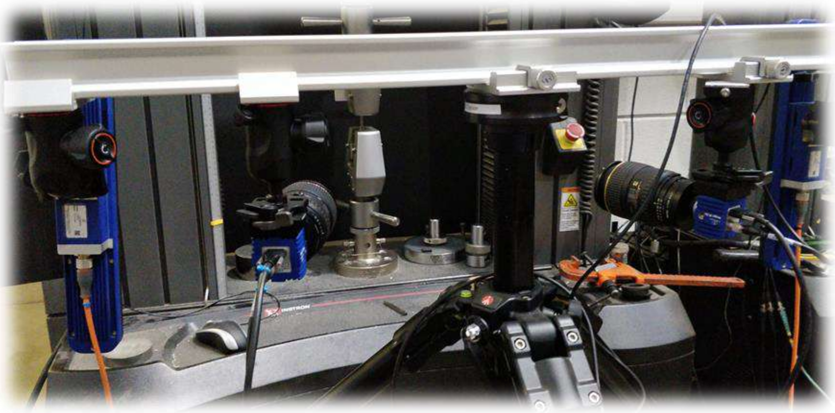
Hydrogen embrittlement - experiments

Permeation



E-chem charging

Desorption



The effect of hydrogen in metals

W. H. Johnson. Proceedings of the Royal Society of London Vol. 23, 168-179 (1875)

II. "On some remarkable Changes produced in Iron and Steel by the Action of Hydrogen and Acids." By WILLIAM H. JOHNSON, B.Sc. Communicated by Prof. Sir WILLIAM THOMSON, LL.D., F.R.S. Received December 7, 1874.

Some three years ago my attention was called to a remarkable change in some of the physical properties of iron caused by its temporary immersion in hydrochloric and sulphuric acids. This change is at once made evident to any one by the extraordinary decrease in toughness and breaking-strain of the iron so treated, and is all the more remarkable as it is

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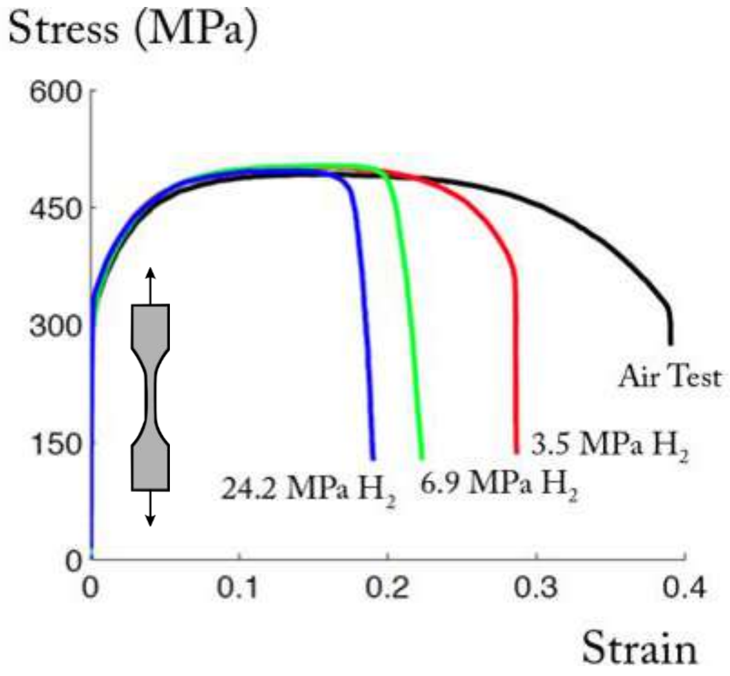
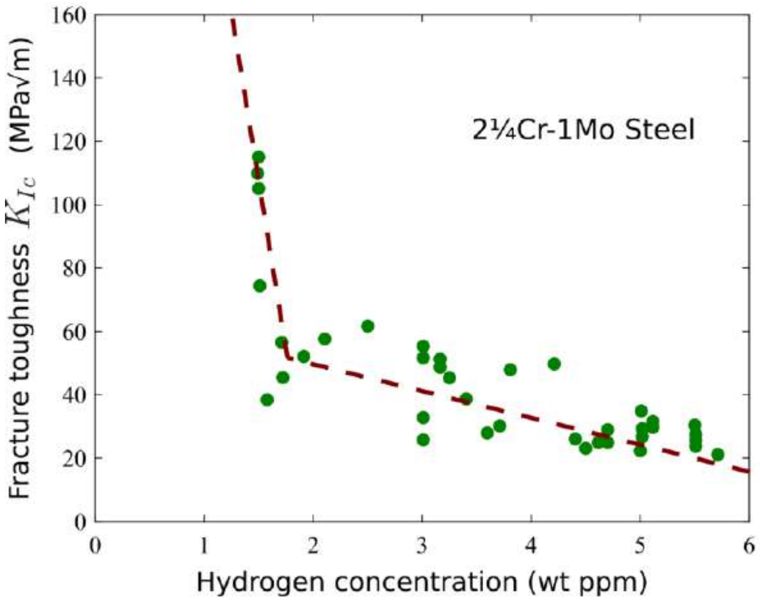
Hydrogen embrittlement

Ductility



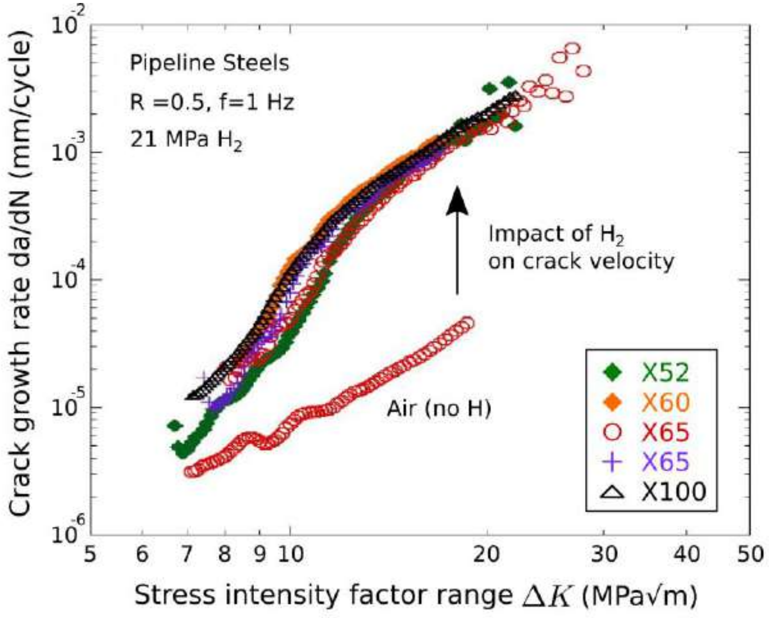
ASME SA106 Steel [Adapted from: Xu and Rana. *2008 Int. Hydrogen Conference* (2009), Anand et al. JMPS (2019)]

Toughness



2¼Cr-1Mo Steel [Adapted from: Hosseini et al. *2016 Int. Hydrogen Conference* (2017)]

Fatigue crack growth



Pipeline steels [Adapted from: San Marchi & Ronevich, 2022 Symposium on Hydrogen- Materials Interactions]

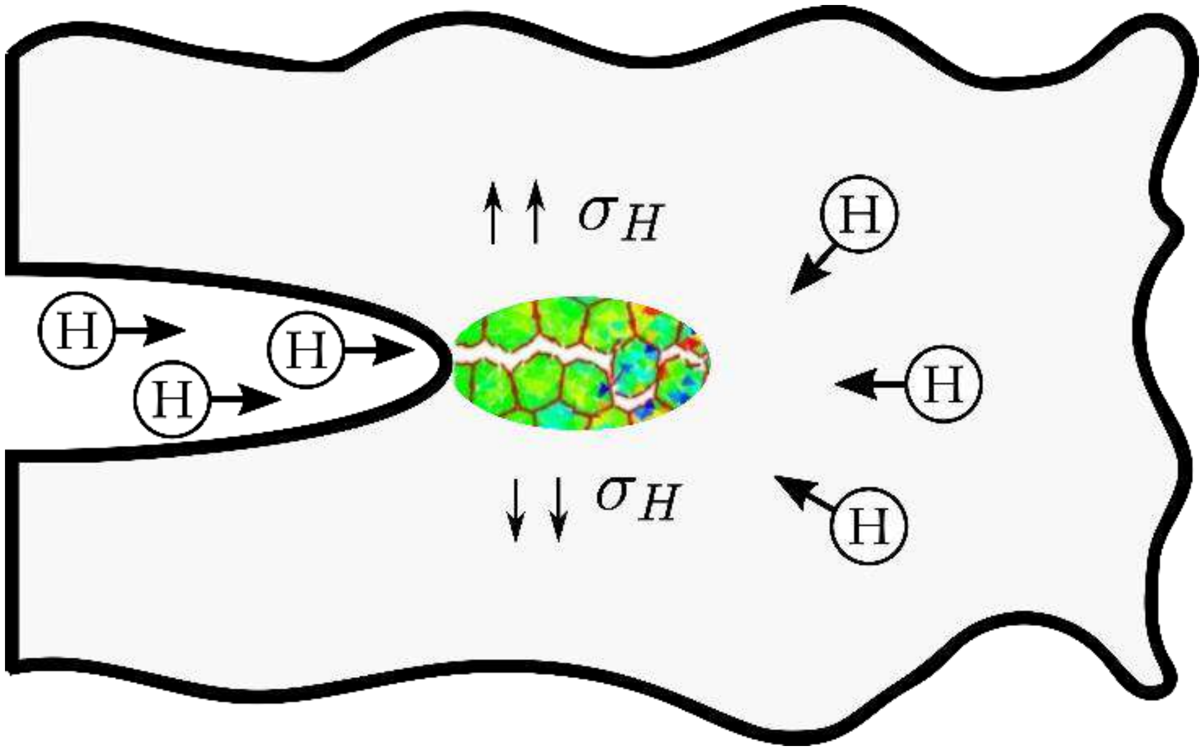
Hydrogen embrittlement: a complex phenomenon

Complex micromechanical and chemical problem, with hydrogen having an impact at multiple scales! [mechanics – chemistry – materials science]

Gas

Electrolyte

Water vapour



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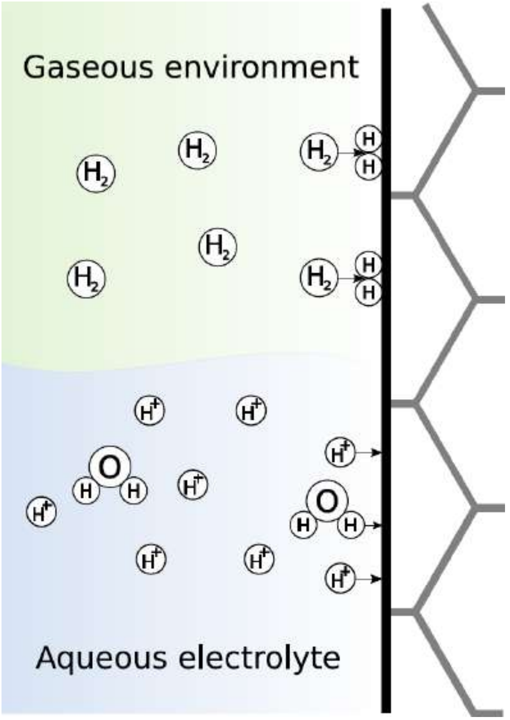
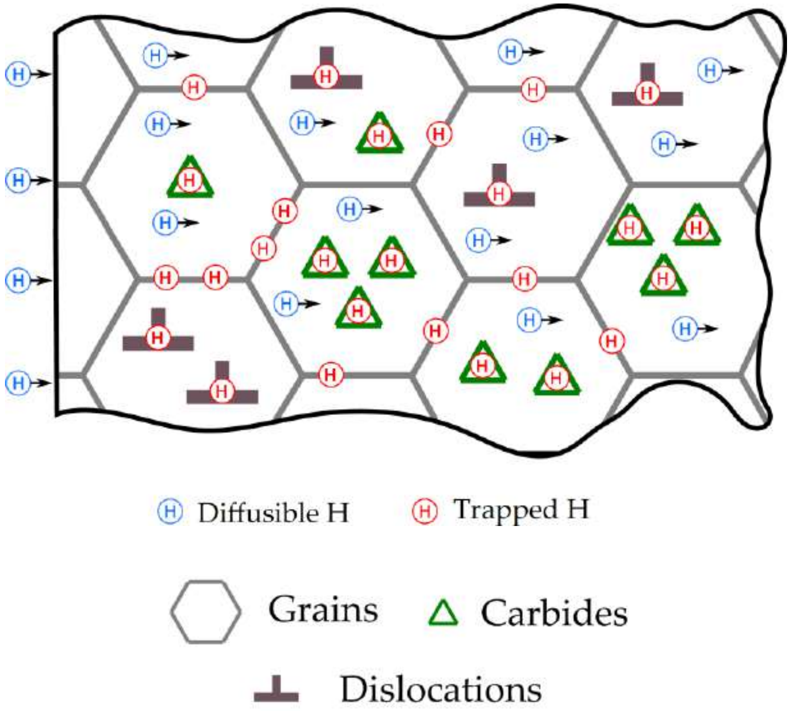
Hydrogen embrittlement stages

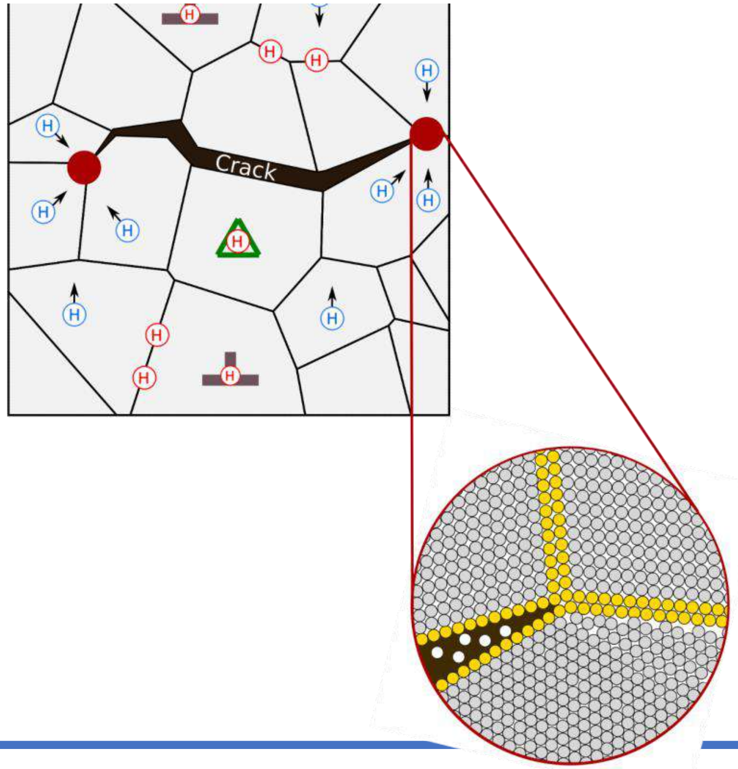
Stage I: H uptake



Stage II: H transport

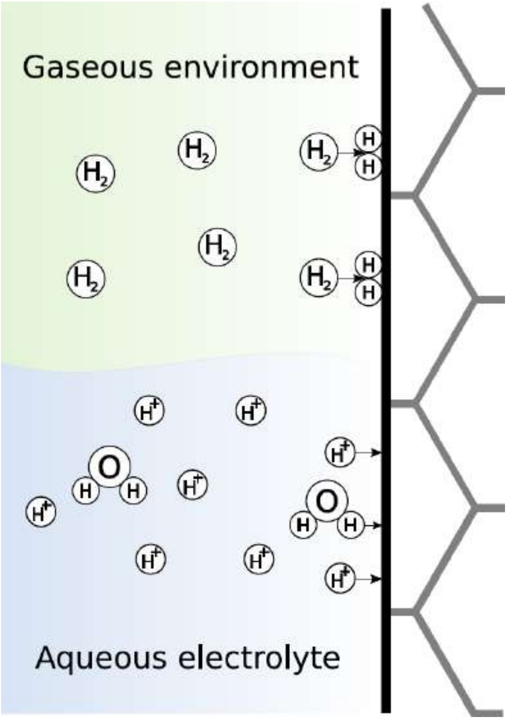


Stage III: H embrittlement



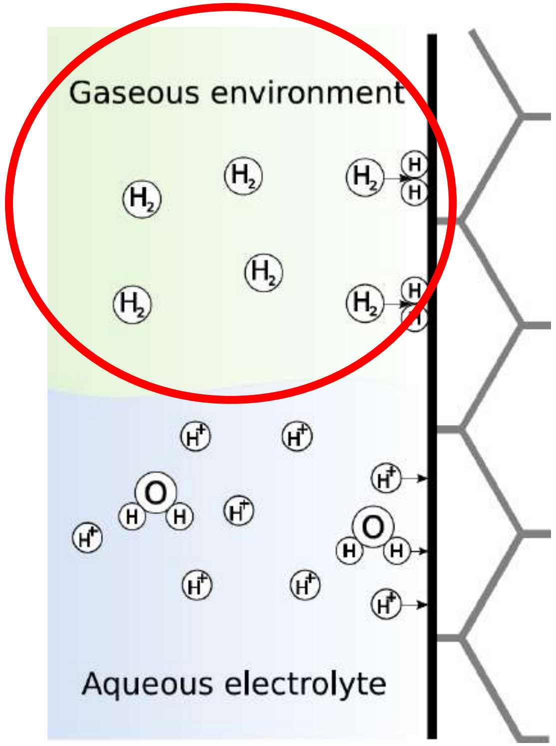
Stage I: H uptake

Stage I: H uptake



Stage I: H uptake, H2 gas

Stage I: H uptake



Gaseous environment (steady state)

$$\frac{1}{2}\mu_{H_2} = \mu_H \qquad \text{with} \qquad \mu_{H_2} = \mu_{H_2}^0 + RT\ln\left(\frac{f_{H_2}}{p^0}\right)$$

Hence: $\mu_H = RT\ln\left(\sqrt{\frac{f_{H_2}}{p^0}}\right)$ and recalling $\mu_L = \mu_L^0 + RT\ln\frac{\theta_L}{1-\theta_L} - \bar{V}_H\sigma_H$

$$C_L = \frac{N_L}{\sqrt{p^0}}\exp\left(-\frac{\mu_L^0}{RT}\right)\exp\left(\frac{\bar{V}_H\sigma_H}{RT}\right)\sqrt{f_{H_2}}$$

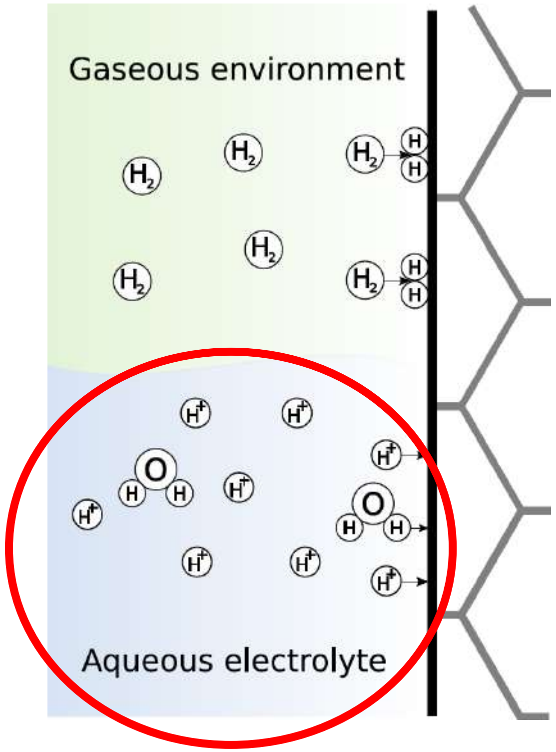
$$C_L = K\sqrt{f_{H_2}} = \exp\left(\frac{\bar{V}_H\sigma_H}{RT}\right)K_{\sigma=0}\sqrt{f_{H_2}}$$ (Sievert's law)

Díaz et al. *Int. J. Mech. Sci.* (2016)

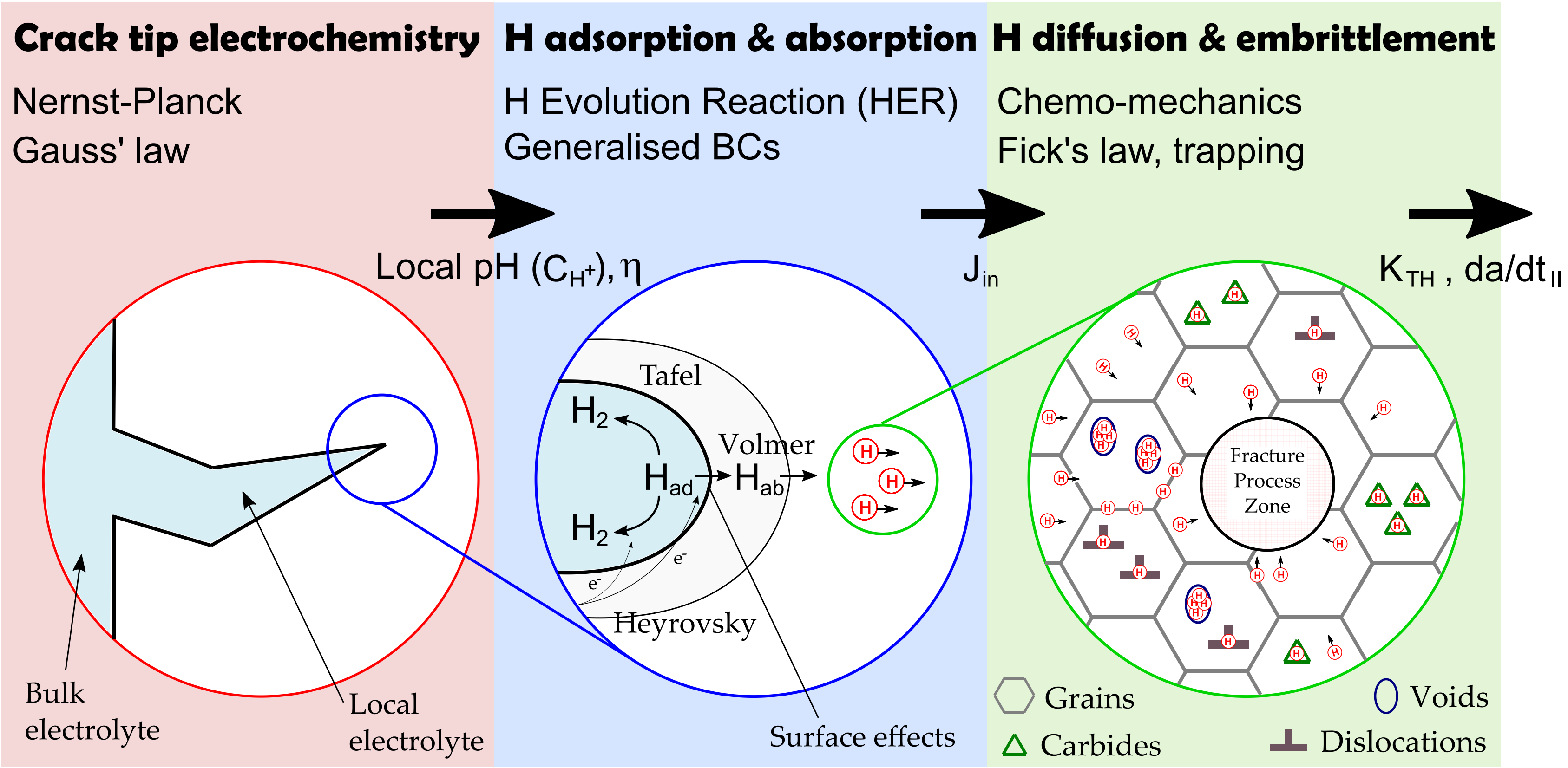
Martínez-Pañeda et al. *Int. J. Hydrogen Energy* (2016)

Stage I: H uptake, aqueous electrolyte

Stage I: H uptake



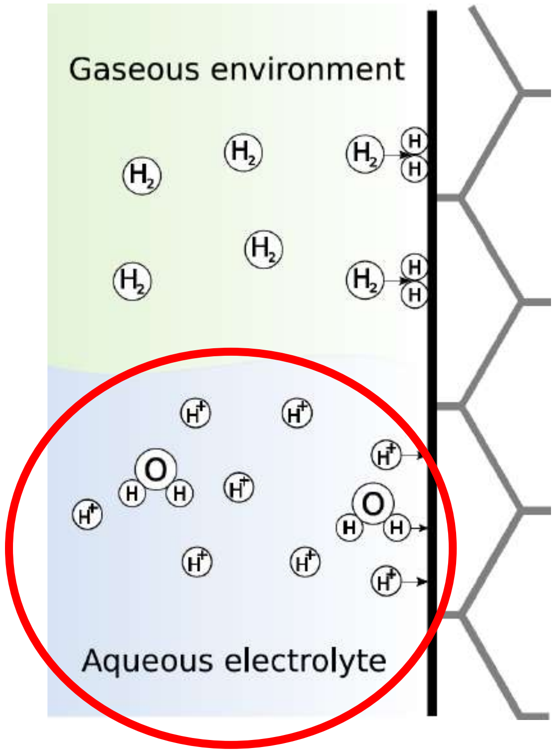
Aqueous electrolyte



Martínez-Pañeda. *RILEM Technical Letters* (2021)

Stage I: H uptake, aqueous electrolyte

Stage I: H uptake



Aqueous electrolyte – a complete electro-chemo-mechanics model

Electrolyte domain

Nernst-Planck: $$\dot{C}_\pi + \underbrace{(\mathbf{v}\cdot\boldsymbol{\nabla})C_\pi}_{\text{transport due to fluid flow}} + \underbrace{\boldsymbol{\nabla}\cdot(-D_\pi \boldsymbol{\nabla} C_\pi)}_{\text{diffusion}} \underbrace{+\frac{z_\pi F}{RT}\boldsymbol{\nabla}\cdot(-D_\pi C_\pi \boldsymbol{\nabla}\varphi)}_{\text{electric potential driven migration}} + \underbrace{R_\pi}_{\text{volume reactions}} = 0$$

Electro-neutrality: $$\sum_\pi z_\pi C_\pi = 0$$

Surface domain

$$H^+ + M + e^- \underset{k'_{Va}}{\overset{k_{Va}}{\rightleftharpoons}} MH_{ads}$$

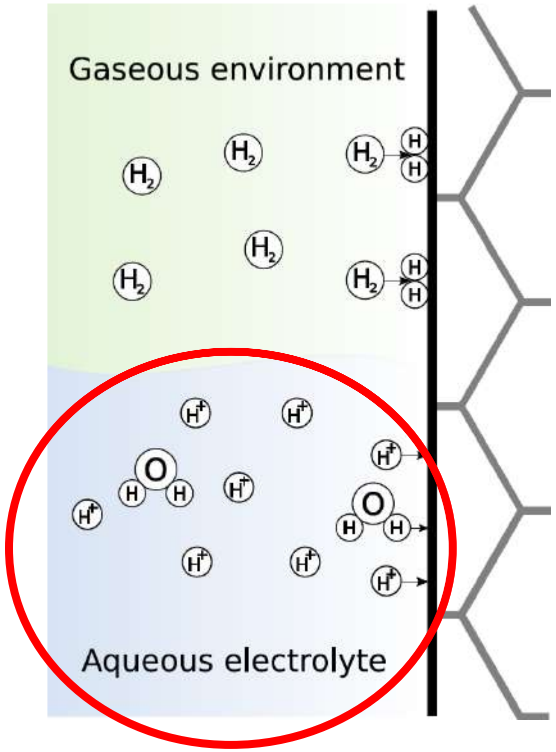
$$H^+ + e^- + MH_{ads} \underset{k'_{Ha}}{\overset{k_{Ha}}{\rightleftharpoons}} M + H_2$$

$$2MH_{ads} \underset{k'_{T}}{\overset{k_{T}}{\rightleftharpoons}} 2M + H_2$$

$$MH_{ads} \underset{k'_{A}}{\overset{k_{A}}{\rightleftharpoons}} MH_{abs}$$

Stage I: H uptake, aqueous electrolyte

Stage I: H uptake



Aqueous electrolyte – a complete electro-chemo-mechanics model

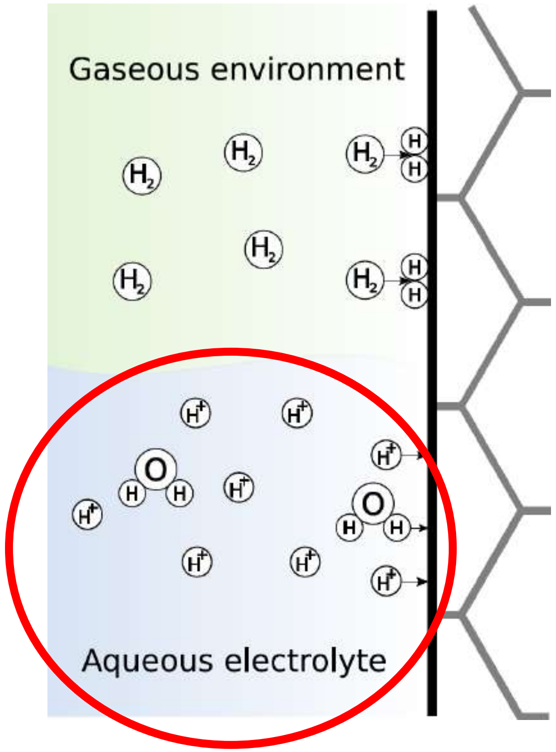
Reaction rates:

	Forward	Backward
Volmer(acid) :	$\nu_{Va} = k_{Va} C_{H^+} (1-\theta_{ads}) \exp\left(-\alpha_{Va}\frac{\eta F}{RT}\right)$	$\nu'_{Va} = k'_{Va}\theta_{ads} \exp\left((1-\alpha_{Va})\frac{\eta F}{RT}\right)$
Heyrovsky(acid) :	$\nu_{Ha} = k_{Ha} C_{H^+} \theta_{ads} \exp\left(-\alpha_{Ha}\frac{\eta F}{RT}\right)$	$\nu'_{Ha} = k'_{Ha}(1-\theta_{ads}) p_{H_2} \exp\left((1-\alpha_{Ha})\frac{\eta F}{RT}\right)$
Tafel :	$\nu_T = k_T \theta_{ads}^2$	$\nu'_T = k'_T (1-\theta_{ads})^2 p_{H_2}$
Absorption :	$\nu_A = k_A (N_L - C_L)\theta_{ads}$	$\nu'_A = k'_A C_L (1-\theta_{ads})$
Volmer(base) :	$\nu_{Vb} = k_{Vb}(1-\theta_{ads}) \exp\left(-\alpha_{Vb}\frac{\eta F}{RT}\right)$	$\nu'_{Vb} = k'_{Vb} C_{OH^-}\theta_{ads} \exp\left((1-\alpha_{Vb})\frac{\eta F}{RT}\right)$
Heyrovsky(base) :	$\nu_{Hb} = k_{Hb}\theta_{ads} \exp\left(-\alpha_{Hb}\frac{\eta F}{RT}\right)$	$\nu'_{Hb} = k'_{Hb}(1-\theta_{ads}) p_{H_2} C_{OH^-} \exp\left((1-\alpha_{Hb})\frac{\eta F}{RT}\right)$

Hageman & Martínez-Pañeda. *Corros. Sci.* (2022)

Stage I: H uptake, aqueous electrolyte

Stage I: H uptake



Aqueous electrolyte – a complete electro-chemo-mechanics model

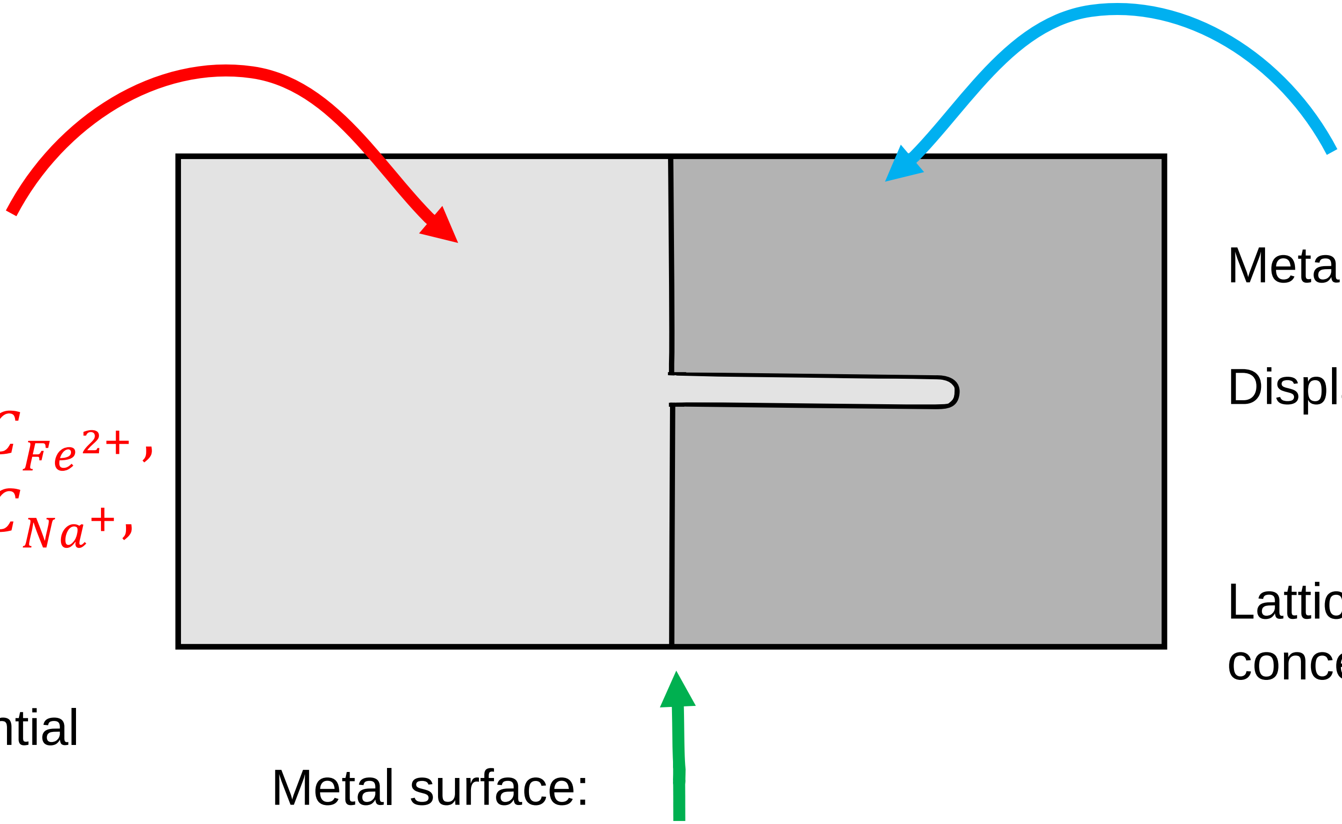
Electrolyte:

Ion species

$C_{H^+}, C_{OH^-}, C_{Fe^{2+}},$
$C_{FeOH^+}, C_{Na^+},$
C_{Cl^-}

Electric potential

φ



Metal surface:
Surface coverage θ_{ads}

Metal:

Displacement

$\mathbf{u}$

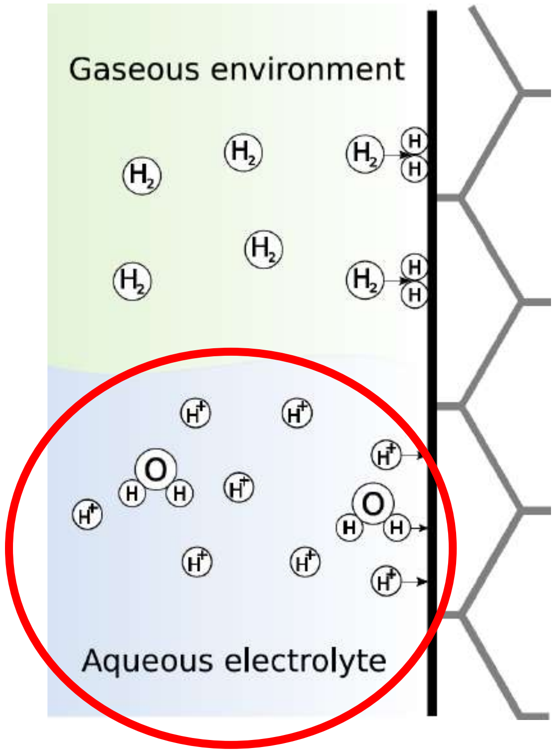
Lattice H concentration

C_L

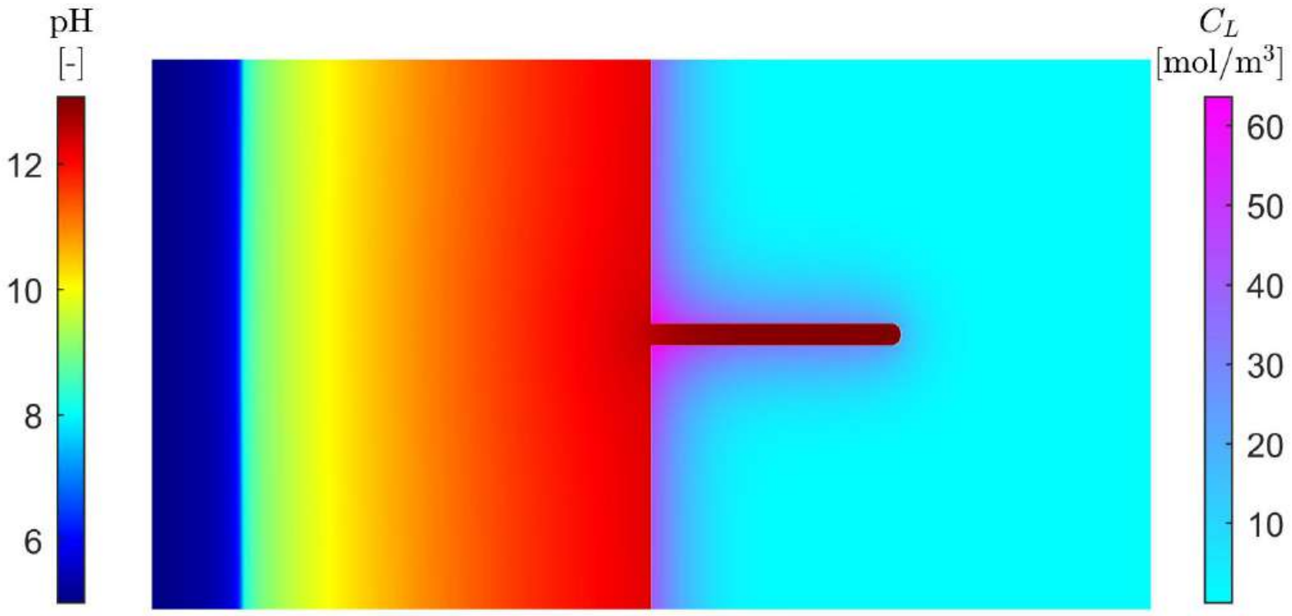
Hageman & Martínez-Pañeda. *Corros. Sci.* (2022)

Stage I: H uptake, aqueous electrolyte

Stage I: H uptake



Aqueous electrolyte – a complete electro-chemo-mechanics model

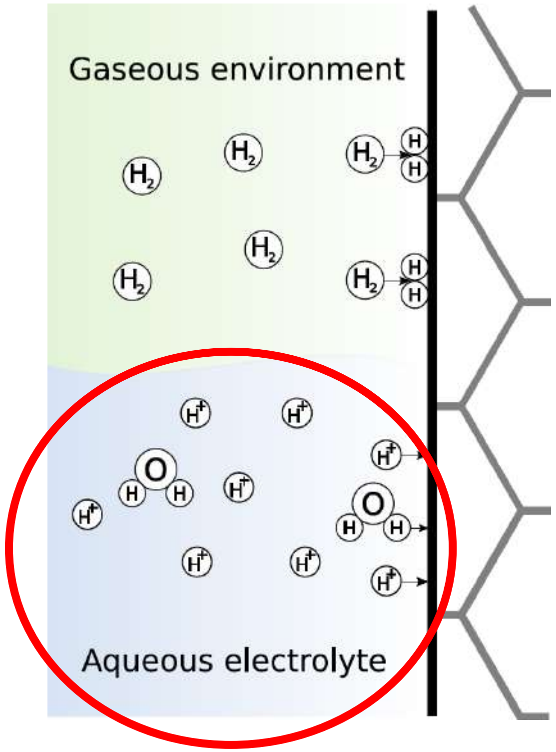


$$E_M = -0.5\ \mathrm{V}_{SHE}$$

Hageman & Martínez-Pañeda. *Corros. Sci.* (2022)

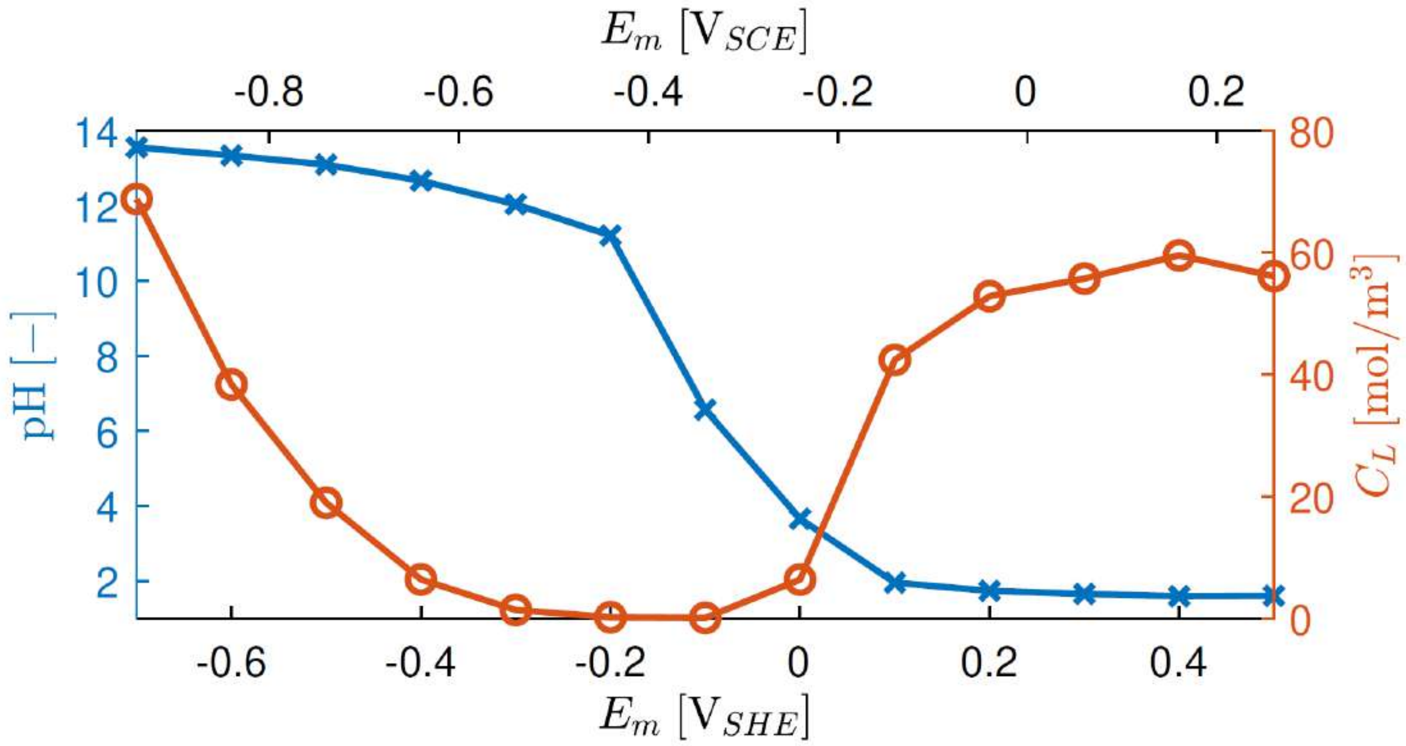
Stage I: H uptake, aqueous electrolyte

Stage I: H uptake



Aqueous electrolyte – a complete electro-chemo-mechanics model

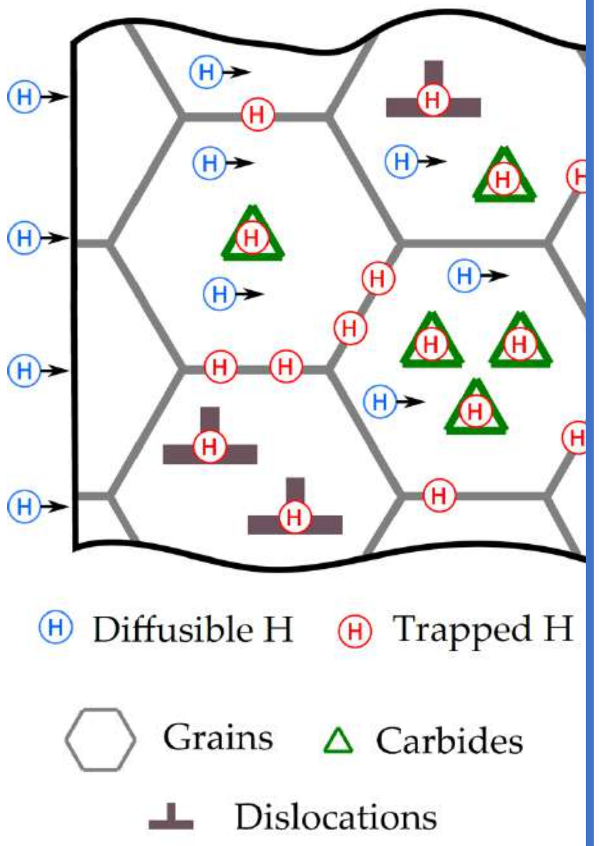
Crack tip estimates:



Hageman & Martínez-Pañeda. *Corros. Sci.* (2022)

Stage II: H diffusion and trapping

Stage II: H transport



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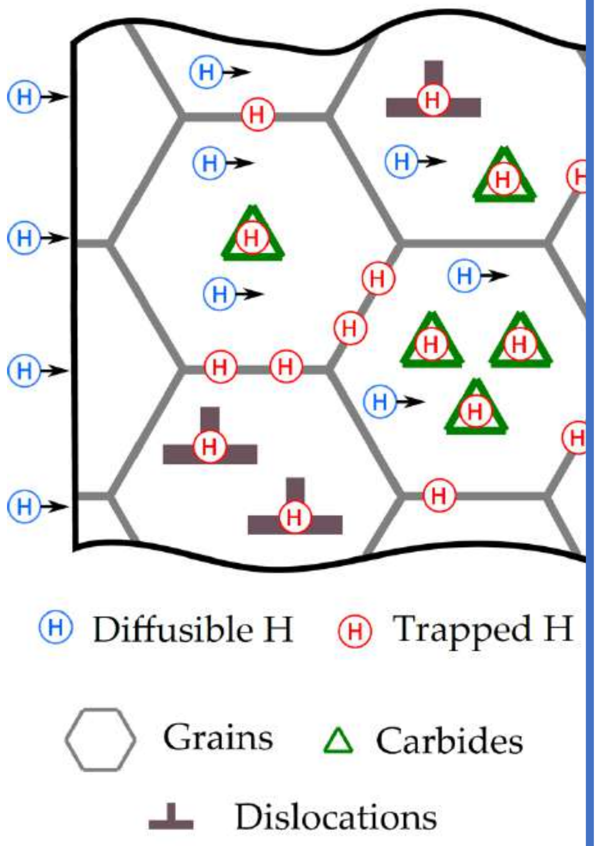

$$\frac{\partial C}{\partial t} - D\nabla^2 C + \nabla \cdot \left(\frac{DC}{RT} \bar{V}_H \nabla \sigma_H \right) = 0$$

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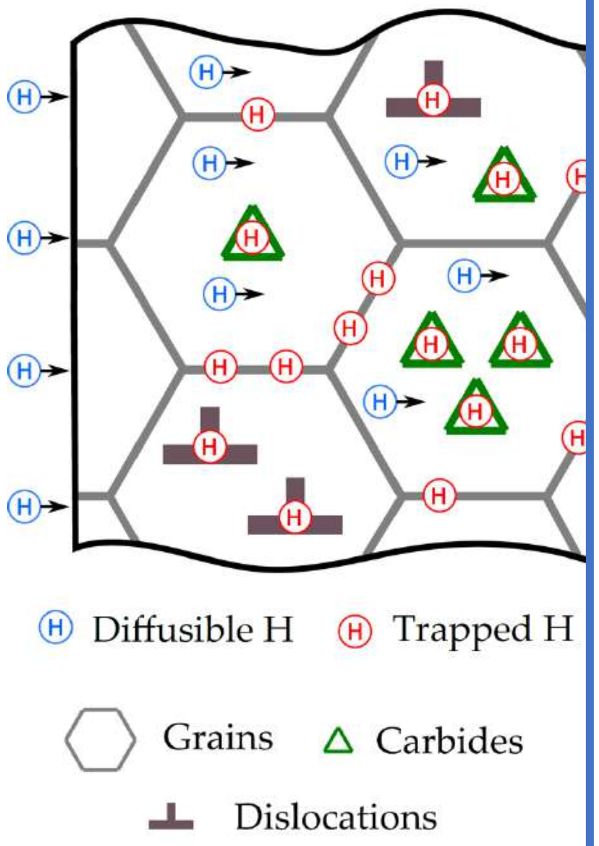
Stage II: H diffusion and trapping

Stage II: H transport

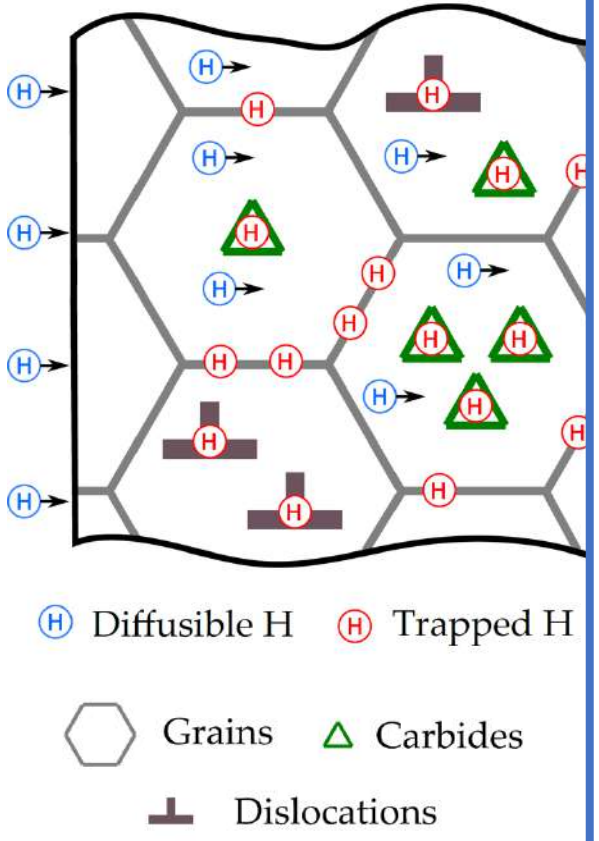


$$\frac{\partial C}{\partial t} - D\nabla^2 C + \nabla \cdot \left(\frac{DC}{RT} \bar{V}_H \nabla \sigma_H \right) = 0$$

At steady-state: $$C_L = C_0 \exp\left(\frac{\bar{V}_H \sigma_H}{RT} \right)$$

Stage II: H diffusion and trapping

Stage II: H transport



Oriani multi-trap

$$C_L = N_L \theta_L \;, \quad C_T = N_T \theta_T \;, \quad D_e = D \frac{C_L}{C_L + \sum_i C_T^{(i)} \left(1 - \theta_T^{(i)}\right)}$$

$$\frac{D_L}{D_e} \frac{\partial C_L}{\partial t} = D_L \nabla^2 C_L + \nabla \cdot \left(\frac{D_L C_L}{RT} \bar{V}_H \nabla \sigma_H \right)$$

Isfandbod & Martínez-Pañeda. *Int. J. Plast.* (2021)

Fernández-Sousa, Betegón, Martínez-Pañeda. *Acta Mat.* (2020)

McNabb-Foster

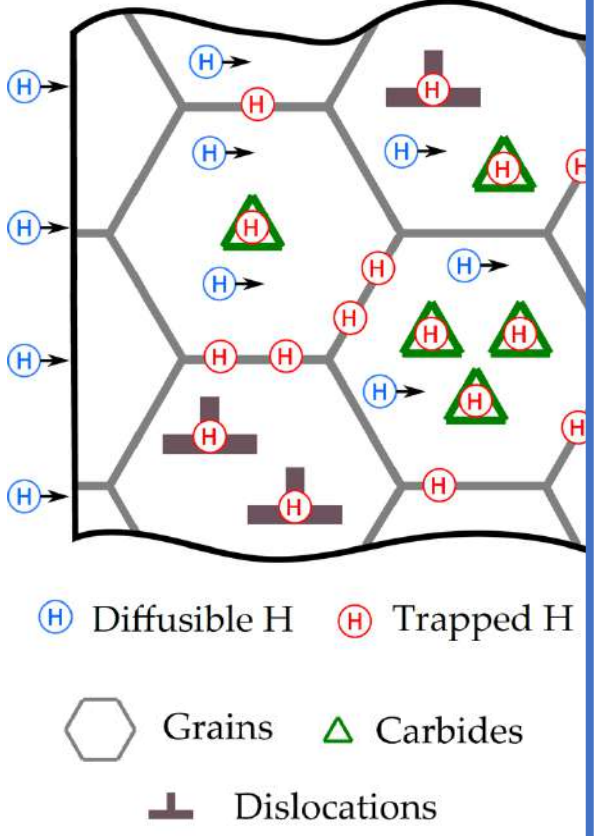
$$\frac{\partial C_L}{\partial t} + \frac{\partial C_T}{\partial t} = D_L \nabla^2 C_L + \nabla \cdot \left(\frac{D_L C_L}{RT} \bar{V}_H \nabla \sigma_H \right)$$

$$\frac{\partial C_T}{\partial t} = N_T \left[k_r C_L (1 - \theta_T) - p_r \theta_T \right]$$

Martínez-Pañeda, Díaz, Wright, Turnbull. *Corros. Sci.* (2020)

Stage II: H diffusion and trapping

Stage II: H transport



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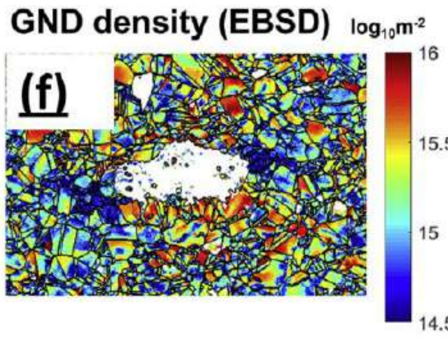
$$\frac{D_L}{D_e} \frac{\partial C_L}{\partial t} = D_L \nabla^2 C_L + \nabla \cdot \left(\frac{D_L C_L}{RT} \bar{V}_H \nabla \sigma_H \right)$$

- Dislocation trap density account for SSDs **and GNDs**:

$$N_T^{(d)} = \frac{\sqrt{2}\rho}{a} \qquad \text{with} \qquad \rho = \rho_{SSD} + \rho_{GND}$$

Taylor (1938): $\rho_{GND} = \bar{r} \frac{\eta^p}{b} \quad \rho_{SSD} = \left(\frac{\sigma_{ref} f(\varepsilon^p)}{0.5 M \mu b} \right)^2$

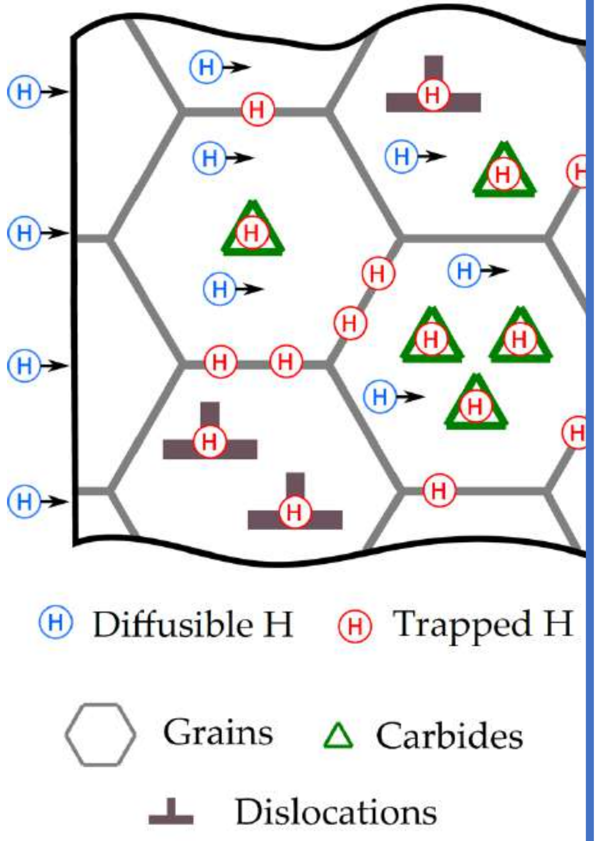


J. Jiang et al., Acta Mater., 2016

Martínez-Pañeda, Niordson, Gangloff. *Acta Mater.* (2016)

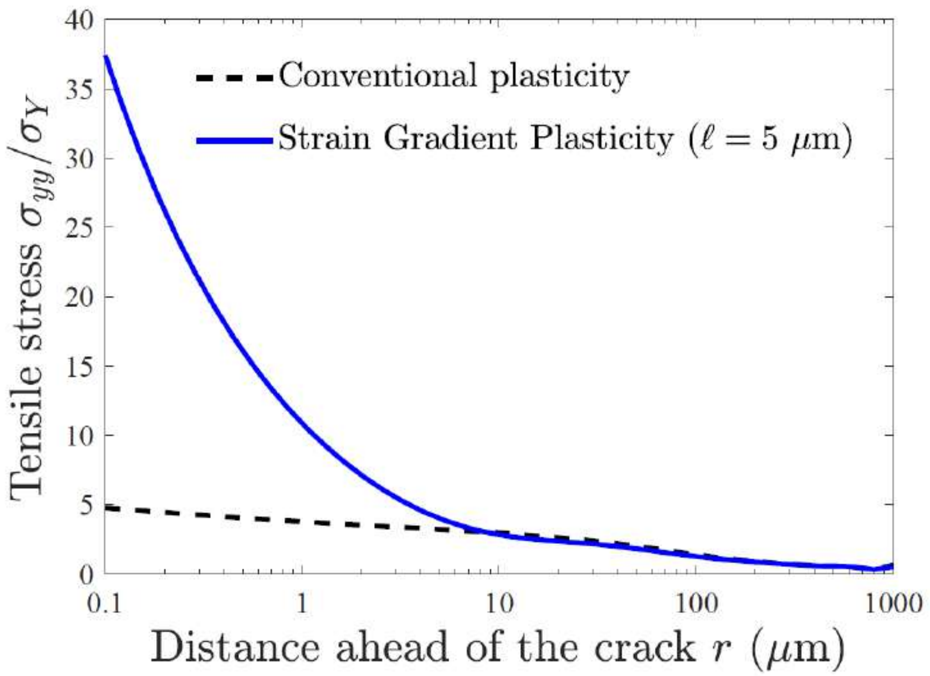
Stage II: H diffusion and trapping

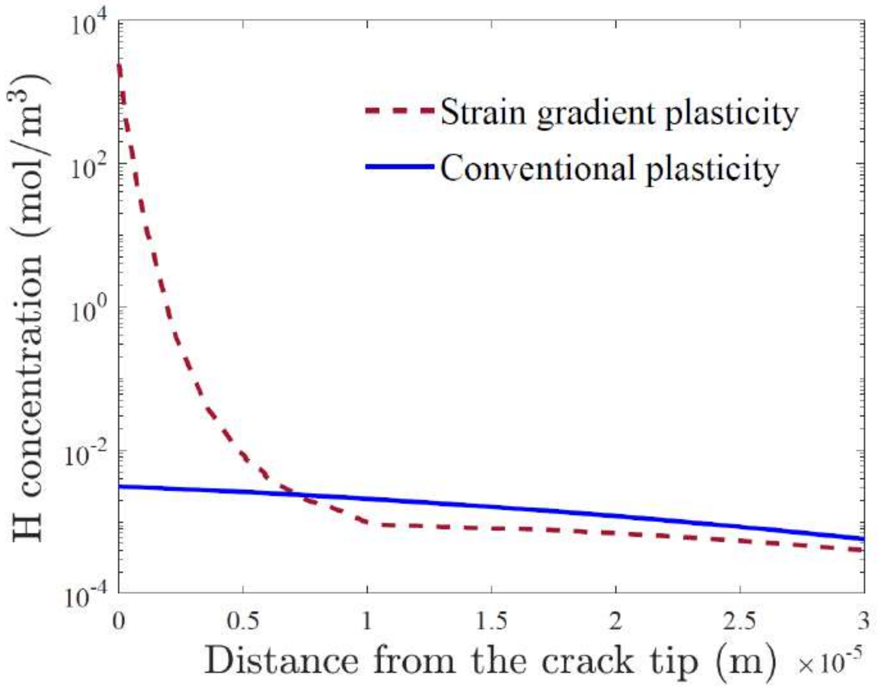
Stage II: H transport



The dual role of GNDs: enhancing trapping and elevating σ_H and C_L

$$\sigma_f = 0.5M\mu b\sqrt{\rho} = 0.5M\mu b\sqrt{\rho_{SSD} + \rho_{GND}}$$

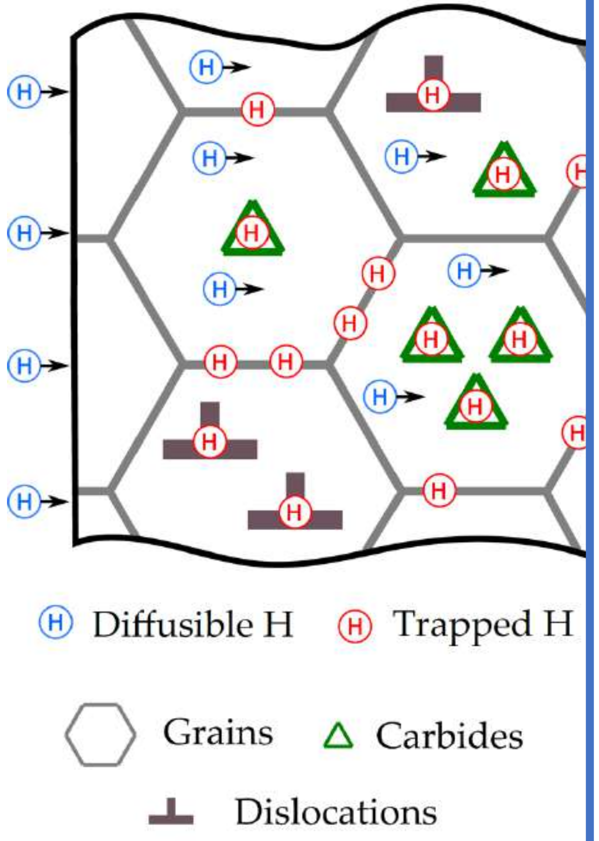




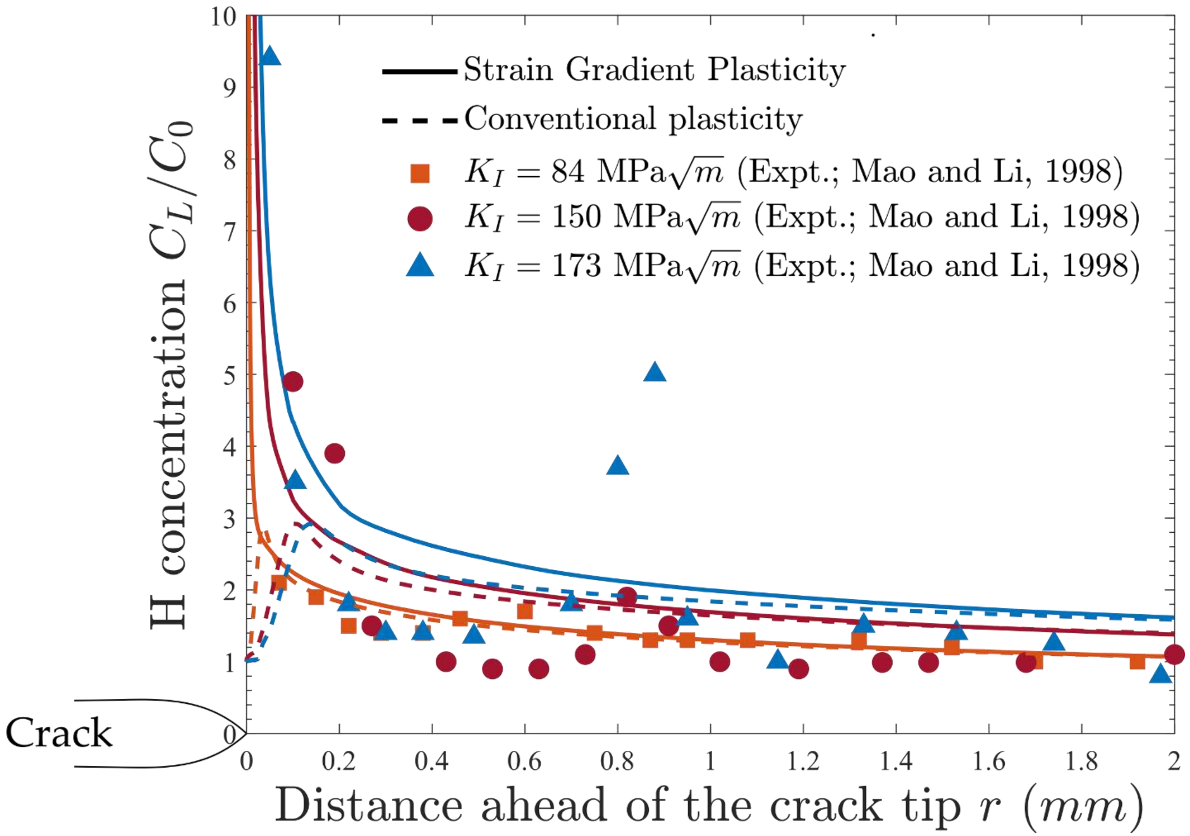
Martínez-Pañeda et al. *Int. J. Hydrogen Energy* (2016)

Stage II: H diffusion and trapping

Stage II: H transport



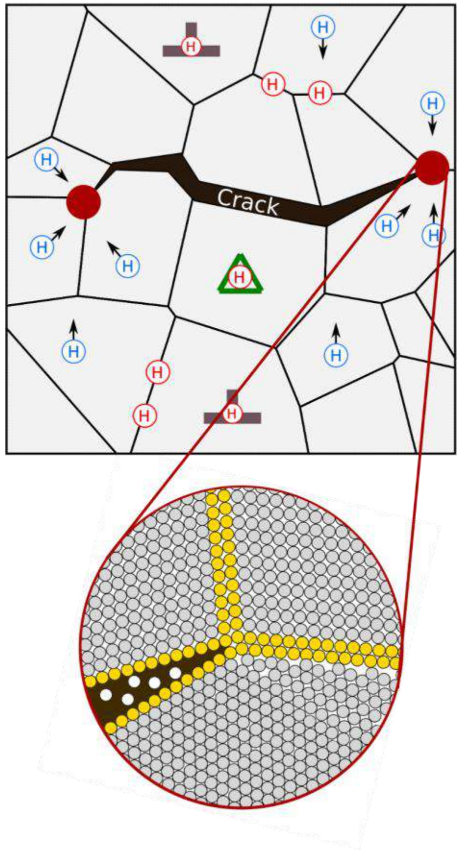
The dual role of GNDs: enhancing trapping and elevating σ_H and C_L



Martínez-Pañeda et al. *Int. J. Hydrogen Energy* (2016)

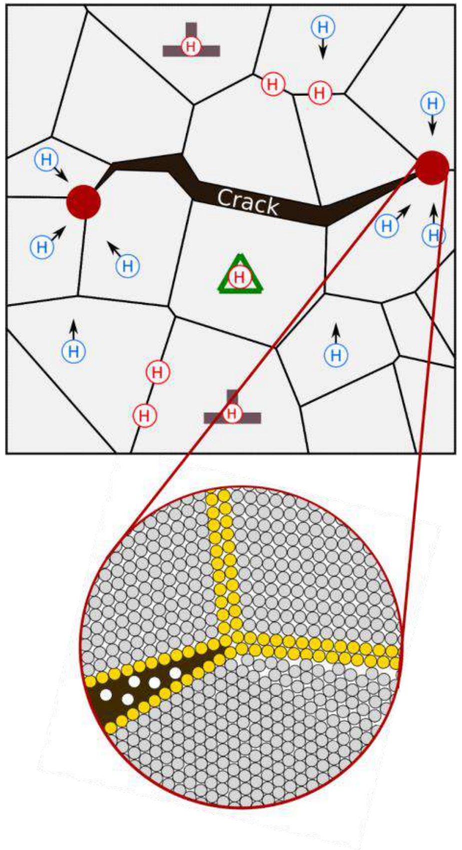
Stage III: Embrittlement

Stage III: Fracture

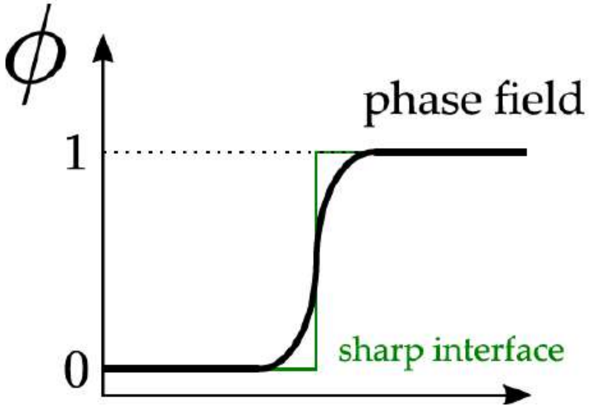


Stage III: Embrittlement

Stage III: Fracture



Phase field modelling



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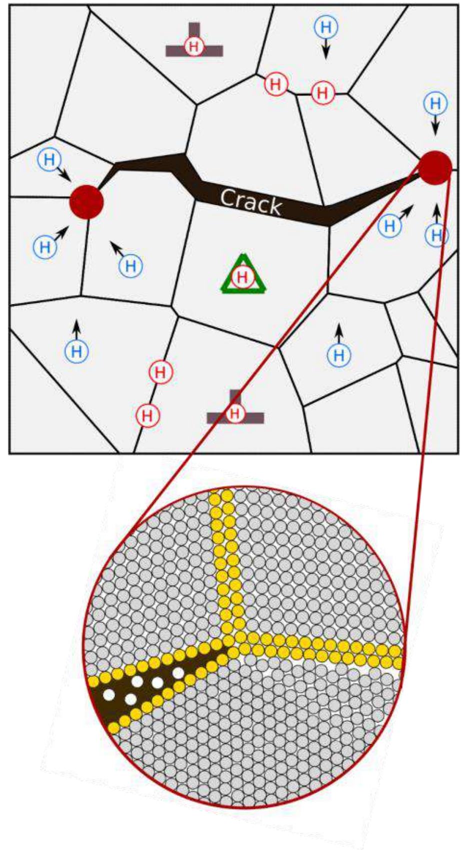
Stage III: Embrittlement

Stage III: Fracture



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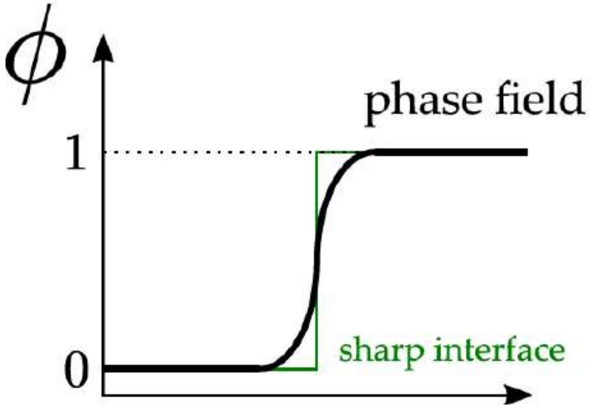
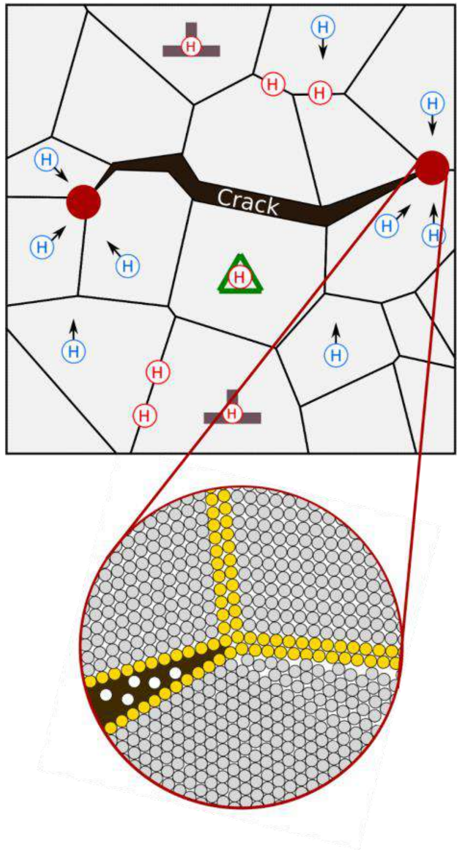


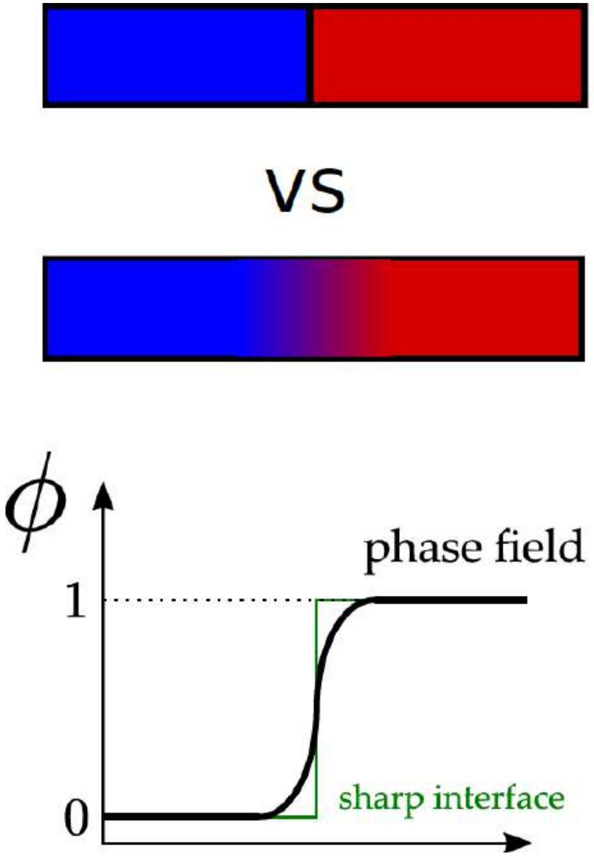
- The interface equation is defined in the entire domain, no special treatment is needed
- Topological changes such as divisions or merging of interfaces can be easily simulated
- The interface equation can be easily combined with equations describing various physical phenomena

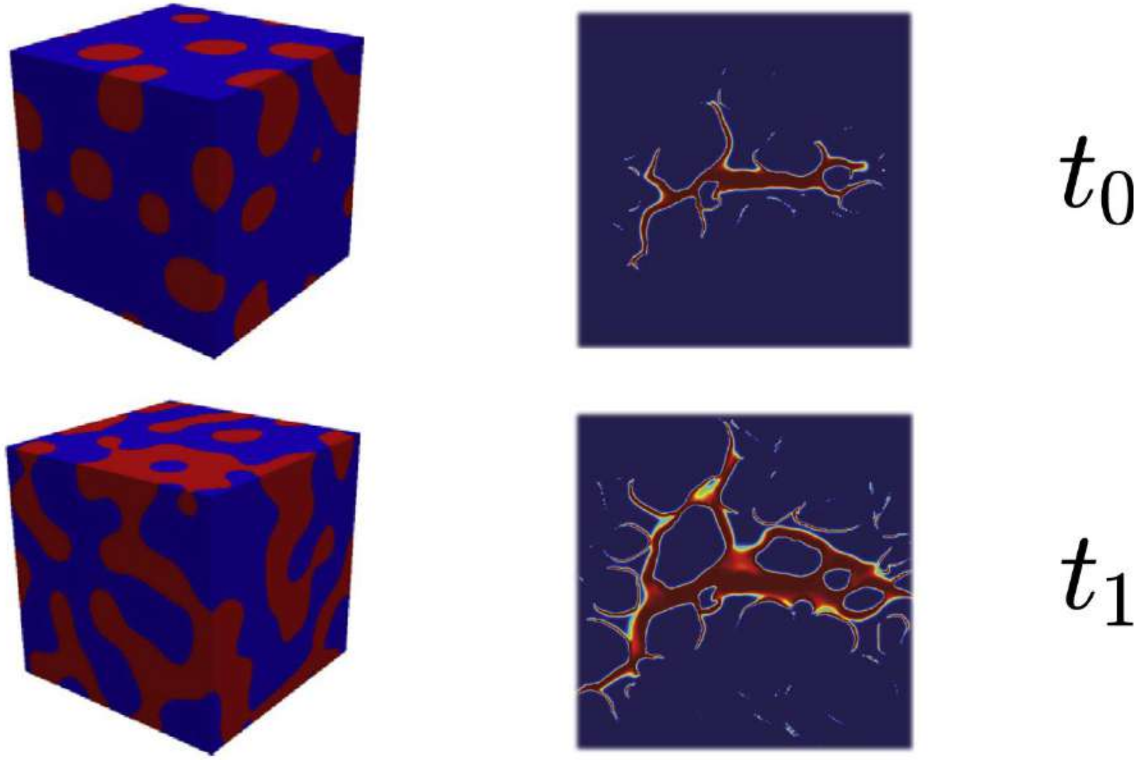
Stage III: Embrittlement

Stage III: Fracture



Phase field modelling



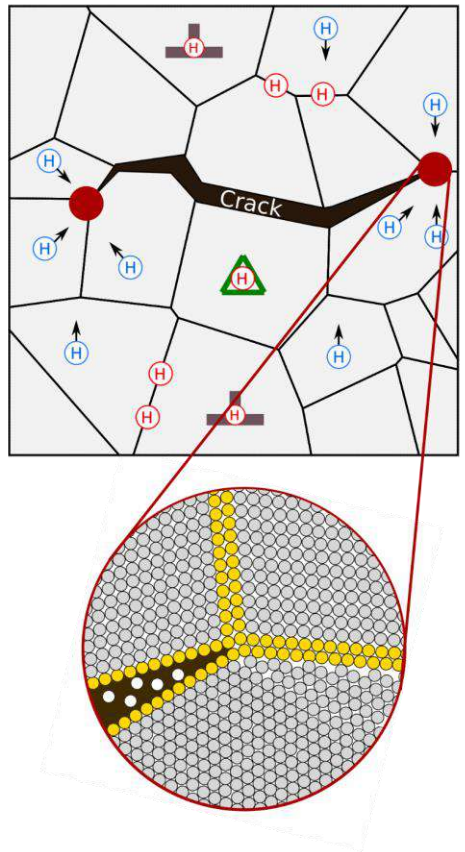


Microstructural evolution

Fracture mechanics

Stage III: Embrittlement

Stage III: Fracture



Phase field fracture

- Griffith's energy balance (Griffith, 1920)

$$\frac{\mathrm{d}\Pi}{\mathrm{d}A} = \frac{\mathrm{d}\Psi\left(\boldsymbol{\varepsilon}\right)}{\mathrm{d}A} + G_c = 0$$

A - crack area

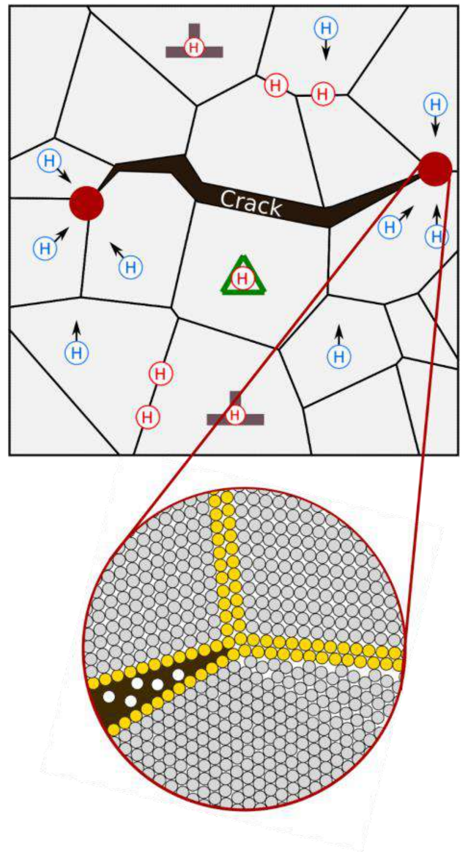
Π - total energy

$\Psi = \int \psi \, \mathrm{d}V$ - strain energy

G_c - critical energy release rate

Stage III: Embrittlement

Stage III: Fracture



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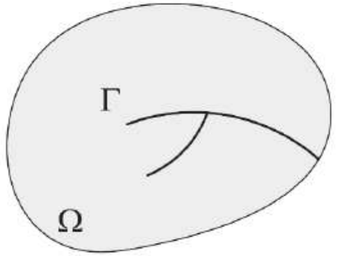
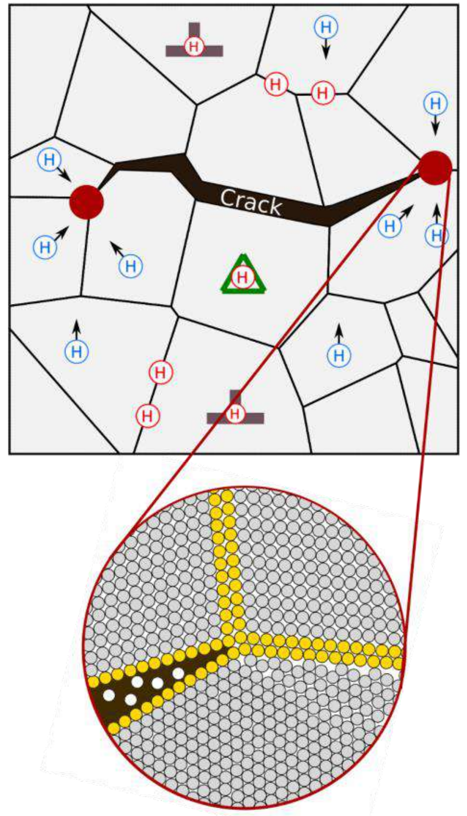
- Variational approach to fracture (Francfort and Marigo, 1998)

$$\Pi = \int_\Omega \psi(\boldsymbol{\varepsilon}) \, \mathrm{d}V + \int_\Gamma G_c \, \mathrm{d}\Gamma$$



Stage III: Embrittlement

Stage III: Fracture



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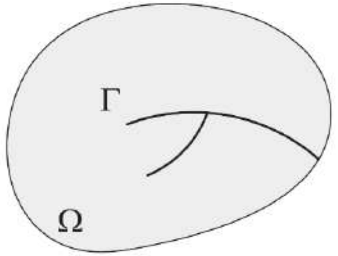
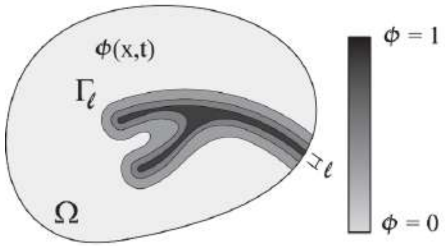


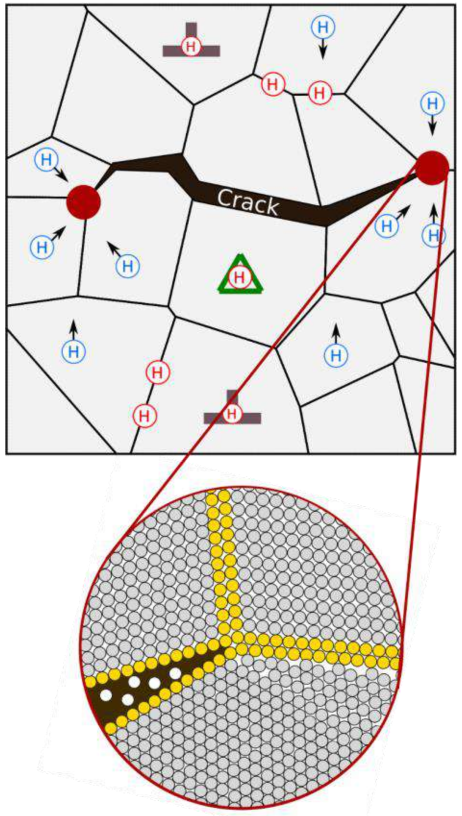
- Phase field fracture (Bourdin et al., 2008; Miehe et al., 2010)

$$\Pi_\ell = \int_\Omega (1-\phi)^2 \psi_0(\boldsymbol{\varepsilon}) \, \mathrm{d}V + \int_\Omega G_c \left(\frac{\phi^2}{2\ell} + \frac{\ell}{2} |\nabla \phi|^2 \right) \mathrm{d}V$$



Stage III: Embrittlement

Stage III: Fracture



Phase field fracture

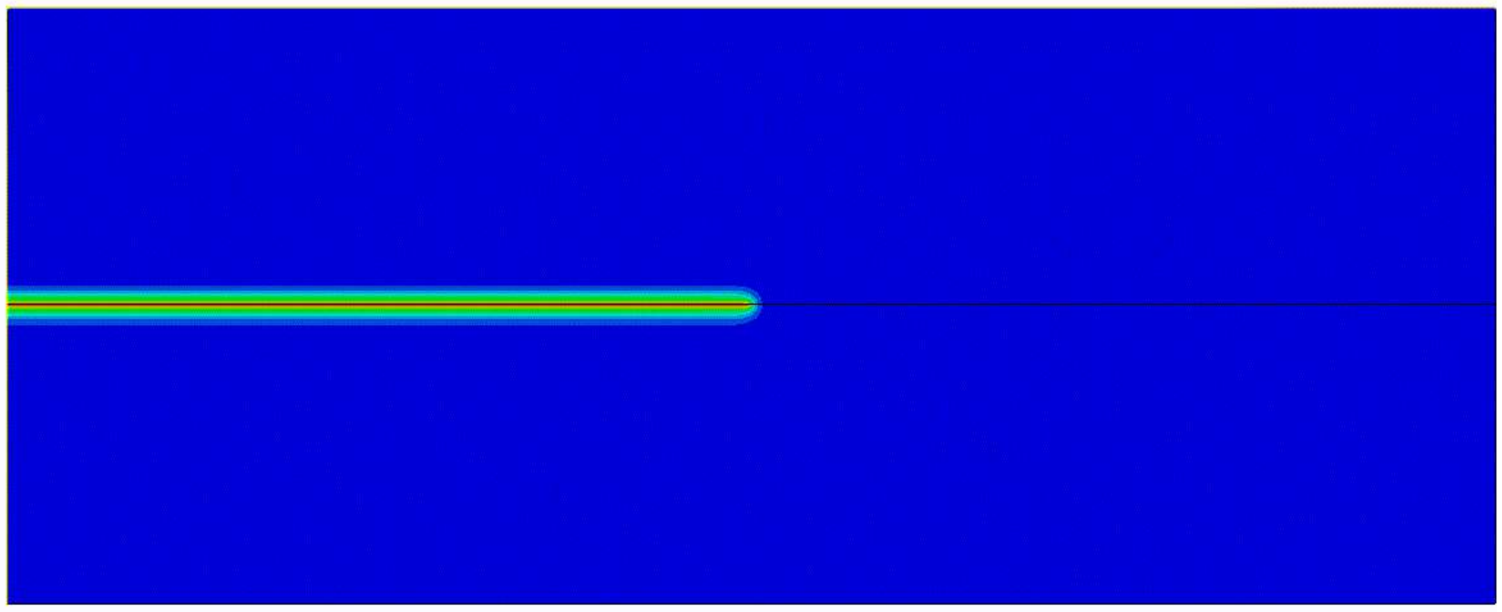
Balance equations:

$$\nabla \cdot \left[(1-\phi)^2 \boldsymbol{\sigma} \right] = \mathbf{0} \quad \text{in} \quad \Omega$$

$$G_c \left(\frac{\phi}{\ell} - \ell \nabla^2 \phi \right) - 2(1-\phi)\, \psi_0(\boldsymbol{\varepsilon}) = 0 \quad \text{in} \quad \Omega$$

red – cracked material

blue – intact material

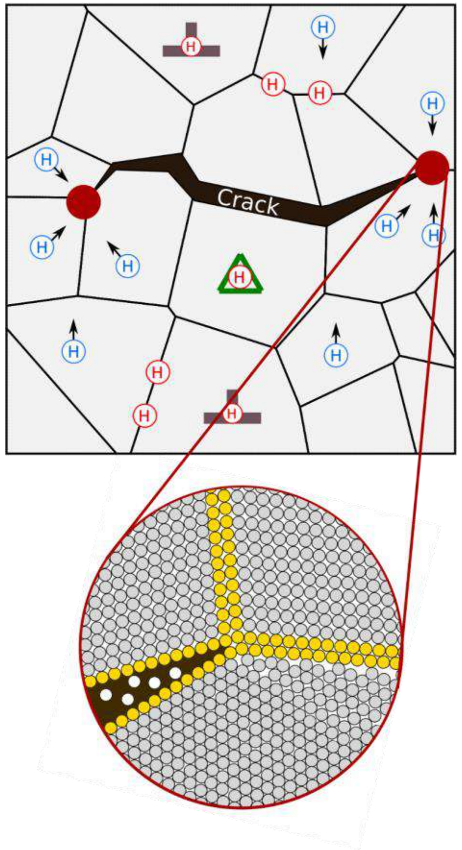


Kristensen, Niordson, Martínez-Pañeda. *Theor. Appl. Fract. Mech.* (2020)

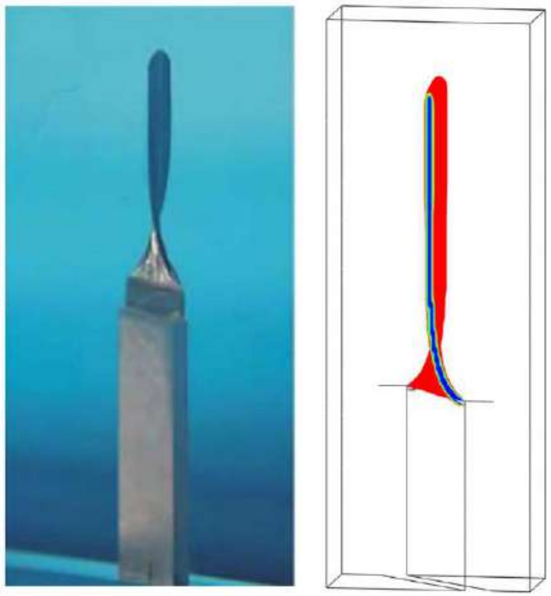
Imperial College London

Stage III: Embrittlement

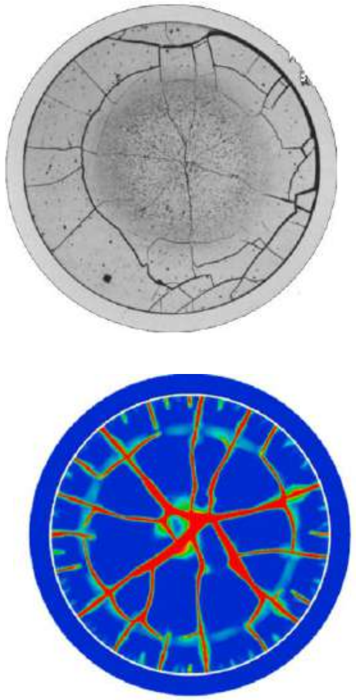
Stage III: Fracture



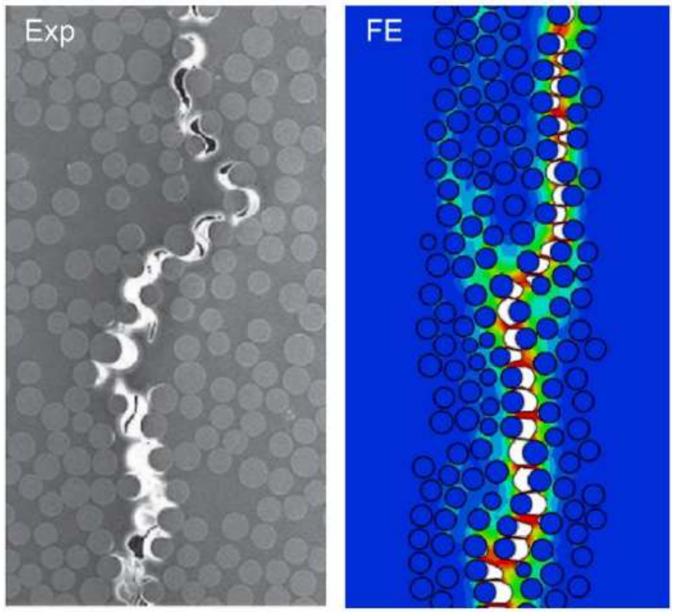
Phase field fracture



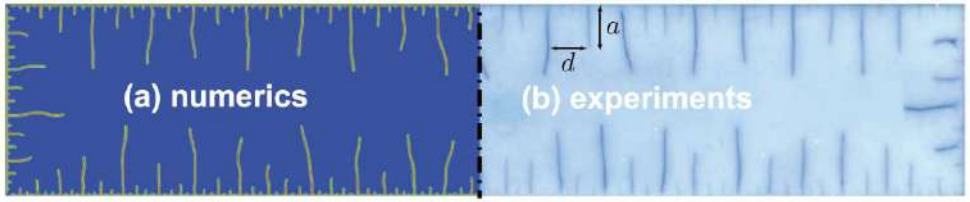
Wu et al., *CMAME* (2021)



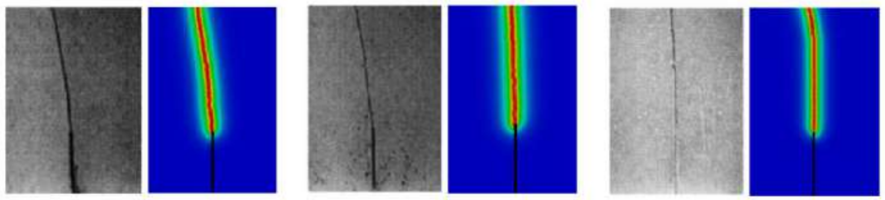
Li & Shirvan, *Ceram. Int.* (2021)



Tan & Martínez-Pañeda, *Compos. Sci. Technol.* (2021)



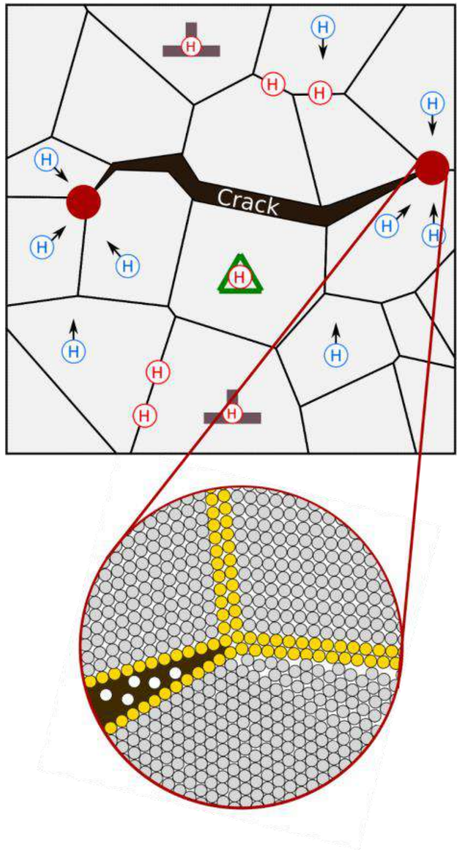
Bourdin et al., *Phys. Rev. Lett.* (2014)



Hirshikesh, Natarajan, Martínez-Pañeda. *Composites, Part B* (2019)

Stage III: Embrittlement

Stage III: Fracture



Phase field modelling of H embrittlement

Deformation of the solid:

$$\nabla \cdot \left[(1-\phi)^2 \boldsymbol{\sigma} \right] = \mathbf{0}$$

Hydrogen transport:

$$\frac{\partial C}{\partial t} - D \nabla^2 C + \nabla \cdot \left(\frac{DC}{RT} \bar{V}_H \nabla \sigma_H \right) = 0$$

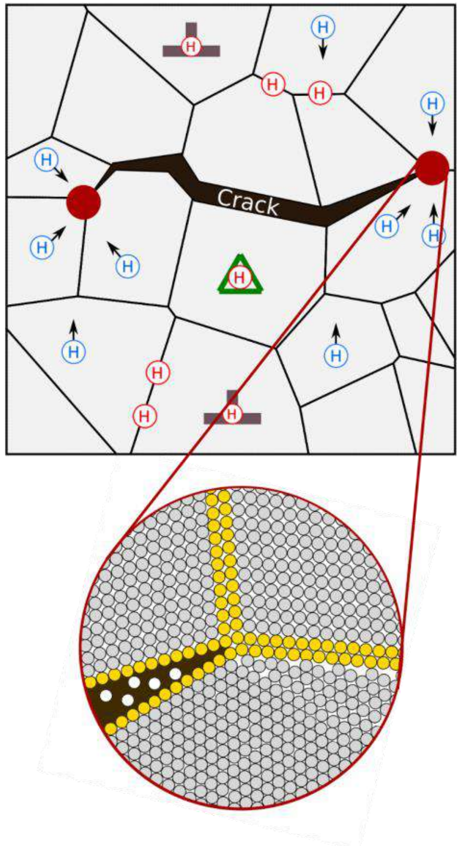
Damage:

$$G_c \left(\frac{\phi}{\ell} - \ell \nabla^2 \phi \right) - 2(1-\phi) \psi(\boldsymbol{\varepsilon}) = 0$$

Martínez-Pañeda et al. CMAME (2018)

Stage III: Embrittlement

Stage III: Fracture



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Damage:

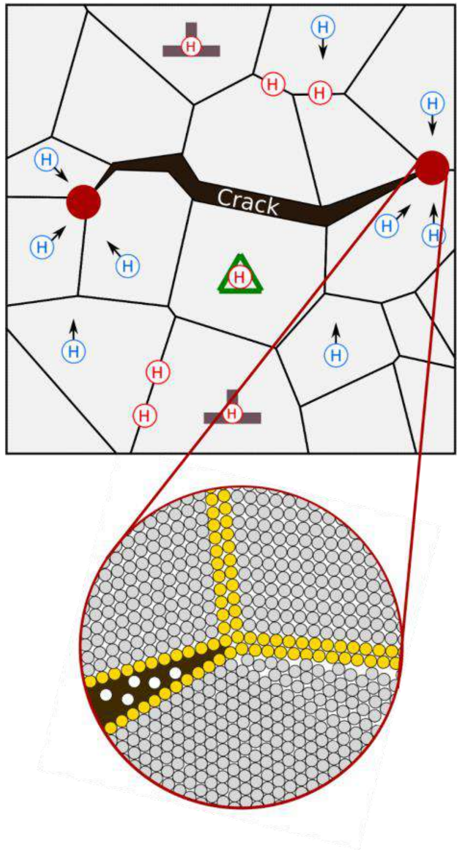
$$G_c(C) \left(\frac{\phi}{\ell} - \ell \nabla^2 \phi \right) - 2(1-\phi)\, \psi(\boldsymbol{\varepsilon}) = 0$$

Martínez-Pañeda et al. CMAME (2018)

Imperial College London

Stage III: Embrittlement

Stage III: Fracture



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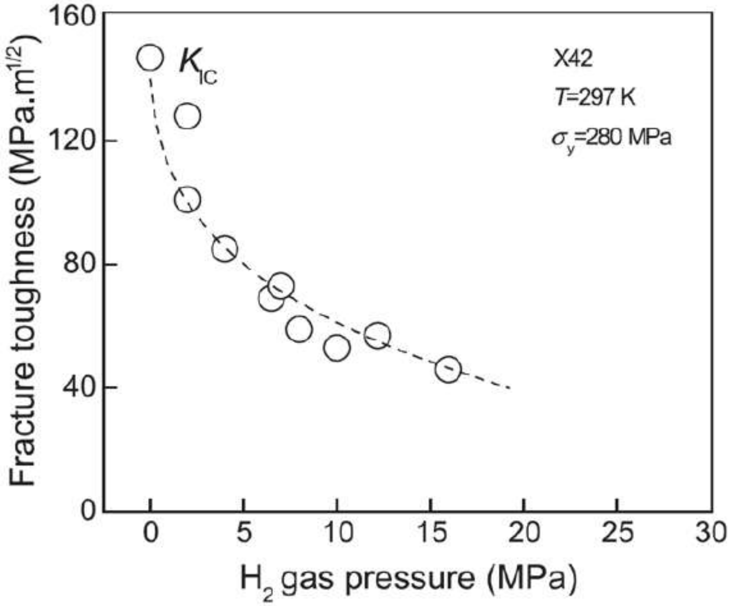


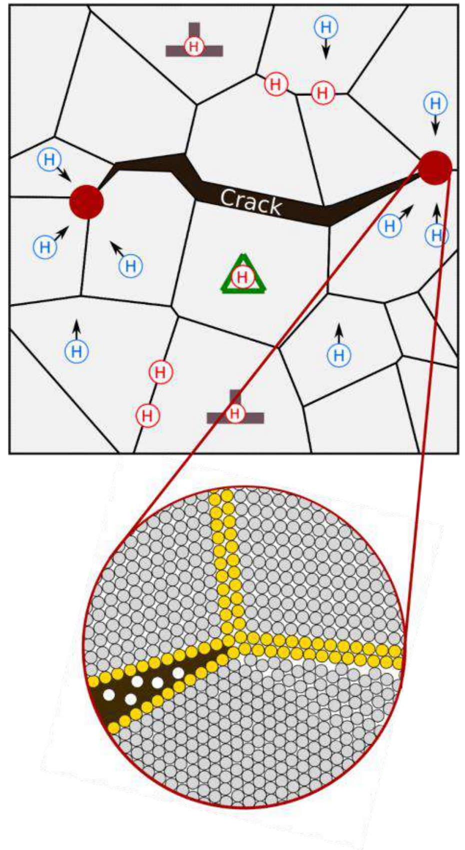
Adapted from Gutierrez-Solana F, Elices M. American Society for Metals; 1982

Martínez-Pañeda et al. CMAME (2018)

Imperial College London

Stage III: Embrittlement

Stage III: Fracture



Phase field modelling of H embrittlement

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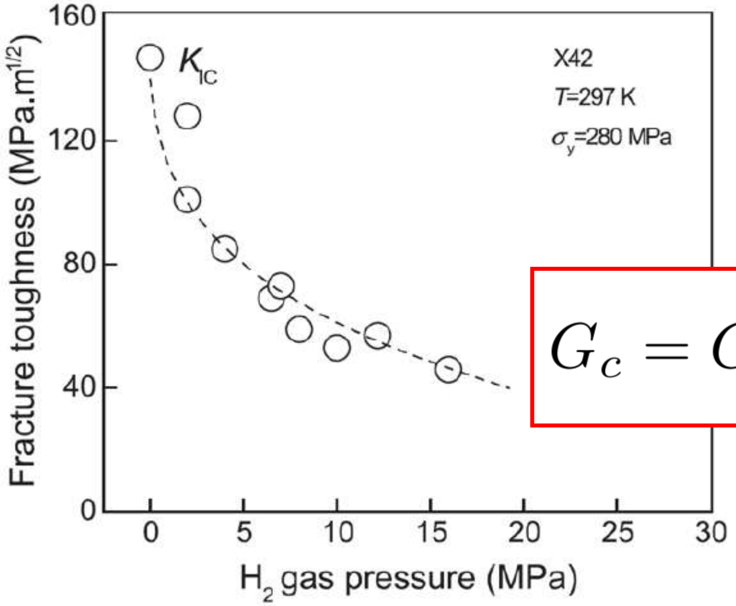


Adapted from Gutierrez-Solana F, Elices M. American Society for Metals; 1982

… and the model can accommodate any mechanistic interpretation:

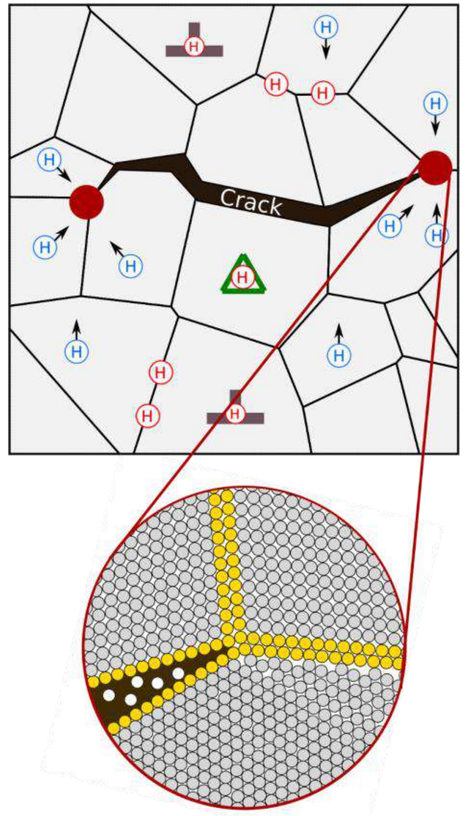
$$G_c = G_c(0)\cdot f\left(C,\, C_L,\, C_T,\, C_T^{gb},\, C_T^{d},\, \rho,\, \varepsilon^p,\, \ldots\right)$$

Martínez-Pañeda et al. CMAME (2018)

Imperial College London

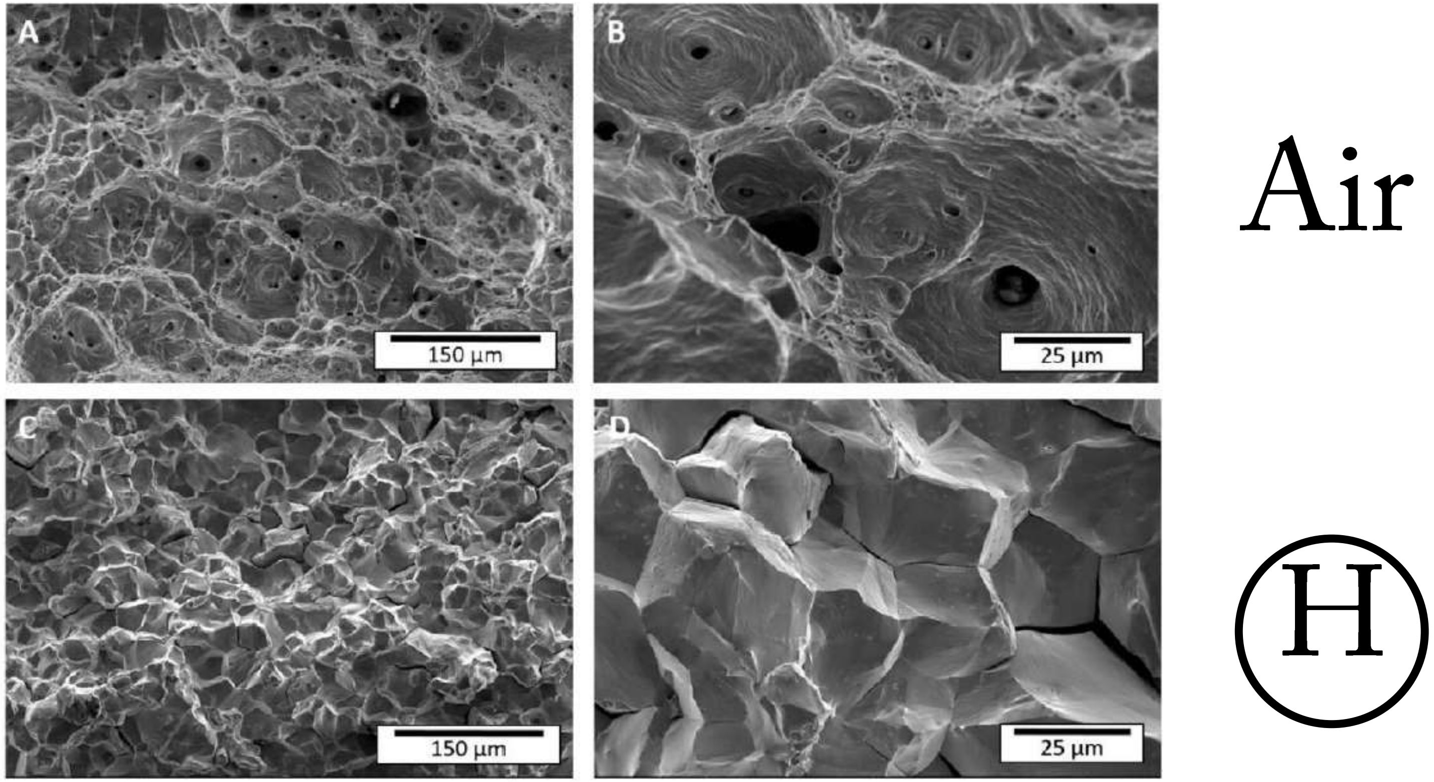
Stage III: Embrittlement

Stage III: Fracture



Phase field modelling of H embrittlement

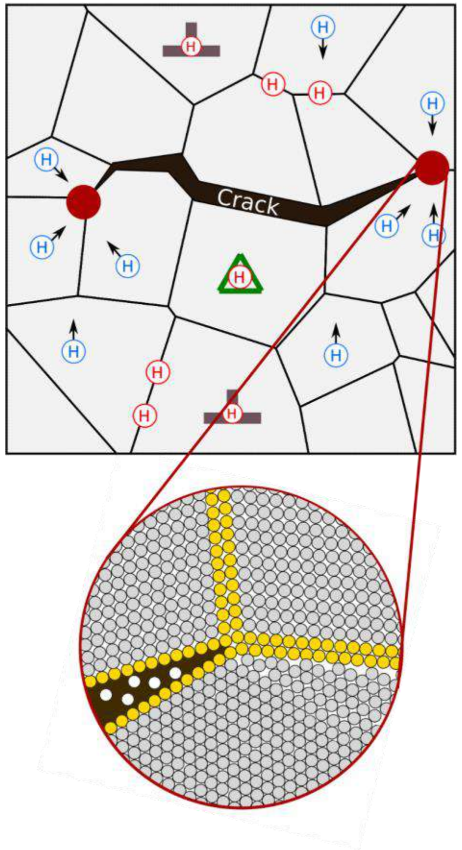
- How does hydrogen make metals brittle?



Harris et al. (Acta Mat., 2018)

Stage III: Embrittlement

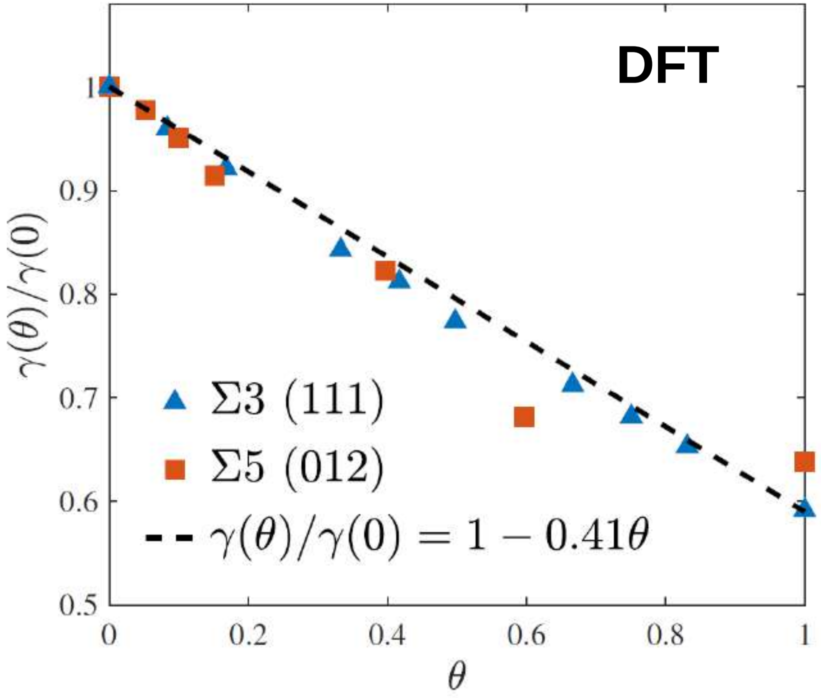
Stage III: Fracture



Phase field modelling of H embrittlement

- Hydrogen atoms strongly reduce the bonding strength between metal atoms.

Fracture energy



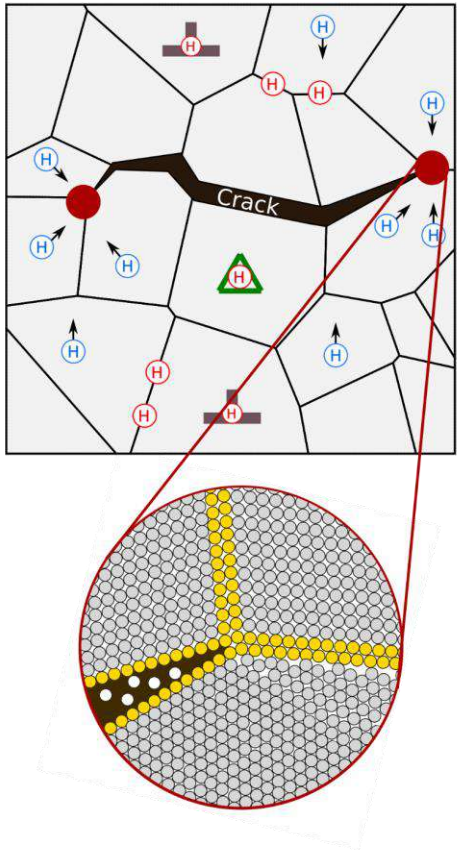
H occupancy

Alvaro et al. IJHE (2016)

Imperial College London

Stage III: Embrittlement

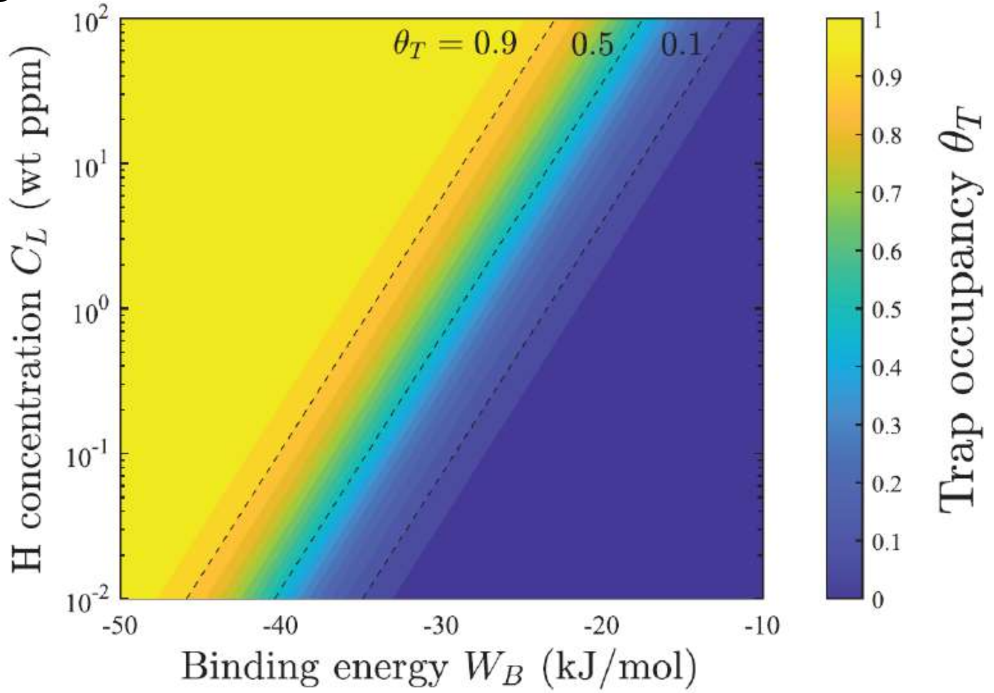
Stage III: Fracture



Phase field modelling of H embrittlement

- Hydrogen atoms strongly reduce the bonding strength between metal atoms.
- Strong traps ($|W_B| > 40$, like grain boundaries or carbides) are filled soon

Trap occupancy as a function of C_L and W_B (Oriani)

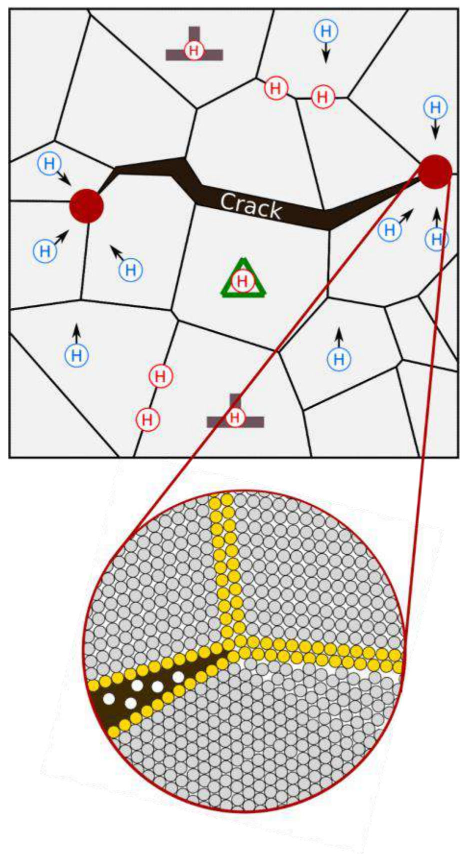


Fernández-Sousa, Betegón, Martínez-Pañeda. *Acta Mat.* (2020)

Imperial College London

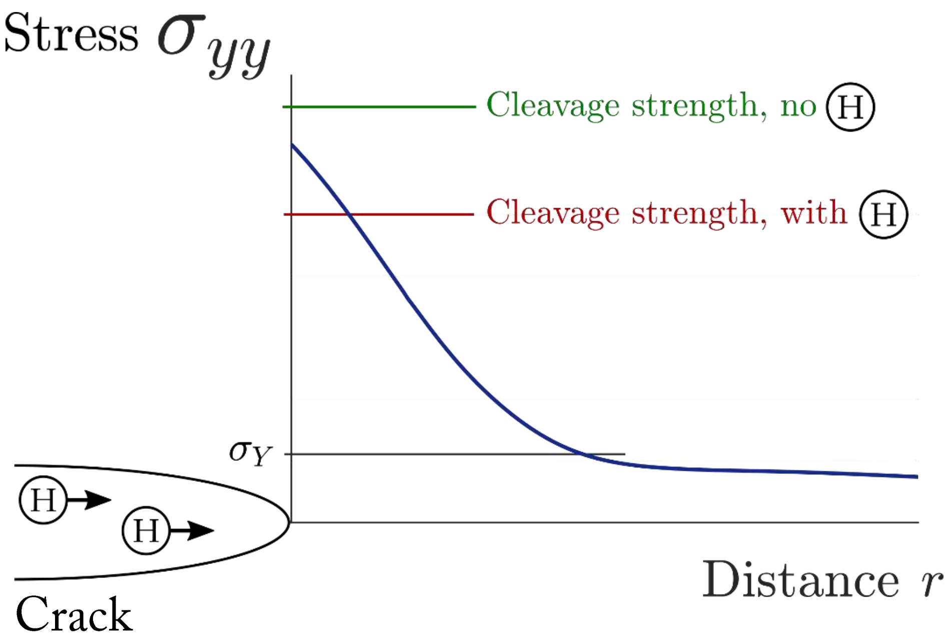
Stage III: Embrittlement

Stage III: Fracture



Phase field modelling of H embrittlement

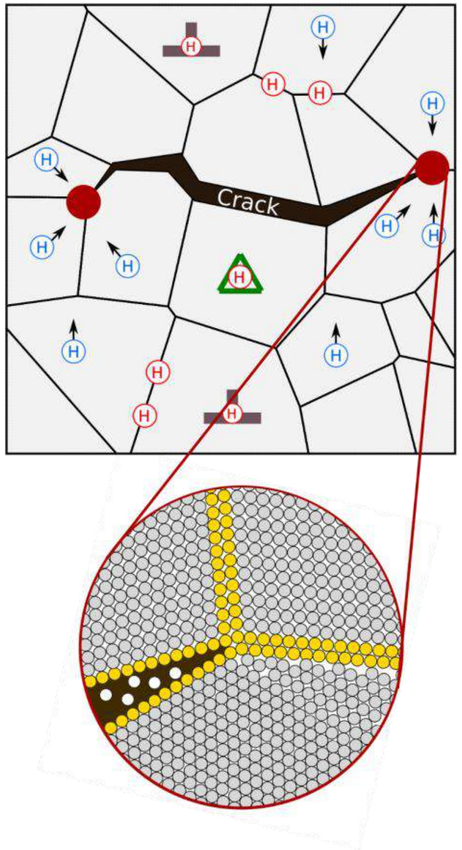
- Hydrogen atoms strongly reduce the bonding strength between metal atoms.
- Strong traps ($|W_B| > 40$, like grain boundaries or carbides) are filled soon
- Gradient-enhanced stresses that are close to the theoretical lattice (or GB) strength ($\hat{\sigma} > 10\sigma_Y$)



Martínez-Pañeda et al., *JMPS (2019)*

Stage III: Embrittlement

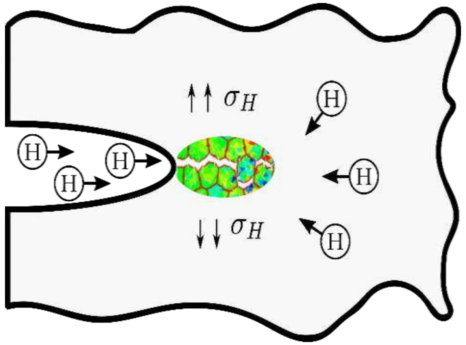
Stage III: Fracture



Phase field modelling of H embrittlement

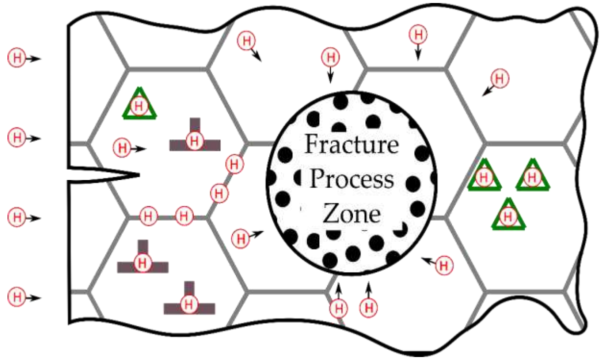
$$G_c(C)\left(\frac{\phi}{\ell}-\ell\nabla^2\phi\right)-2(1-\phi)\,\psi_0(\boldsymbol{\varepsilon})=0$$

Stress-assisted diffusion



Lattice hydrogen concentration C_L

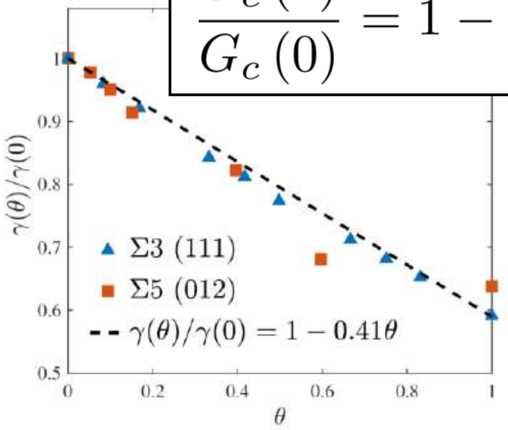
Trapping thermodynamics



Trap occupancy θ

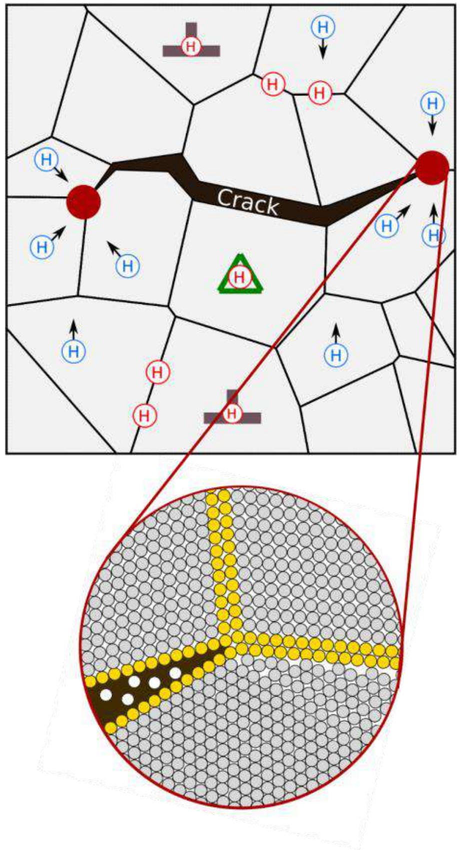
Atomistic calculations

$$\frac{G_c(\theta)}{G_c(0)}=1-\chi\theta$$



Stage III: Embrittlement

Stage III: Fracture



Phase field modelling of H embrittlement

- *Moving* chemical boundary conditions

ϕ - Crack phase field

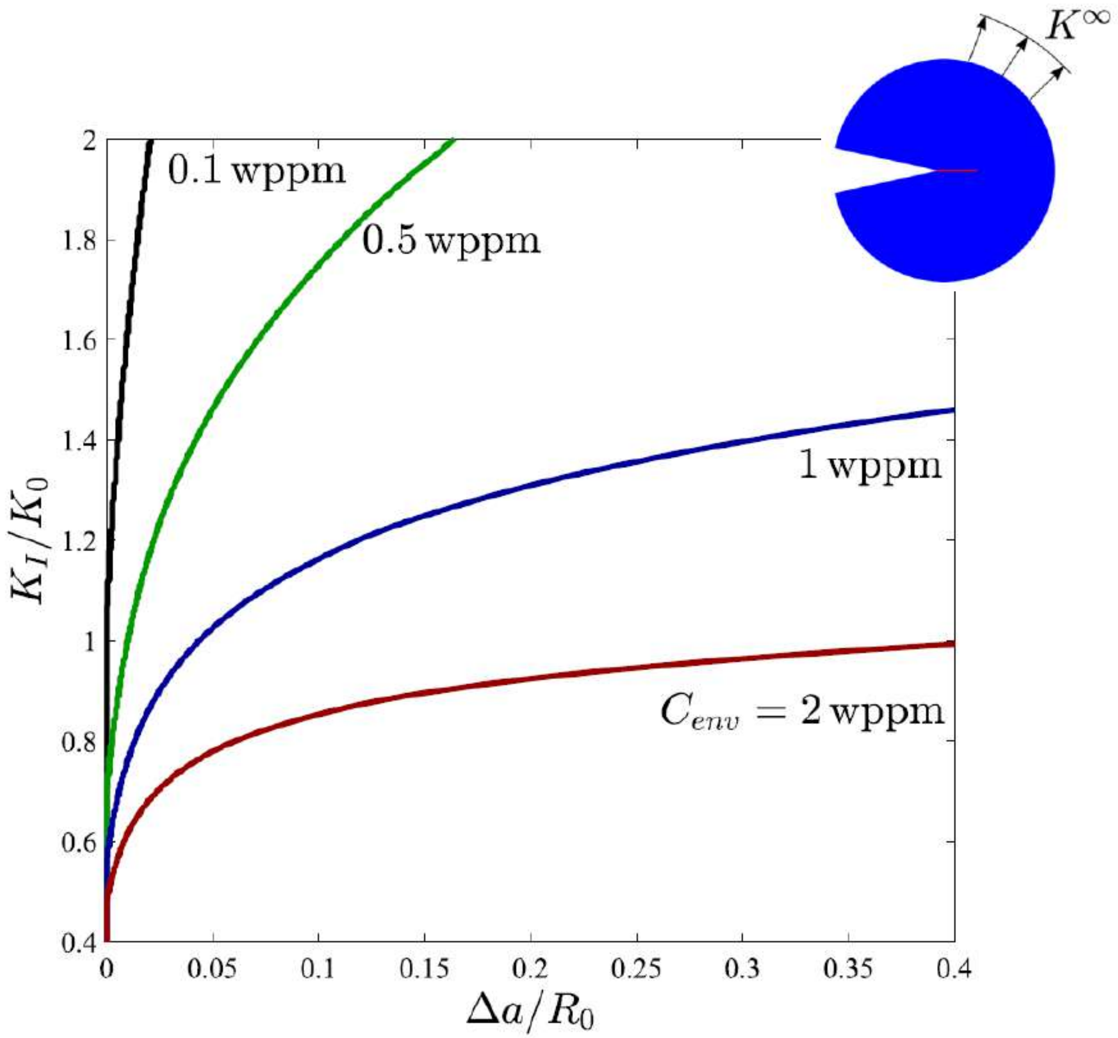
red – cracked material

blue – intact material

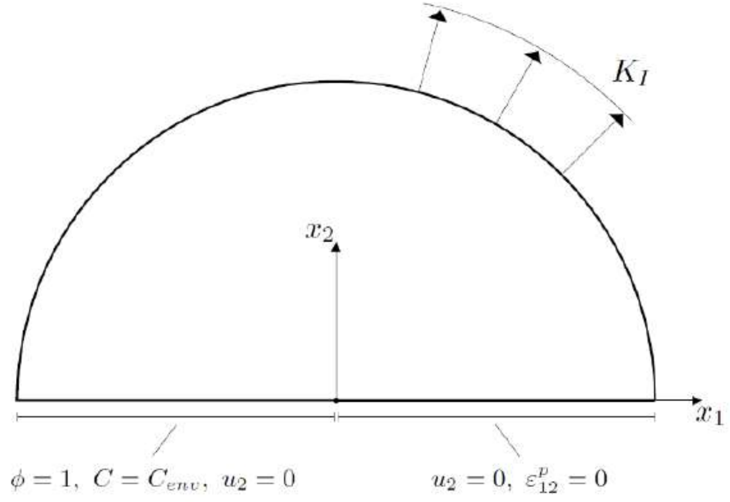
C - H concentration

Kristensen et al., *JMPS* (2020)

Results: R-curves



- Influence of the H content

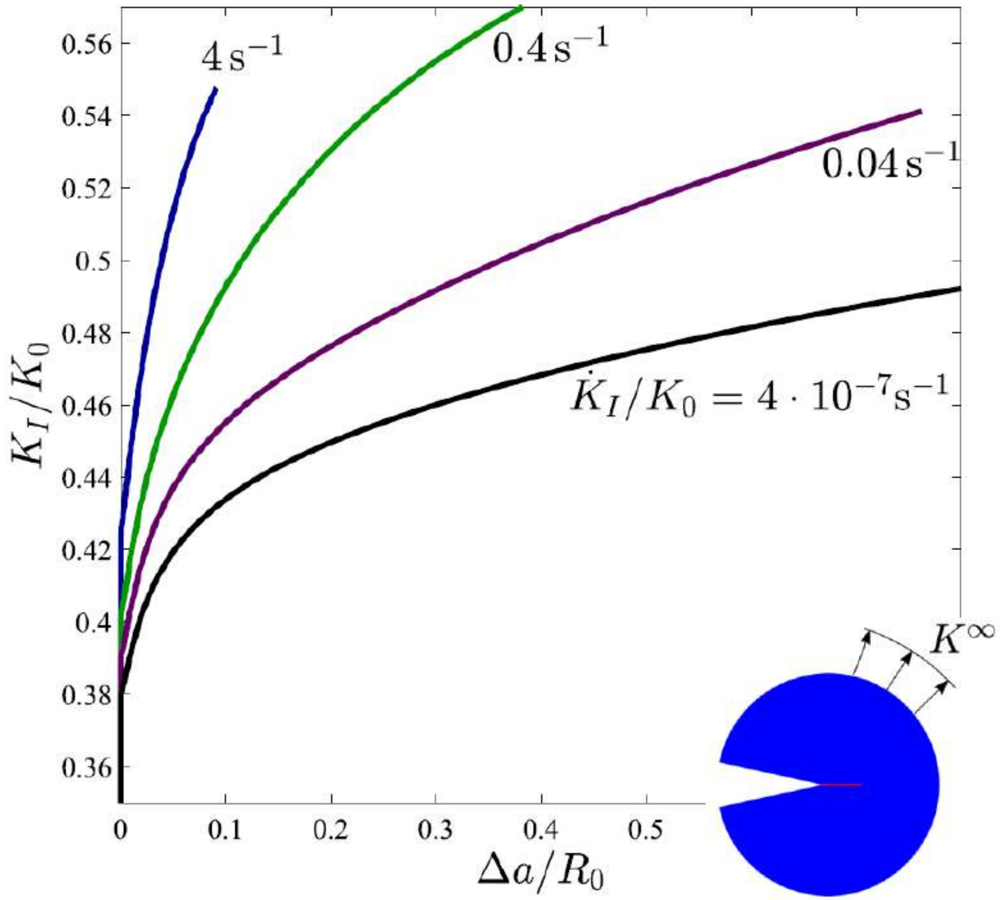


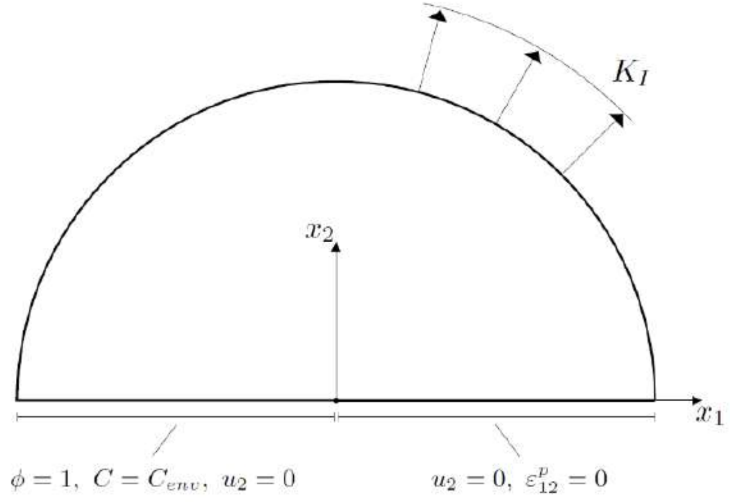
$$K_0 = \sqrt{\frac{EG_c}{1-\nu^2}} \qquad R_0 = \frac{1}{3\pi\left(1-\nu^2\right)}\frac{G_c E}{\sigma_y^2}$$

Kristensen, Niordson, Martínez-Pañeda. *JMPS (2020)*

Results: R-curves

- Influence of the loading rate





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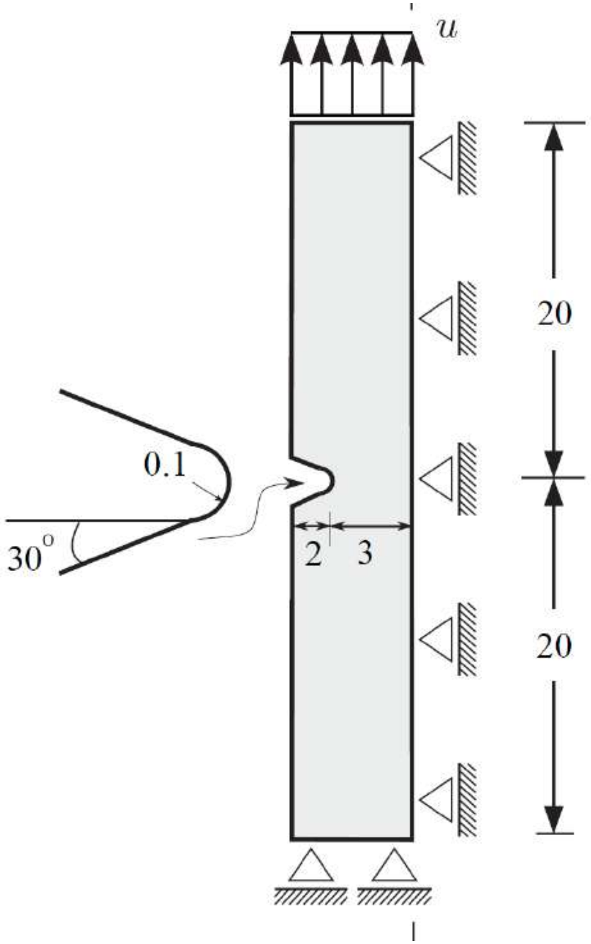
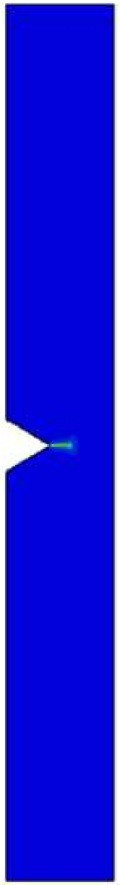
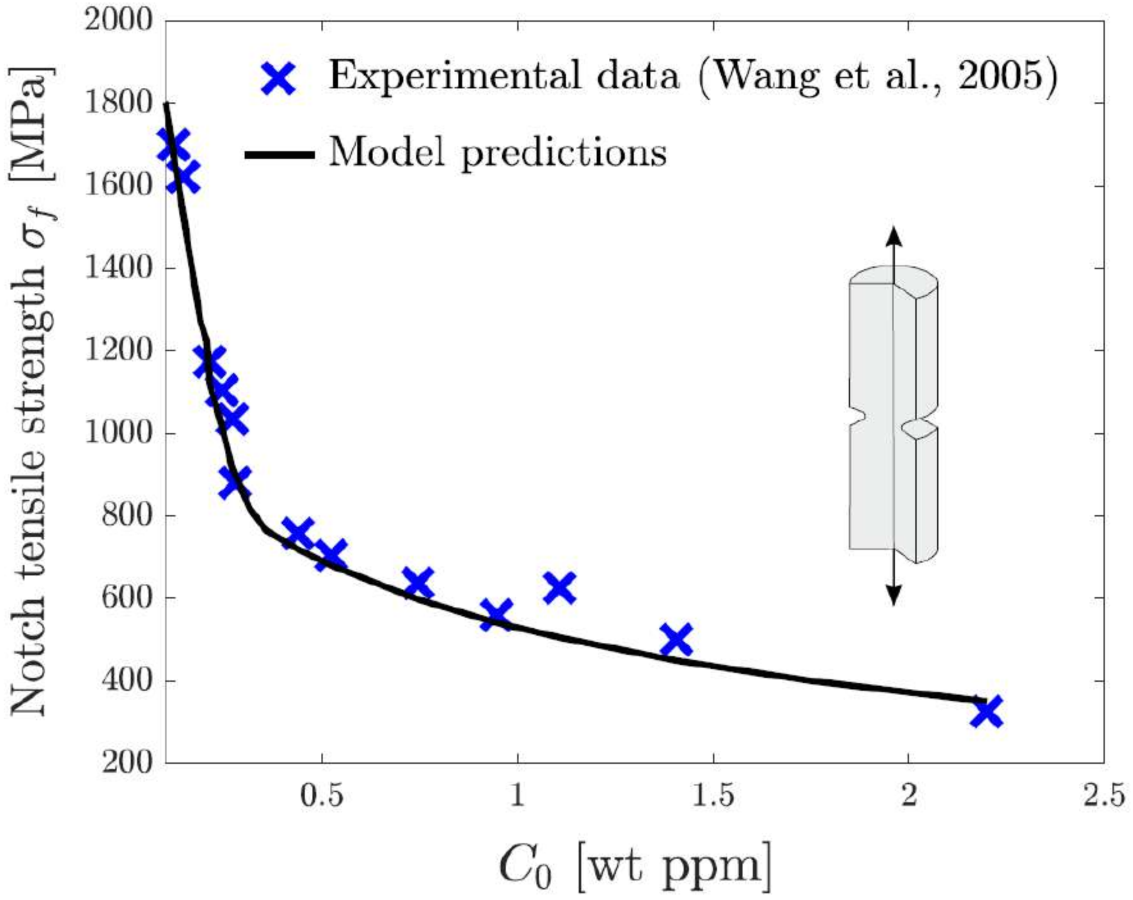
Kristensen, Niordson, Martínez-Pañeda. *JMPS (2020)*

Results: pre-charged steel bars



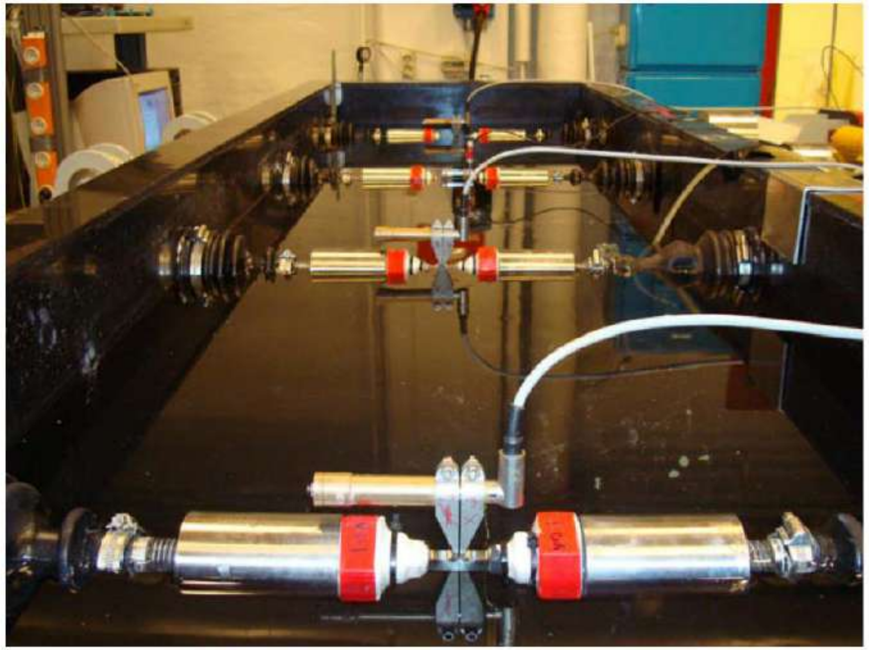




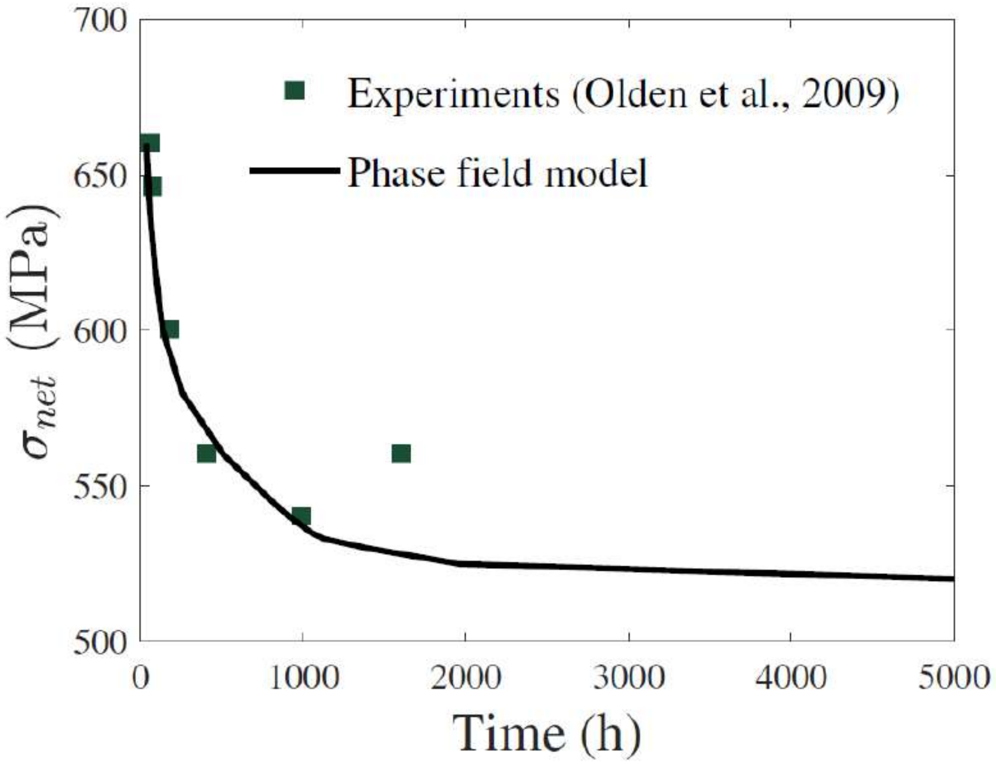
Isfandbod & Martínez-Pañeda. *Int. J. Plasticity (2021)*

Imperial College London

Results: steel samples at constant load



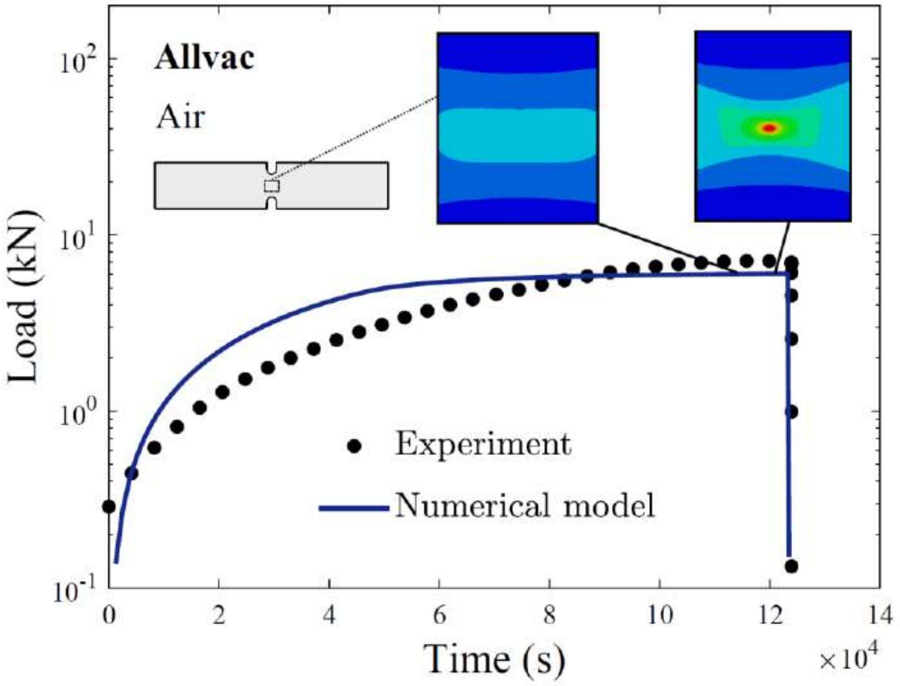
SINTEF

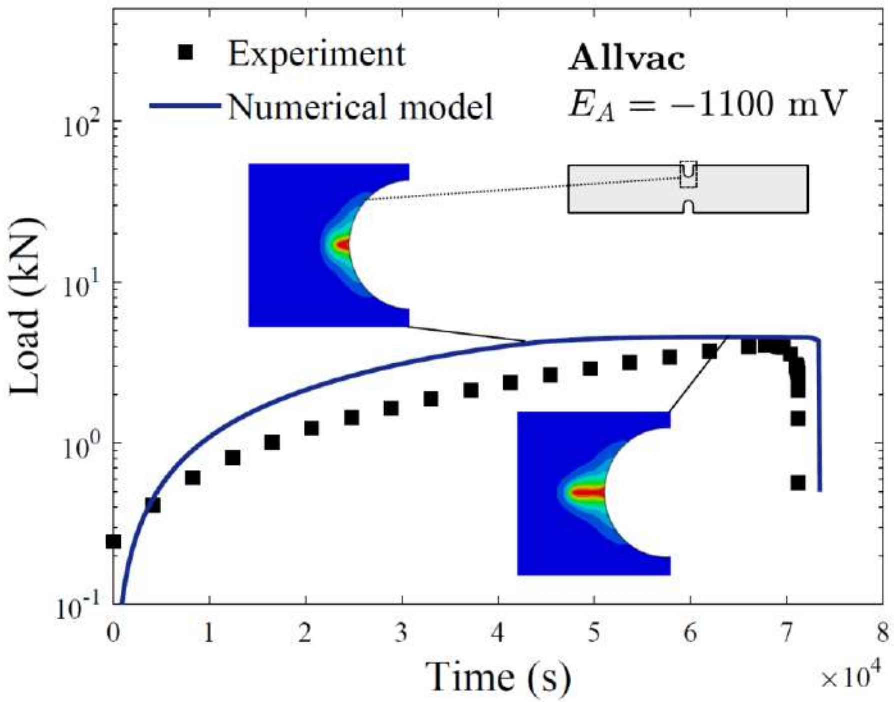


✓ Virtual experiments enable predictions over large time scales

Martínez-Pañeda et al., *CMAME* (2018)

Results: are SSRT experiments suitable?



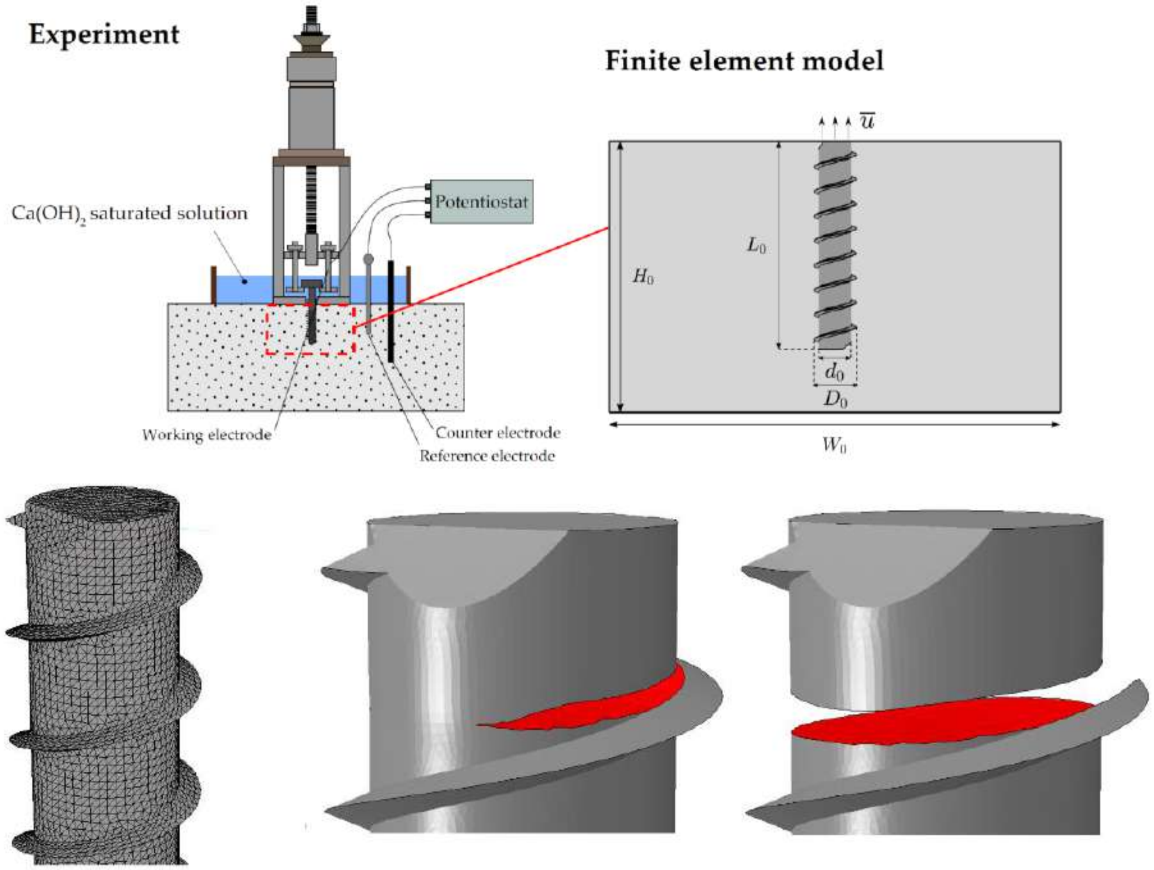


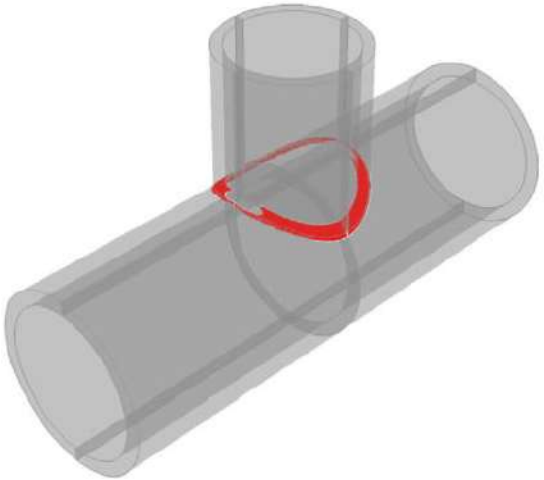
- Early cracking occurs in SSRTs – time to failure is not a valid measure

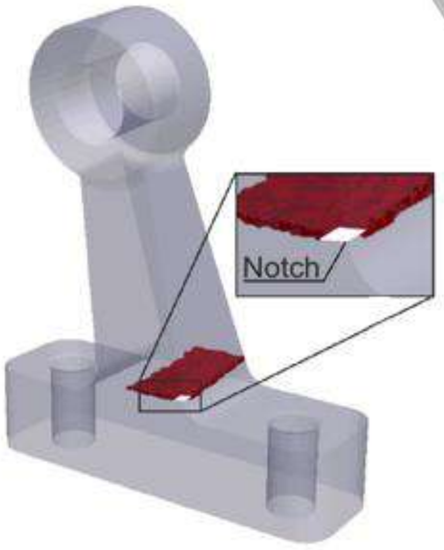
Martínez-Pañeda et al., *Corros. Sci.* (2020)

Results: *Virtual Testing*

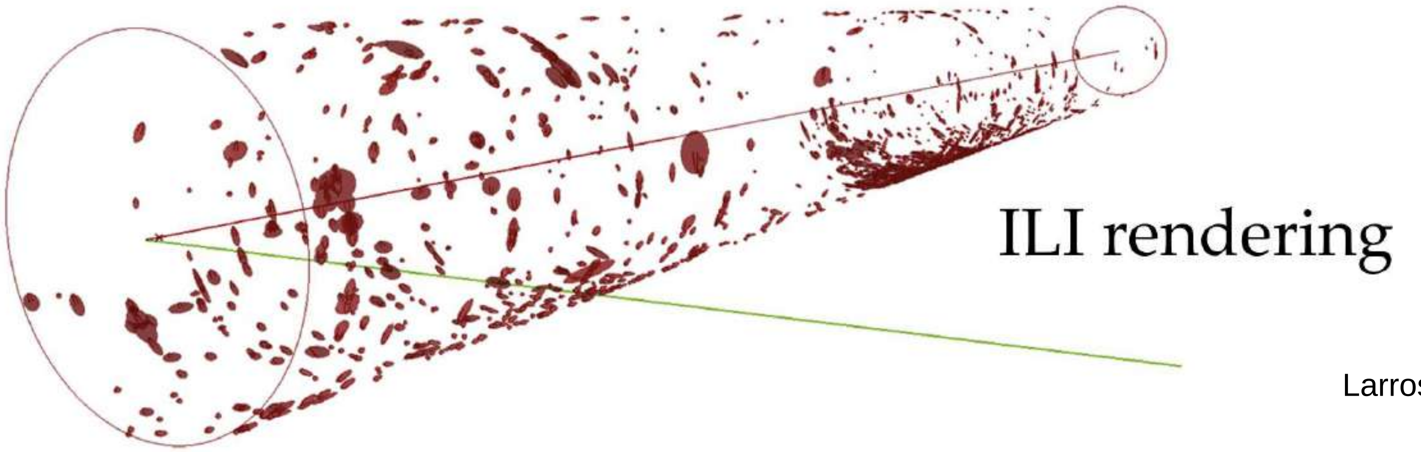
ASTM E488: SCC Strength of Anchors in Concrete



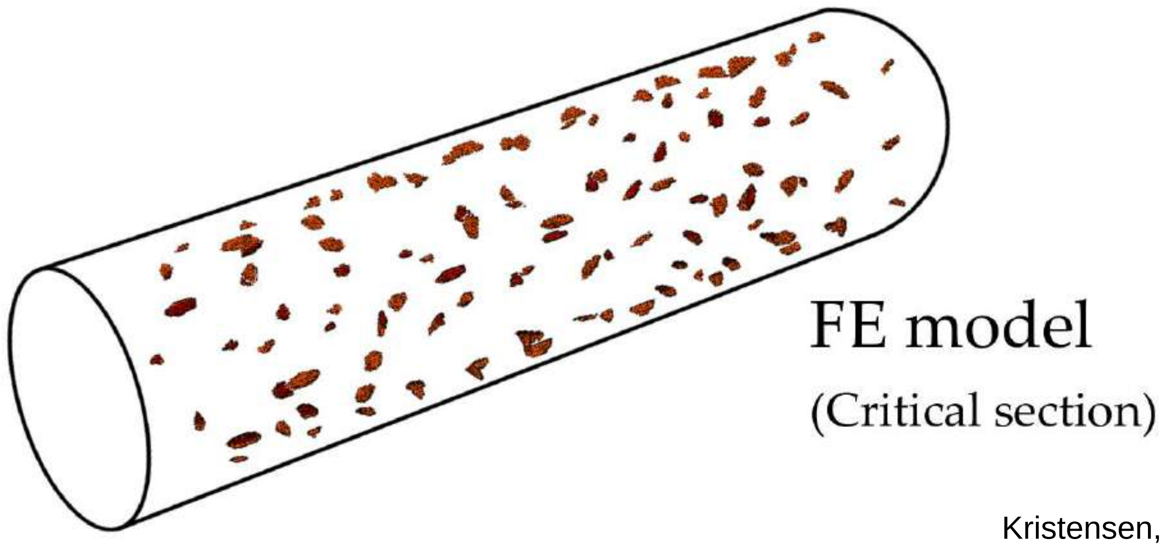




Results: *Virtual Testing*

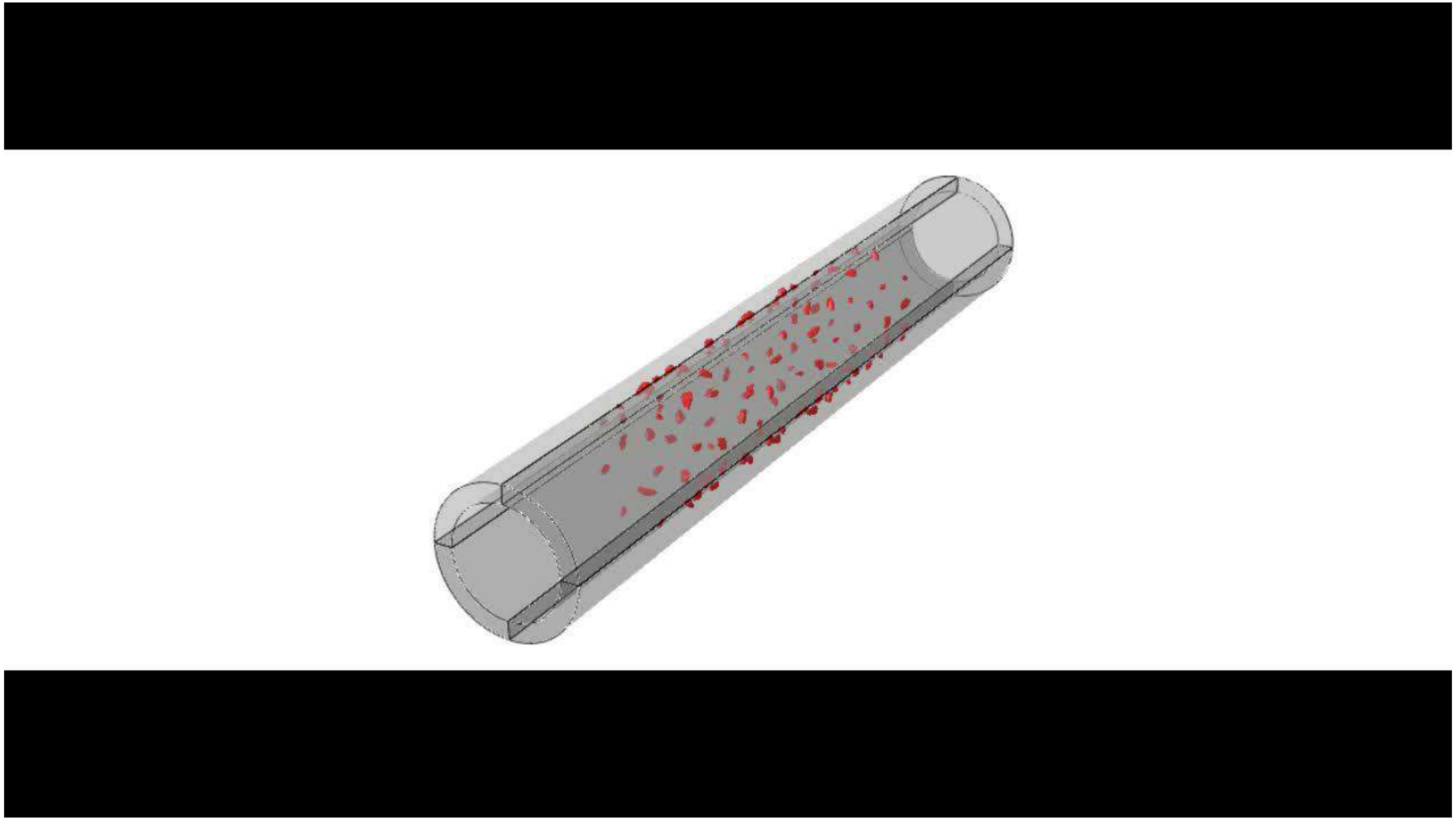


Larrosa et al. *Theor. Appl. Fract. Mech.* (2018)

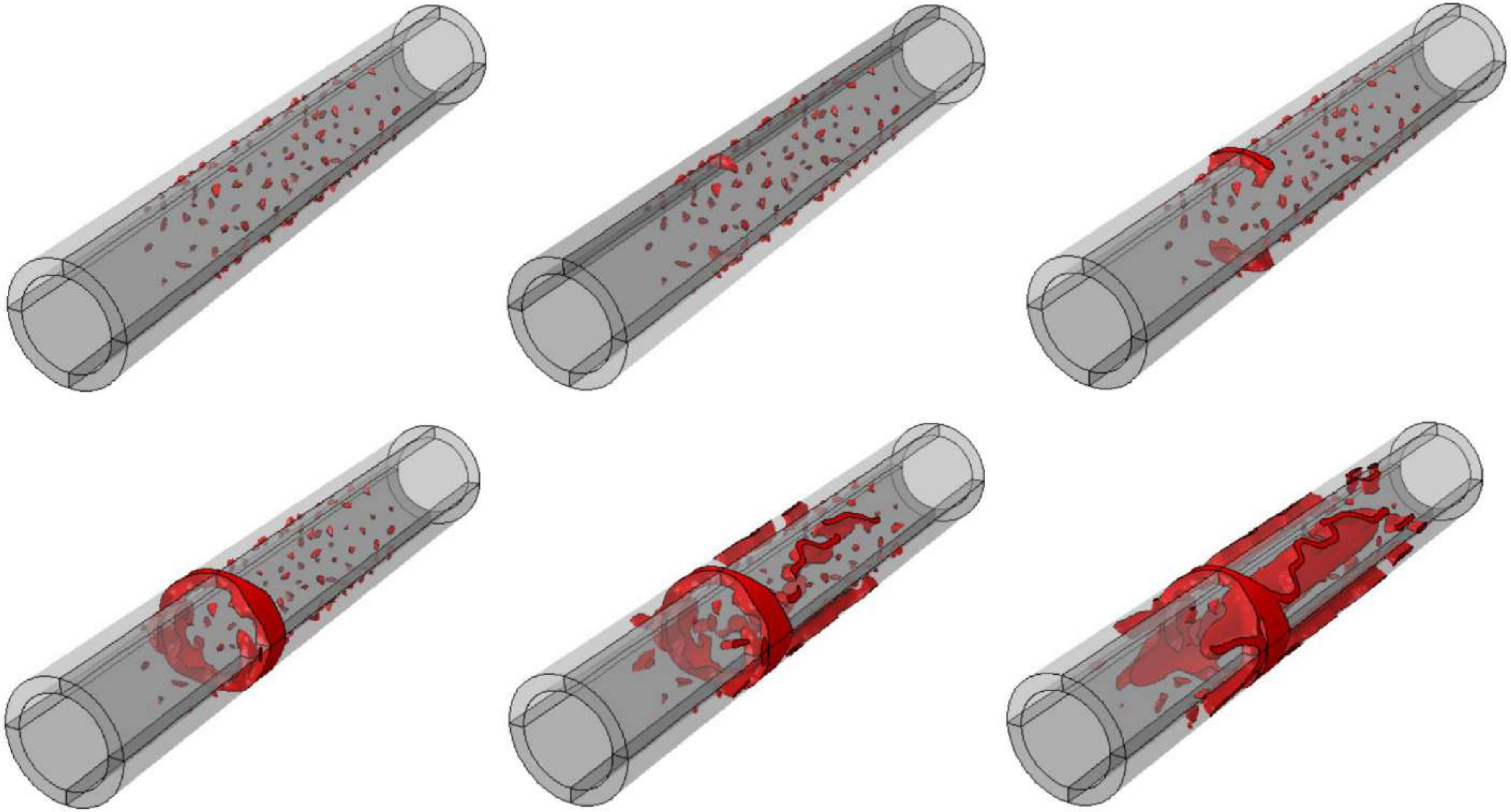


Kristensen, Niordson, Martínez-Pañeda. *Theor. Appl. Fract. Mech.* (2020)

Results: *Virtual Testing*



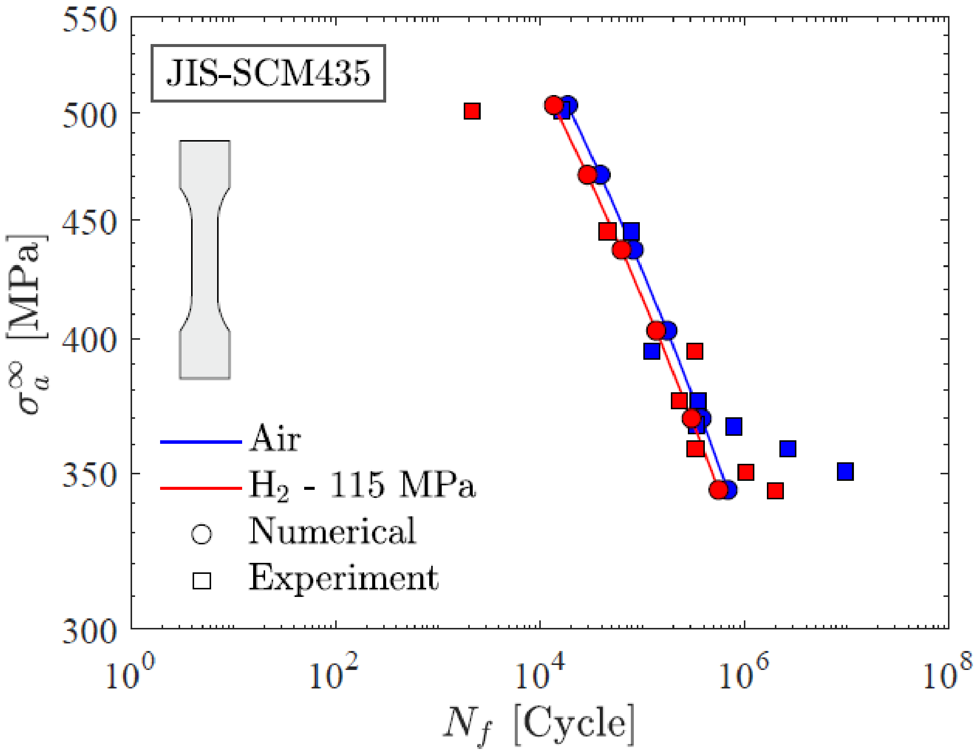
Results: *Virtual Testing*

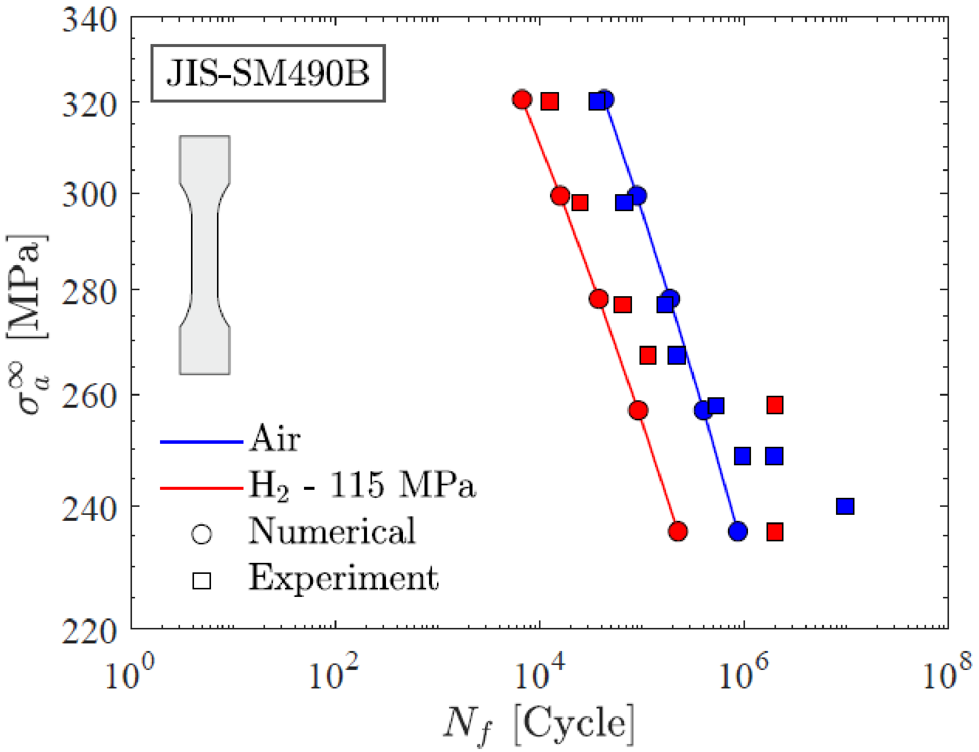


Kristensen, Niordson, Martínez-Pañeda. *Theor. Appl. Fract. Mech.* (2020)

Results – Hydrogen-assisted Fatigue

$$f(\bar{\alpha}(t))G_c(C)\left(\frac{\phi}{\ell}-\ell\nabla^2\phi\right)-2\,(1-\phi)\,\psi\,(\varepsilon)=0 \quad \text{in} \quad \Omega$$

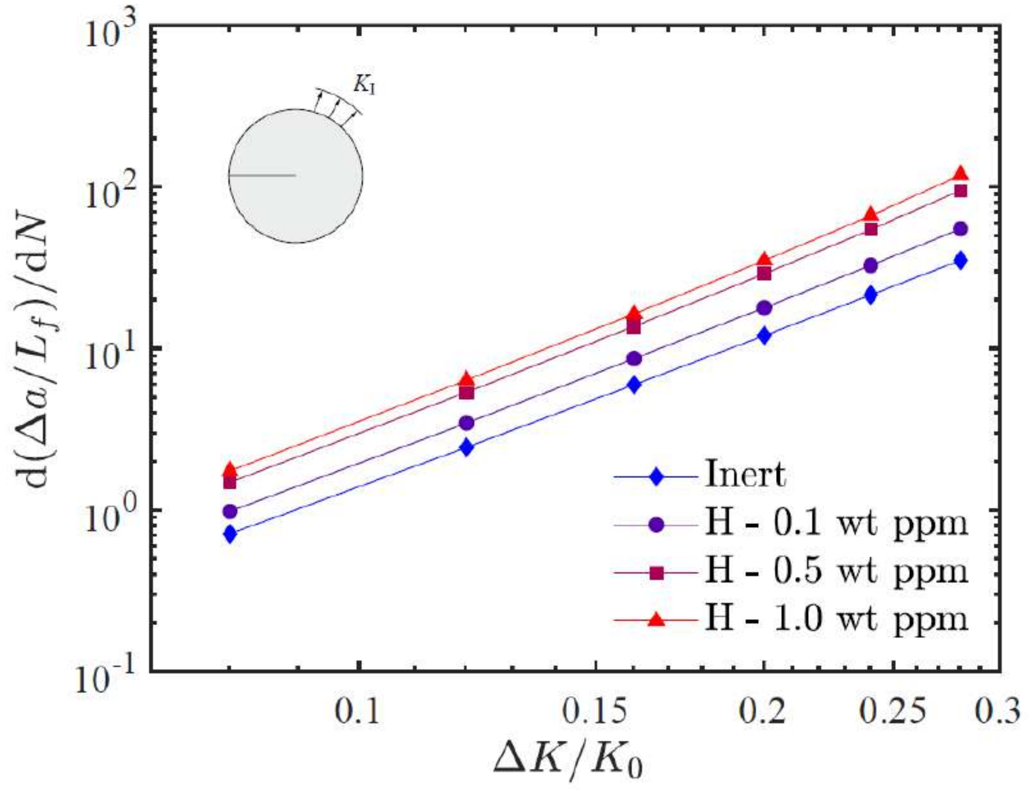




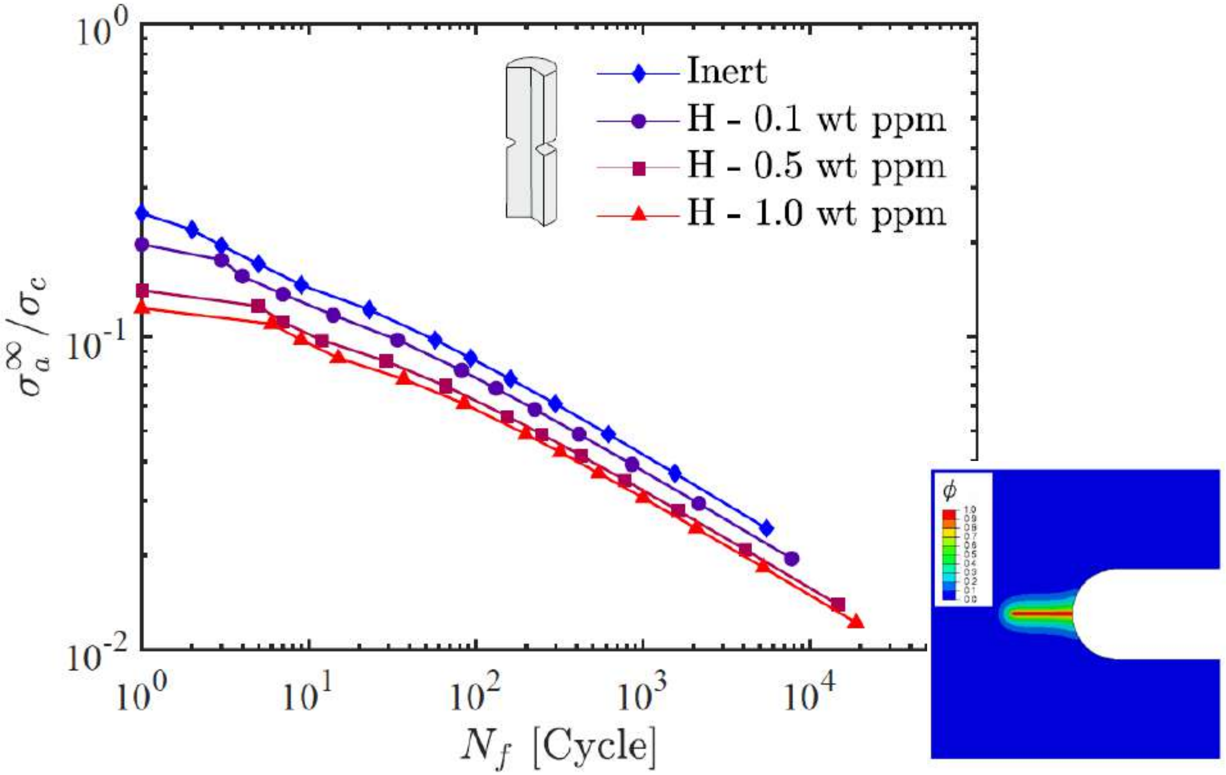
Golahmar, Kristensen, Niordson, Martínez-Pañeda. *Int. J. Fatigue* (2022)

Results – Hydrogen-assisted Fatigue

Paris law behaviour



Virtual S-N curves



Golahmar, Kristensen, Niordson, Martínez-Pañeda. *Int. J. Fatigue* (2022)

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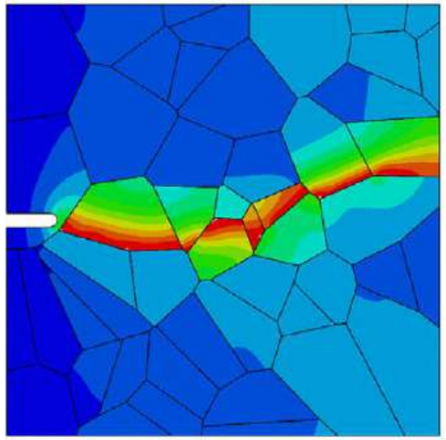
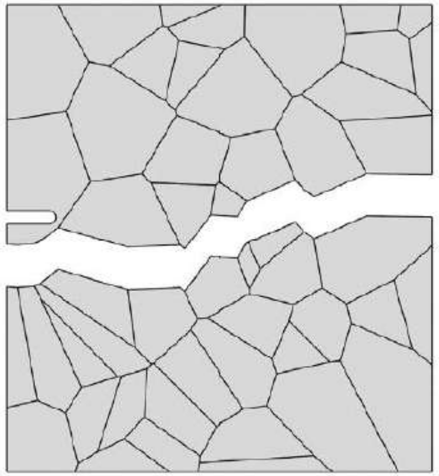
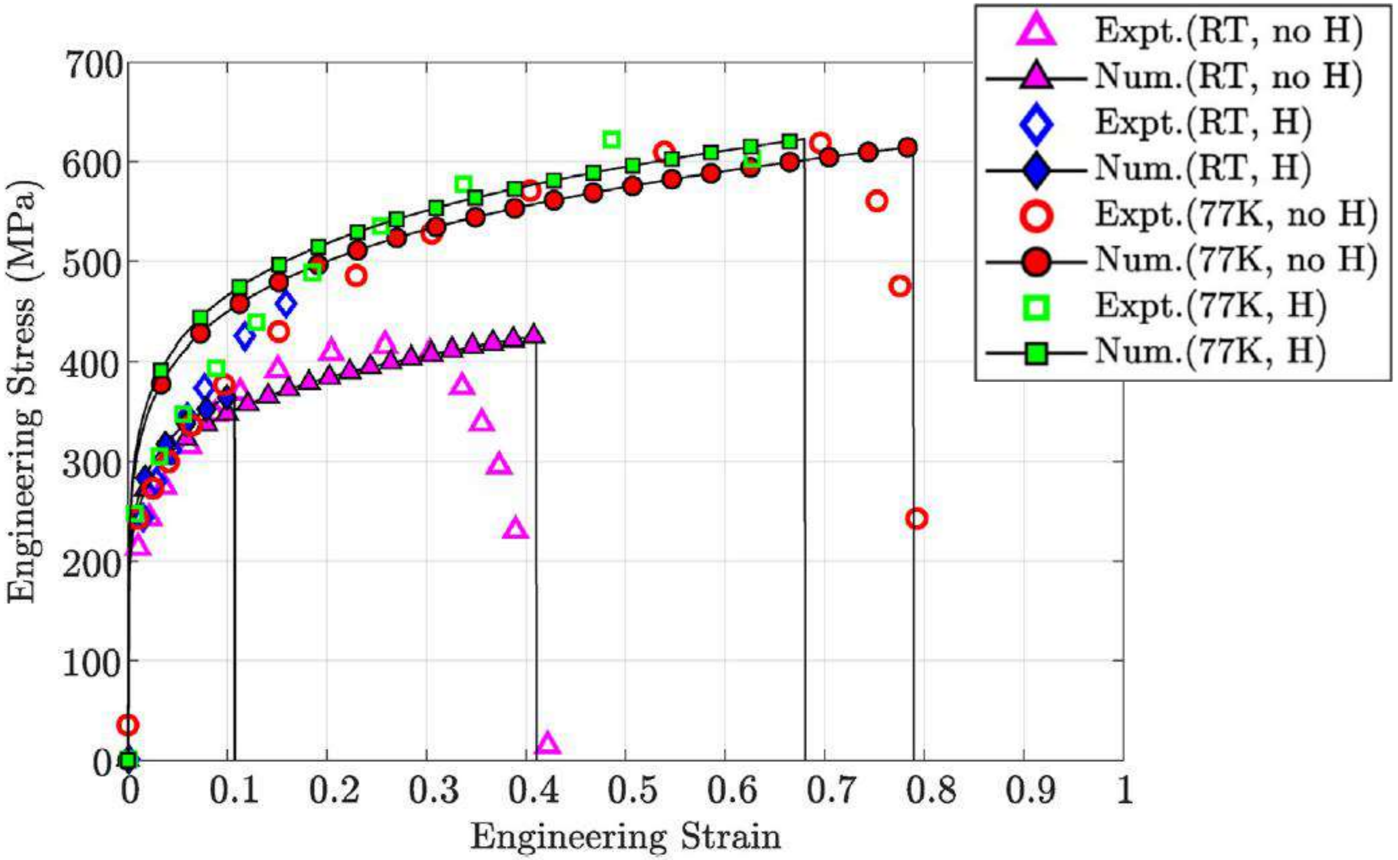
Results – Intergranular cracking

Phase field:
Ductile transgranular cracking



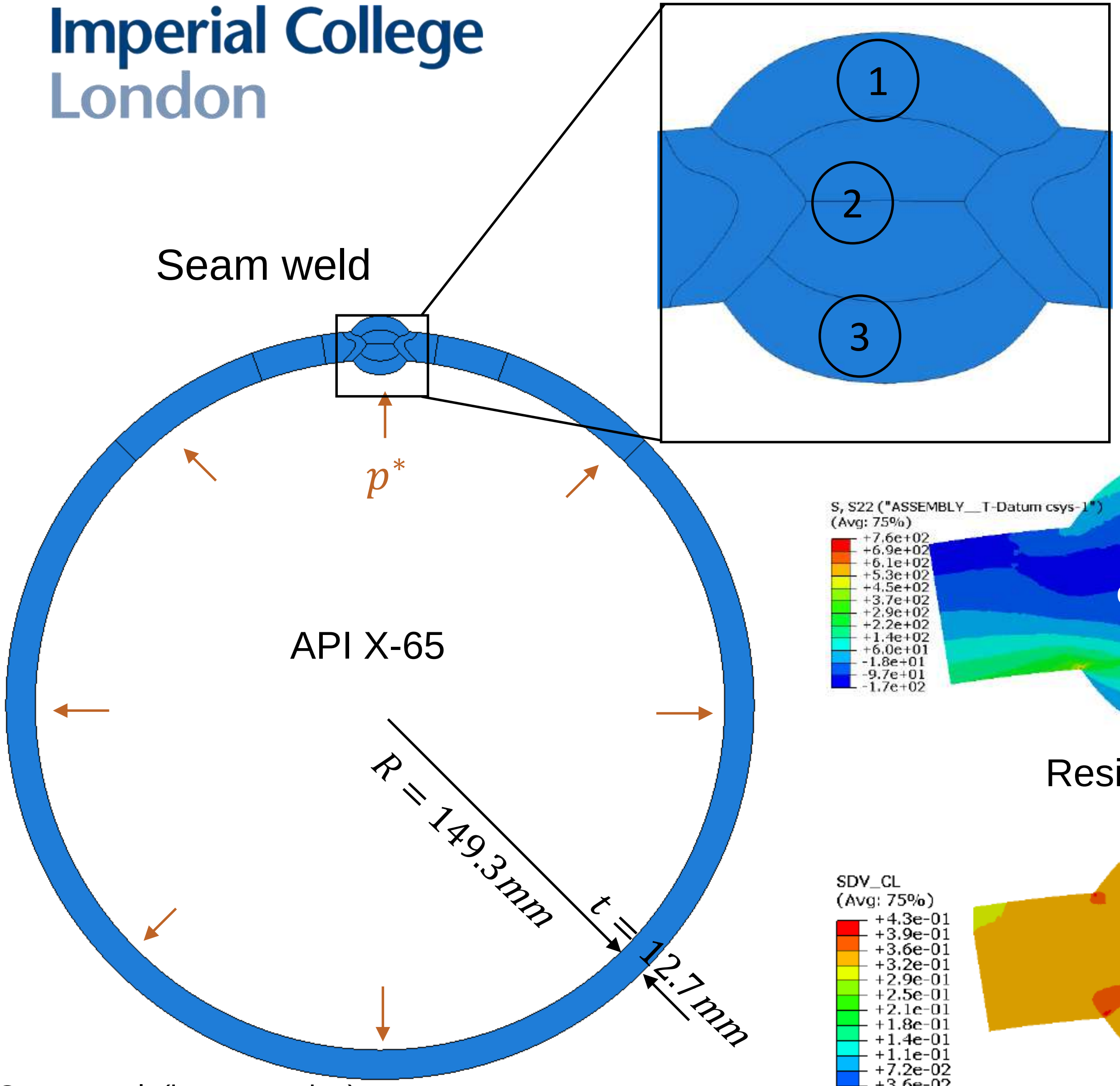
Cohesive zone model:
Brittle intergranular cracking

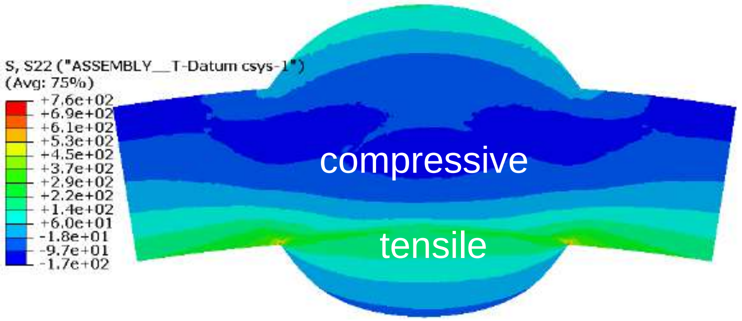




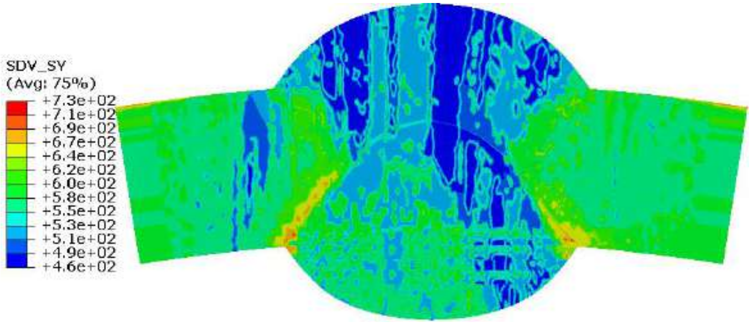
Valverde-González, Martínez-Pañeda *et al.*. *Int. J. Hydrogen Energy* (2022)

Results – Welded joints

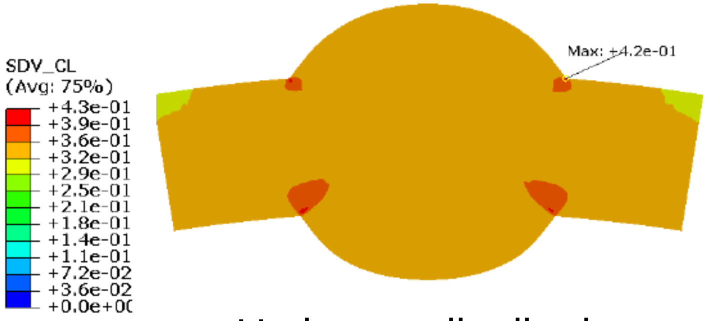




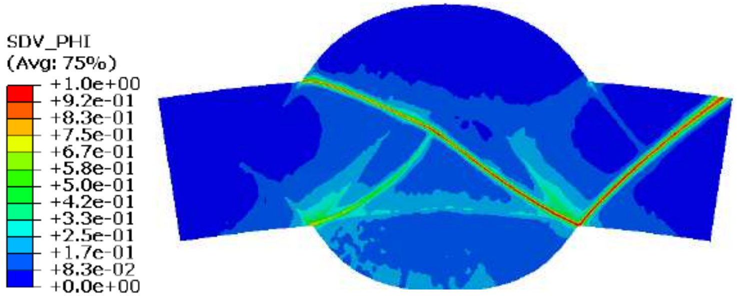
Residual stresses



Microstructural variation



Hydrogen distribution



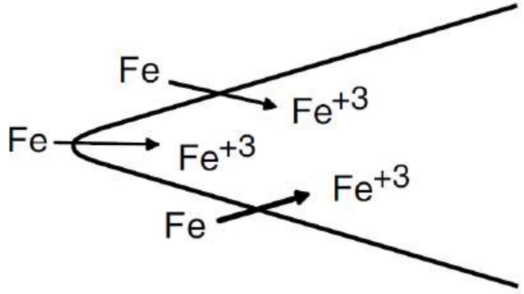
Cracking

Castro et al. (in preparation)
Mandal et al. (in preparation)

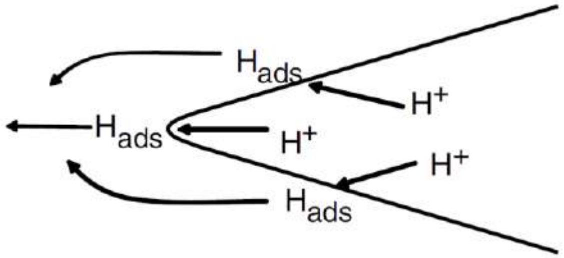
Imperial College London

Environmentally assisted cracking

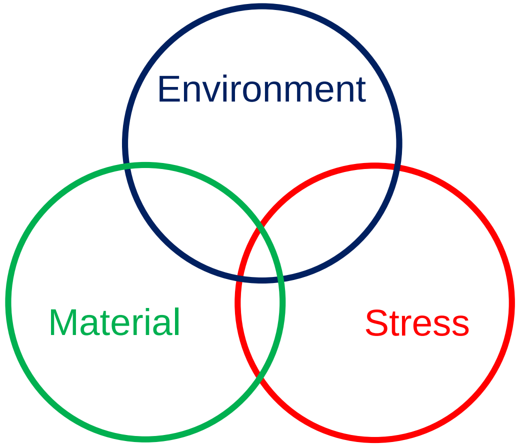
- Stress Corrosion Cracking (SCC)
  - Anodic-dissolution cracking



  - Hydrogen embrittlement

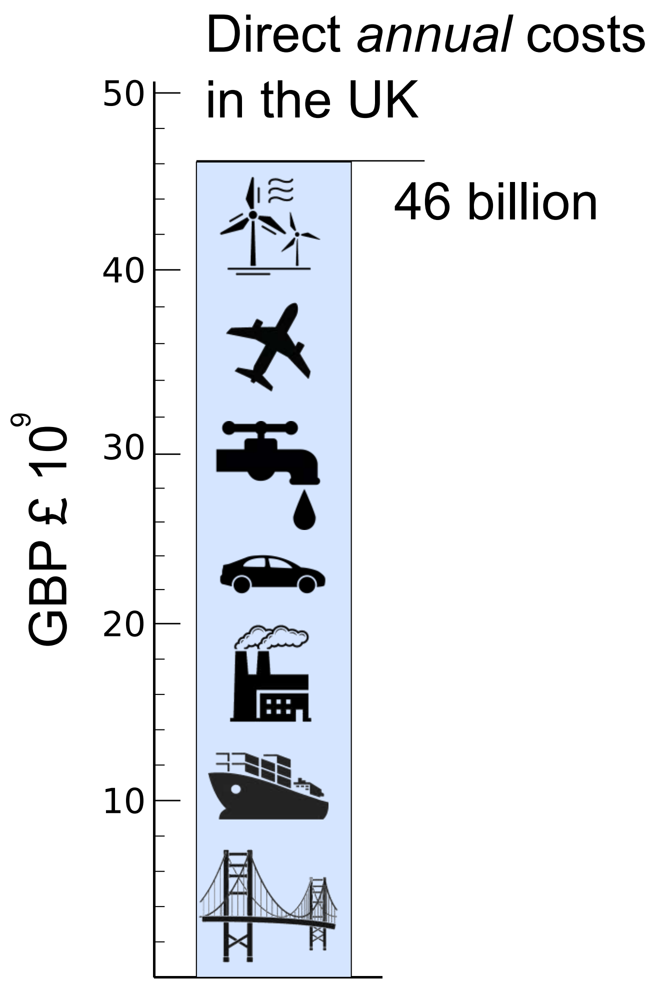


- Hydrogen embrittlement
- Liquid Metal Embrittlement
- Oxidation fatigue, *etc*.



Corrosion – everyone's problem

- Massive societal cost: Globally, US$2.5 trillion per year
- Biggest threat to the durability and sustainability of materials
- Often resulting in catastrophic failures
- Long-standing scientific and technological challenge



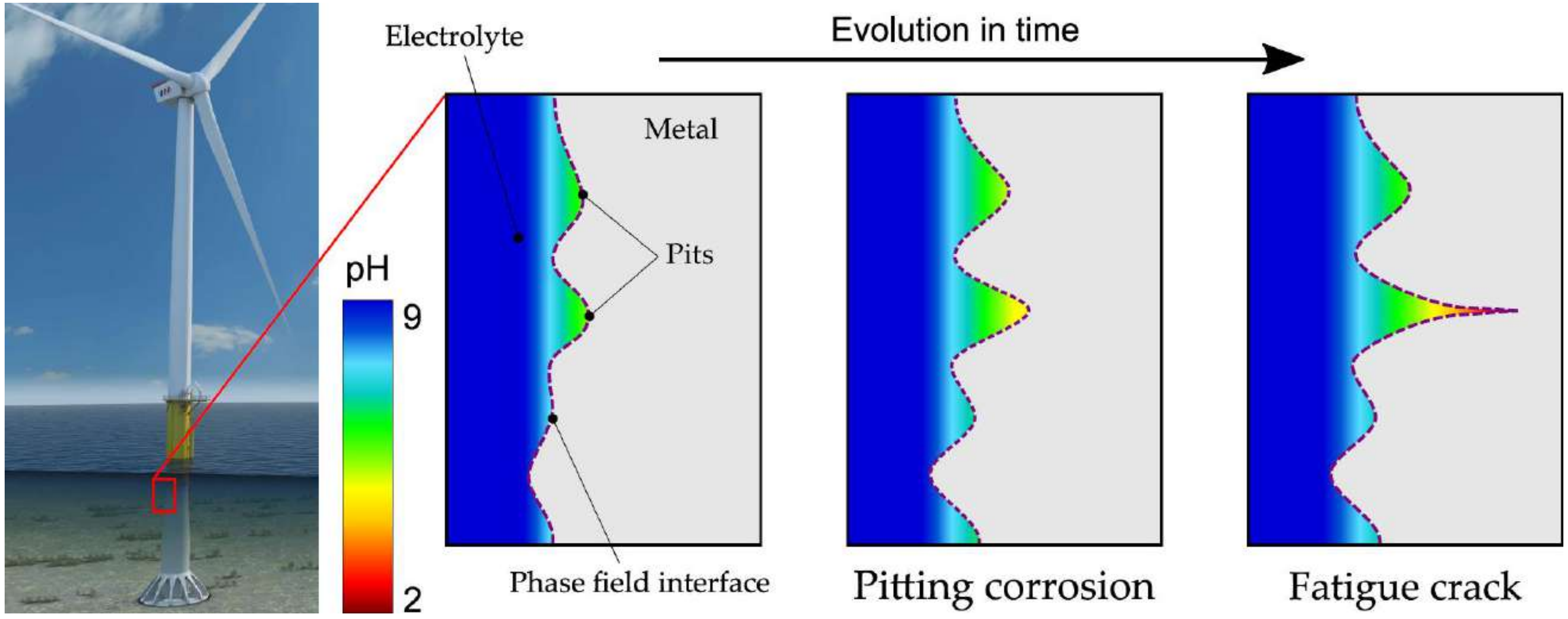
Morandi bridge collapse (Italy)

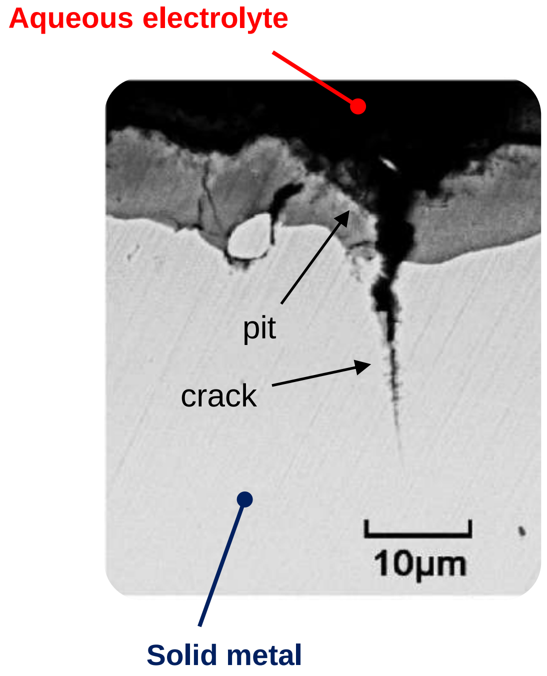
Prestige disaster (Spain)

FedEx landing gear failure (FLL airport)

Imperial College London

A new phase field paradigm: corrosion

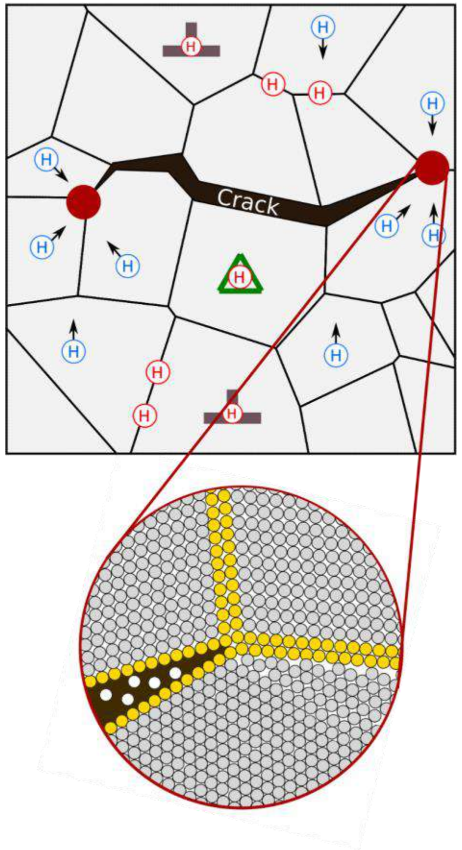




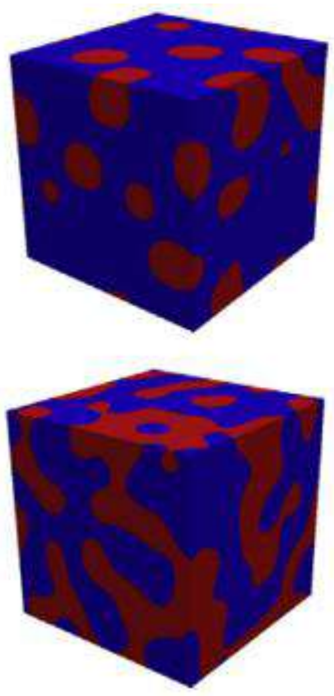
Martínez-Pañeda (RILEM Technical Letters, 2021)

A new phase field paradigm: corrosion

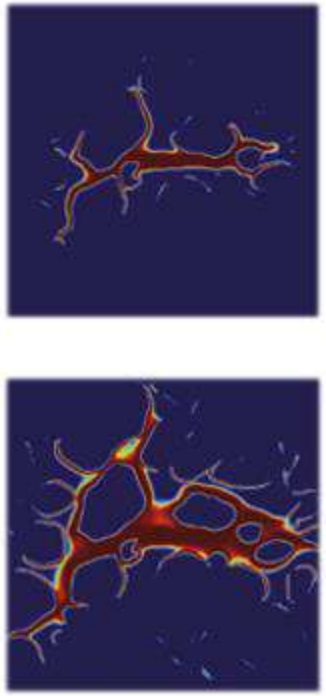
Stage III: Fracture



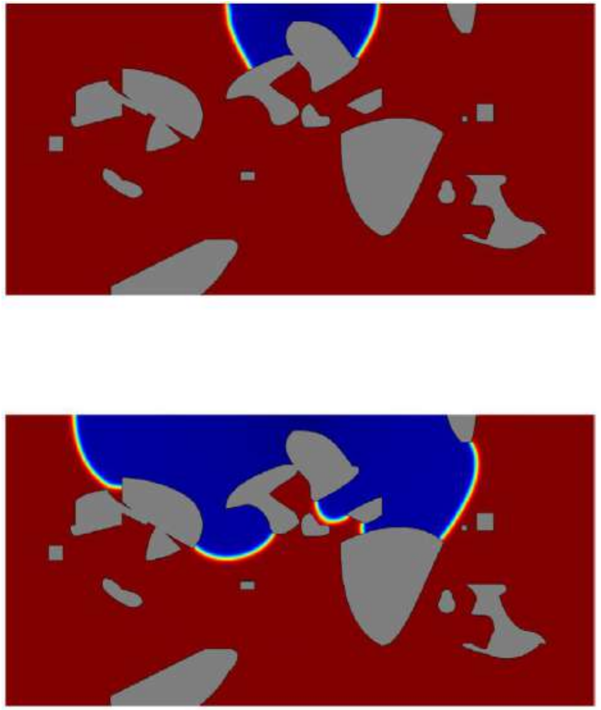
Phase field modelling



Microstructural evolution



Fracture mechanics



Corrosion

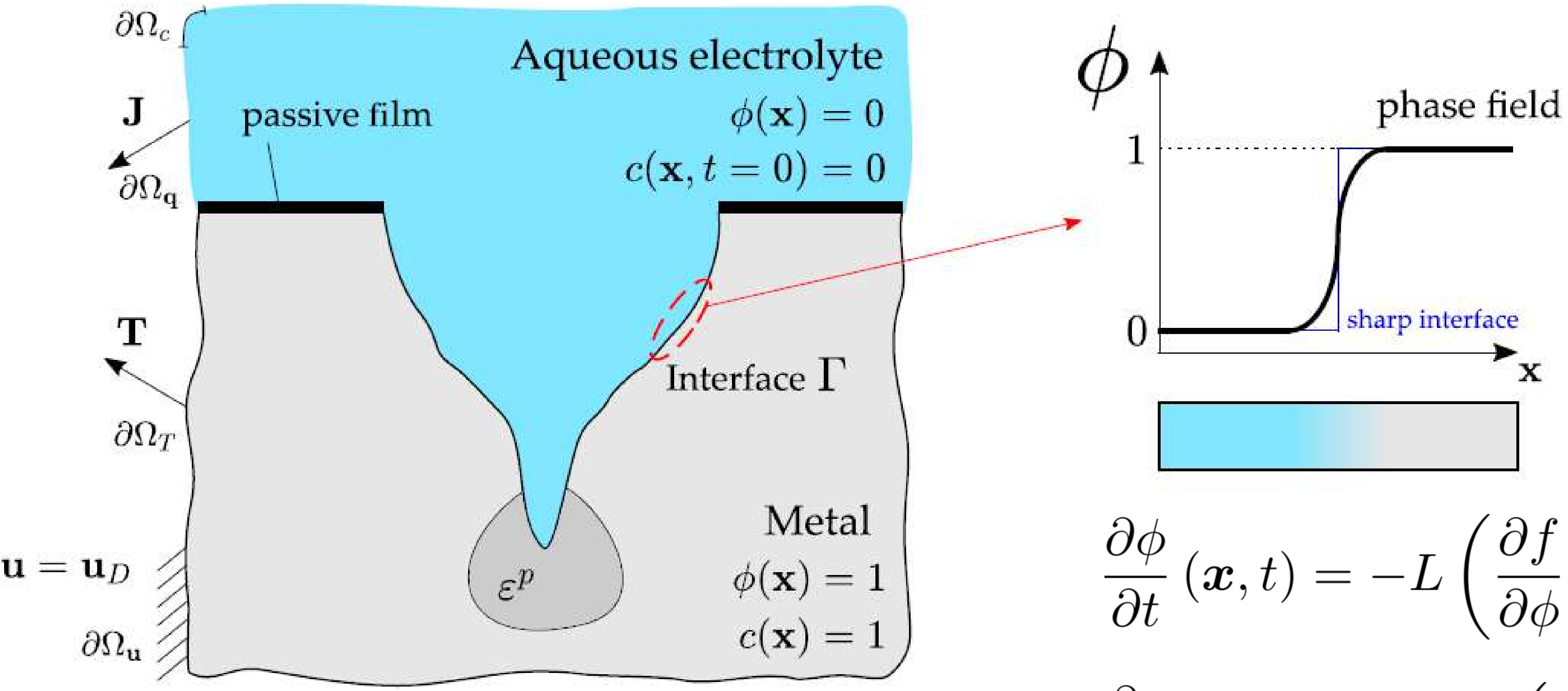
t_0

t_1

Kristensen, Niordson, Martínez-Pañeda. *Philosophical Transactions of the Royal Society A (2021)*

Imperial College London

A new phase field paradigm: corrosion



$$\frac{\partial \phi}{\partial t}(\boldsymbol{x}, t) = -L\left(\frac{\partial f}{\partial \phi} - \alpha \nabla^2 \phi\right)$$

$$\frac{\partial c}{\partial t}(\boldsymbol{x}, t) = \nabla \cdot M\left(\nabla \frac{\partial f}{\partial c}\right)$$

Cui, Ma, Martínez-Pañeda. *JMPS* (2021)

A phase field description of the corrosion front

Imperial College London

Phase field evolution (interface reaction)

$$\frac{\partial \phi}{\partial t}(\boldsymbol{x}, t) = -L\left(\frac{\partial f}{\partial \phi} - \alpha \nabla^2 \phi\right)$$

$$\frac{d\phi}{dt} + L\left(-2A\left[c - h(\phi)(c_{\mathrm{Se}} - c_{\mathrm{Le}}) - c_{\mathrm{Le}}\right](c_{\mathrm{Se}} - c_{\mathrm{Le}})h'(\phi) + wg'(\phi) - \alpha \nabla^2 \phi\right) = 0$$

Concentration of metal ions

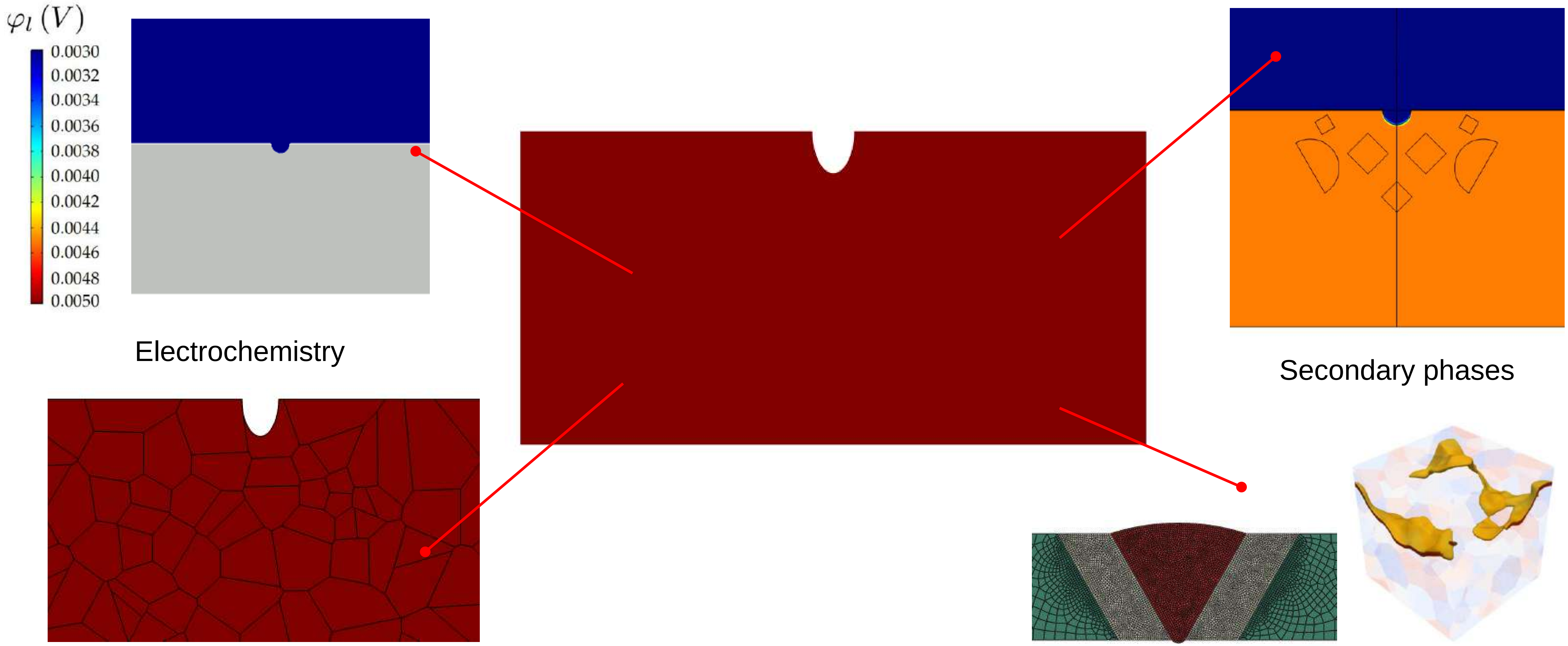
$$\frac{\partial c}{\partial t}(\boldsymbol{x}, t) = \nabla \cdot M\left(\nabla \frac{\partial f}{\partial c}\right)$$

$$\frac{\partial c}{\partial t} - \nabla \cdot D \nabla\left[c - h(\phi)(c_{Se} - c_{Le}) - c_{Le}\right] = 0$$

A new phase field paradigm: corrosion

Cui, Ma, Martínez-Pañeda. *JMPS* (2021)

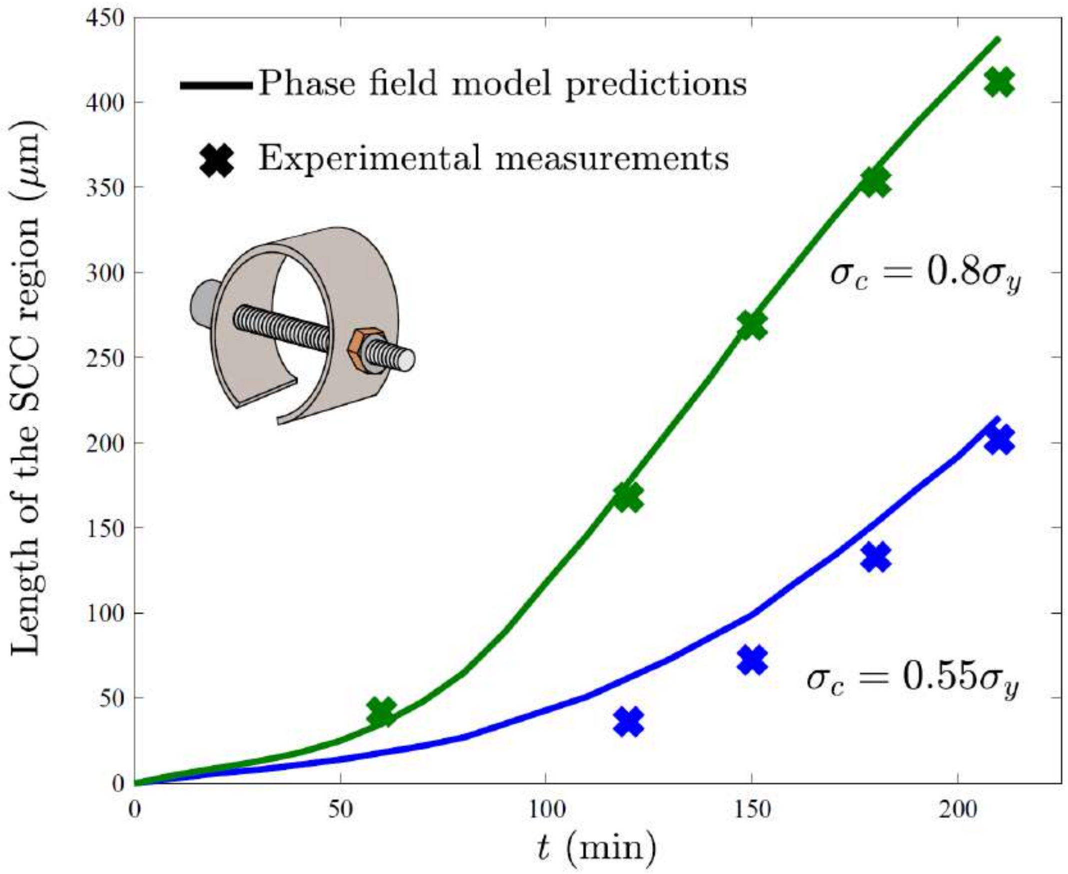
A new phase field paradigm: corrosion

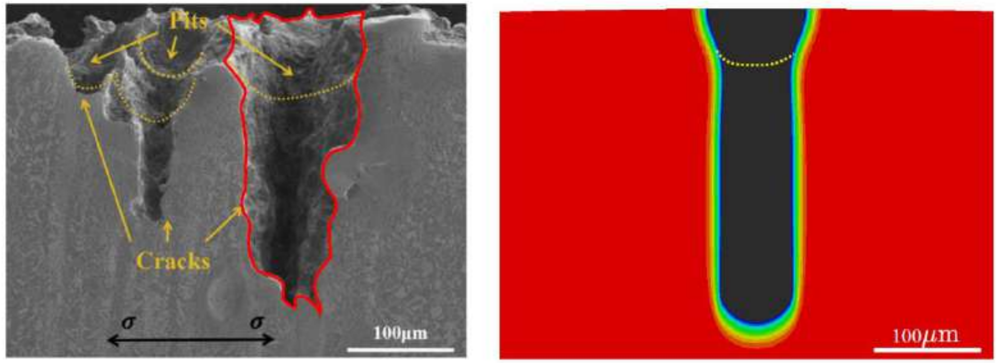


Microstructural anisotropy

Structural integrity analysis

Representative result: C-ring test



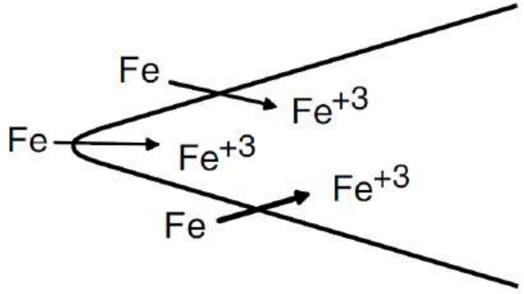


- The model quantitatively captures the sensitivity of corrosion kinetics to applied mechanical load

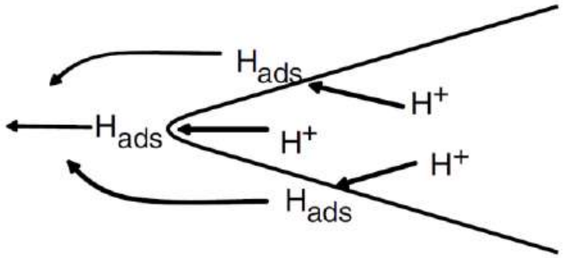
Cui, Ma, Martínez-Pañeda. *JMPS* (2021)

Environmentally assisted cracking

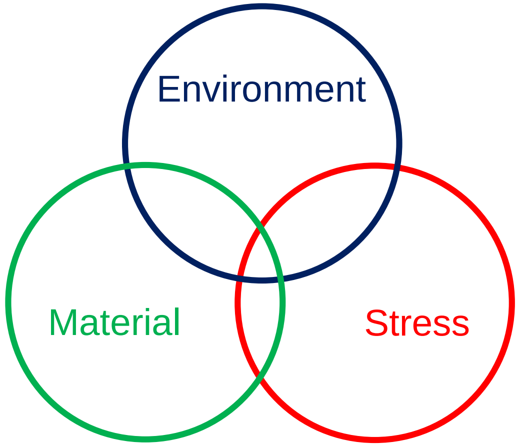
- ❑ Stress Corrosion Cracking (SCC)
  - ❑ Anodic-dissolution cracking



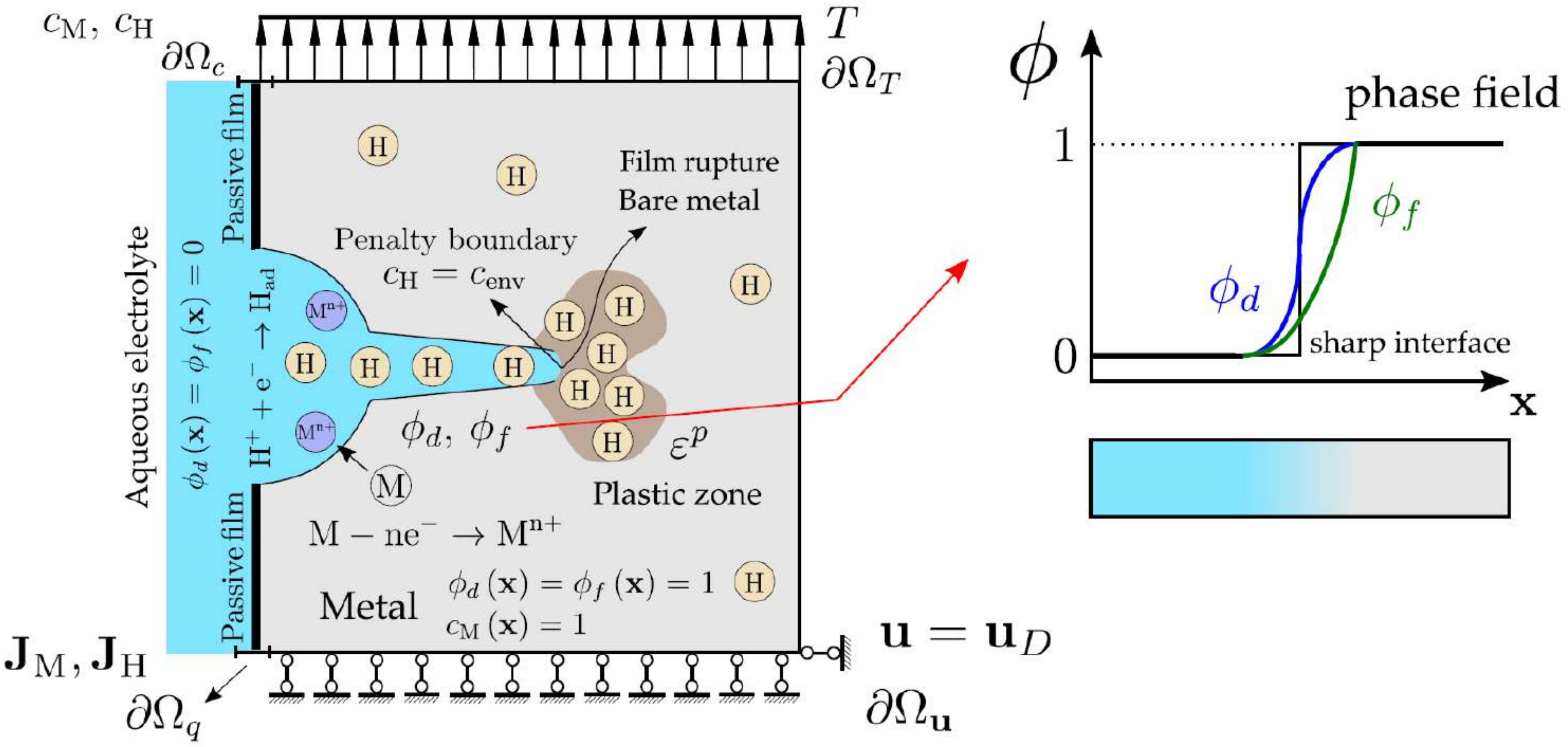
  - ❑ Hydrogen embrittlement



- ❑ Hydrogen embrittlement
- ❑ Liquid Metal Embrittlement
- ❑ Oxidation fatigue, *etc*.



A generalised model for SCC



Cui, Ma, Martínez-Pañeda (JMPS, 2022)

A generalised model for SCC

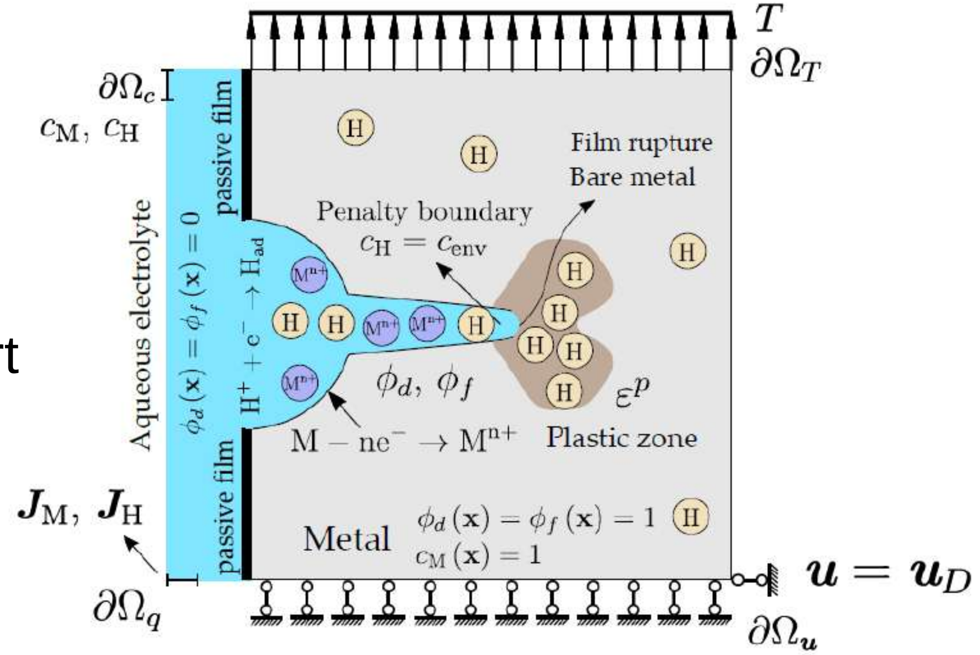
$$\nabla \cdot [h_d(\phi_d) h_f(\phi_f) \boldsymbol{\sigma}] = \mathbf{0}$$ Displacement

$$h'_f(\phi_f)\, h_d(\phi_d)\, \psi_0^m - G_c(c_{\mathrm{H}}) \left(\frac{1-\phi_f}{\ell_f} + \ell_f \nabla^2 \phi_f \right) = 0$$ Fracture

$$\frac{\mathrm{d}c_{\mathrm{H}}}{\mathrm{d}t} - D_{\mathrm{H}} \nabla c_{\mathrm{H}} + \frac{D_{\mathrm{H}} c_{\mathrm{H}}}{RT} \overline{V}_{\mathrm{H}} \nabla \sigma_h = 0$$ H diffusion

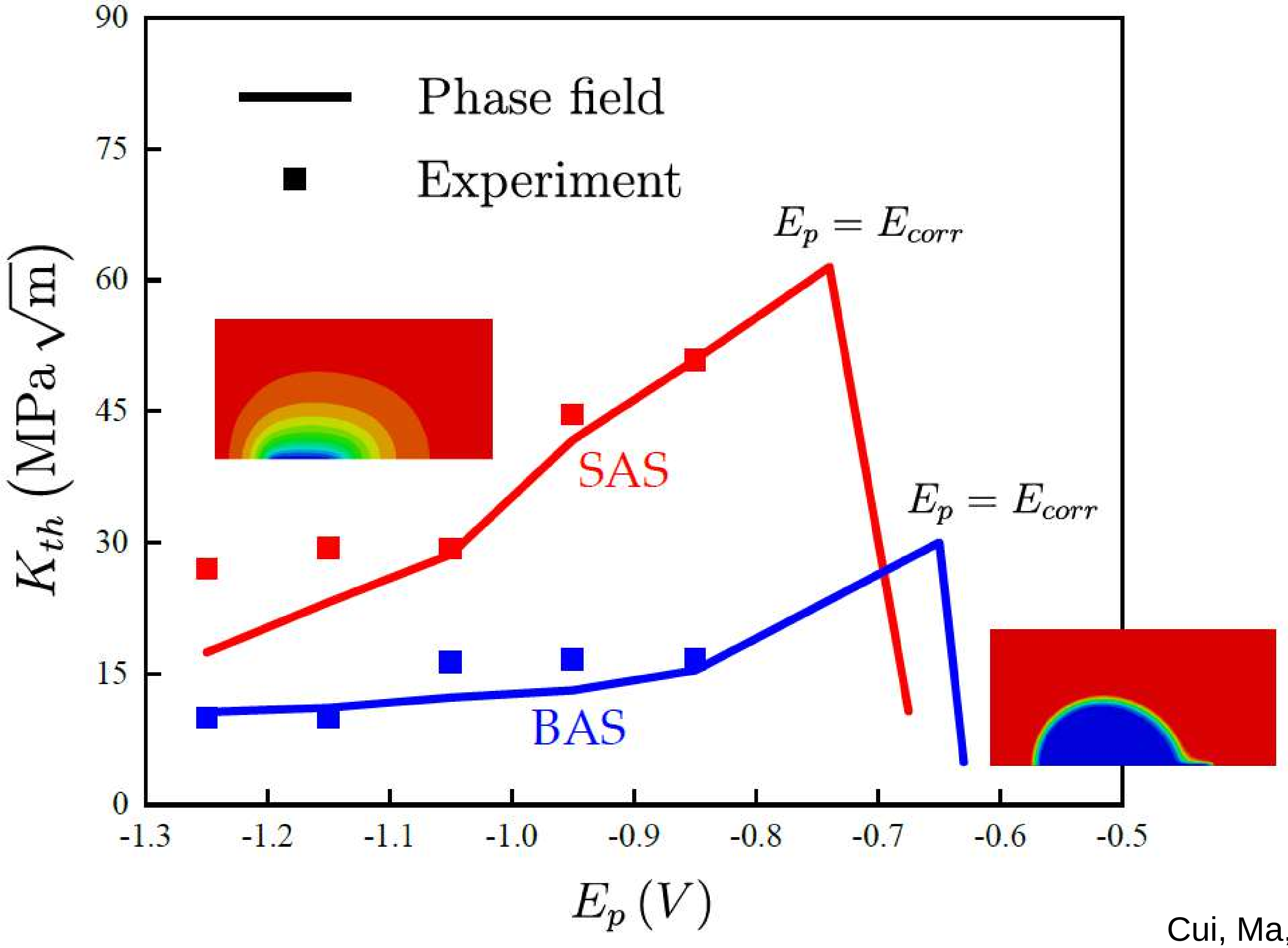
$$\frac{\mathrm{d}c_{\mathrm{M}}}{\mathrm{d}t} - \nabla \cdot D_{\mathrm{M}} \nabla \left[(c_{\mathrm{M}} - h_d(\phi_d)(c_{\mathrm{Se}} - c_{\mathrm{Le}}) - c_{\mathrm{Le}}) \right] = 0$$ Ionic transport

$$\frac{\mathrm{d}\phi_d}{\mathrm{d}t} + L(\varepsilon^p, \sigma_h) \left(\frac{\partial \psi^{ch}}{\partial \phi_d} - \alpha \nabla^2 \phi_d \right) = 0$$ Corrosion



Cui, Ma, Martínez-Pañeda (JMPS, 2022)

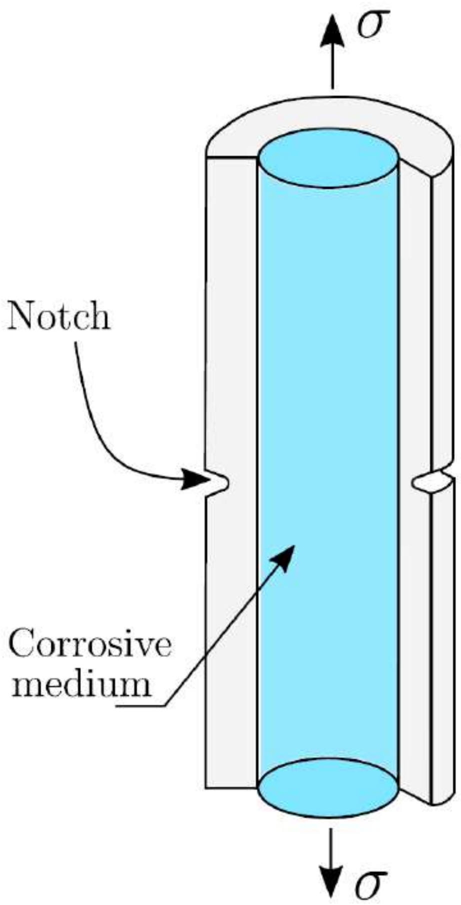
A generalised model for SCC

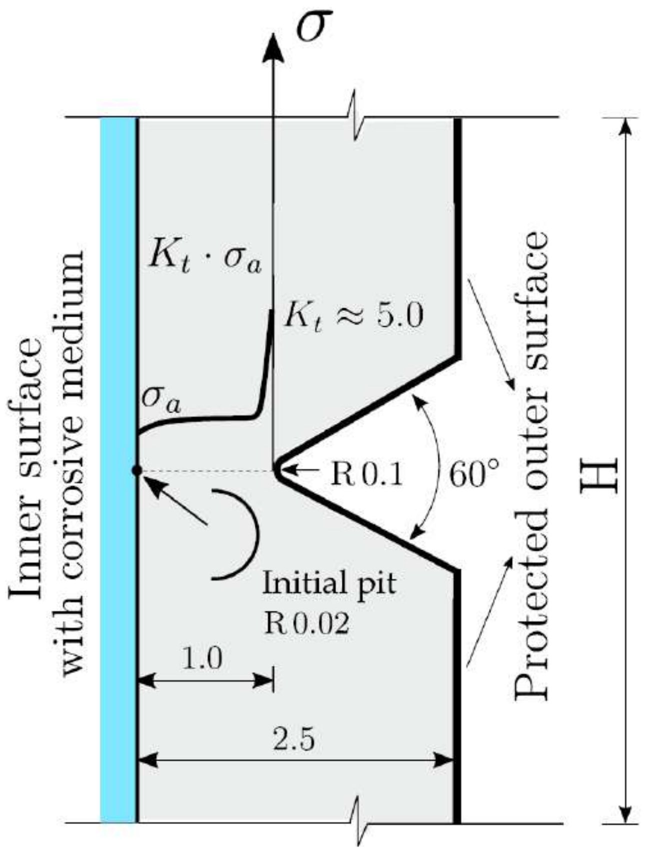


Cui, Ma, Martínez-Pañeda (JMPS, 2022)

A generalised model for SCC

Gruhl (1984) experiments in Al alloys

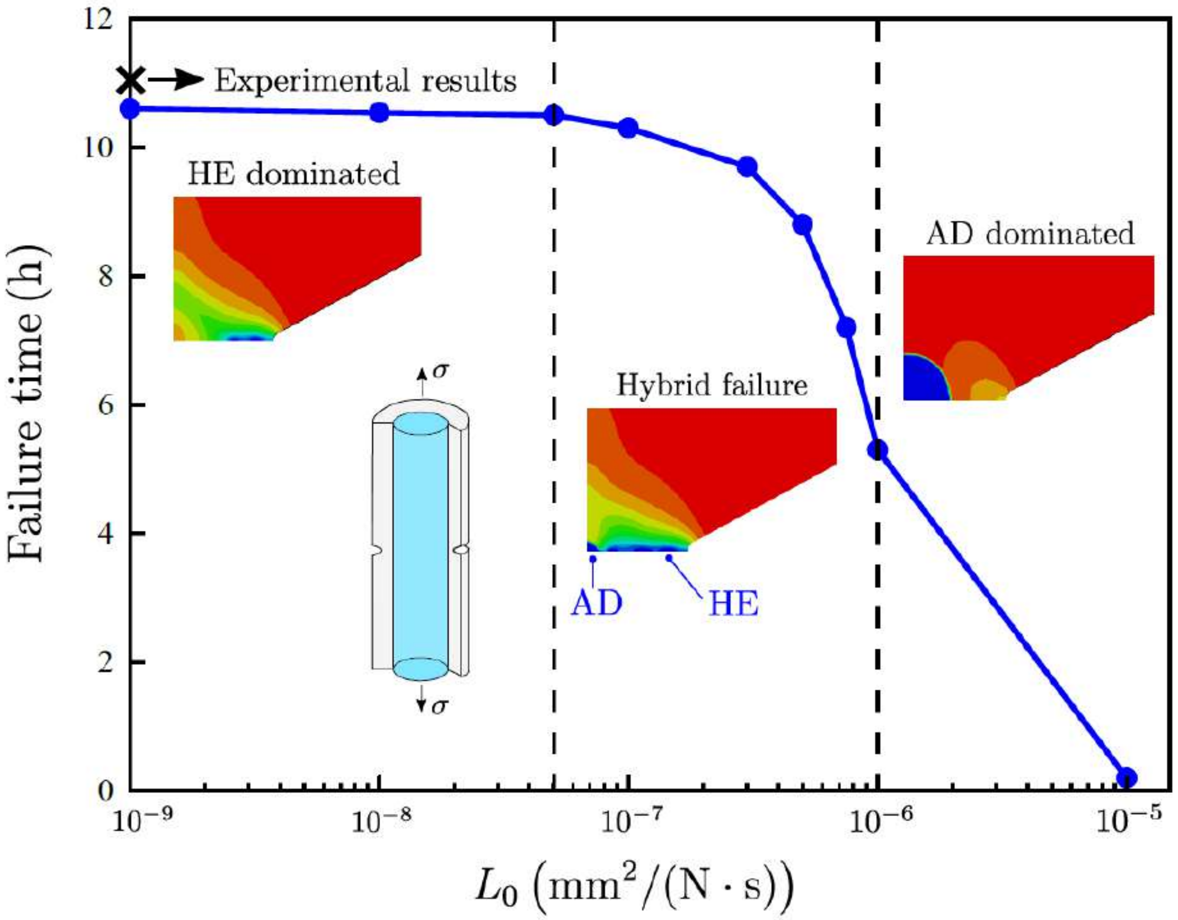




Cui, Ma, Martínez-Pañeda (JMPS, 2022)

A generalised model for SCC

Gruhl (1984) experiments in Al alloys



Cui, Ma, Martínez-Pañeda (JMPS, 2022)

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Concluding remarks

- Phase field and multi-physics modelling can be combined to develop a mechanistic computational framework that resolves the physics processes of hydrogen embrittlement

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Concluding remarks

- Phase field and multi-physics modelling can be combined to develop a mechanistic computational framework that resolves the physics processes of hydrogen embrittlement

- The computational framework developed can predict fracture (and fatigue) in laboratory tests and practical applications *(Virtual Testing)*

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Concluding remarks

- Phase field and multi-physics modelling can be combined to develop a mechanistic computational framework that resolves the physics processes of hydrogen embrittlement

- The computational framework developed can predict fracture (and fatigue) in laboratory tests and practical applications *(Virtual Testing)*

- The framework is general, can accommodate any mechanistic interpretation of H embrittlement and can readily be extended (microstructure, welds, stress corrosion cracking, *etc*.)

Concluding remarks

- Phase field and multi-physics modelling can be combined to develop a mechanistic computational framework that resolves the physics processes of hydrogen embrittlement

- The computational framework developed can predict fracture (and fatigue) in laboratory tests and practical applications *(Virtual Testing)*

- The framework is general, can accommodate any mechanistic interpretation of H embrittlement and can readily be extended (microstructure, welds, stress corrosion cracking, *etc*.)

- The combination of phase field and multi-physics modelling enables developing computational models that can resolve the physical processes of corrosion damage

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Thank you

- Codes are openly shared! www.imperial.ac.uk/mechanics-materials

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