A multi-scale approach to characterize the Hydrogen Induced Cracking (HIC) resistance of (pipeline) steels

Workshop

03-04.09.2024

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Agenda

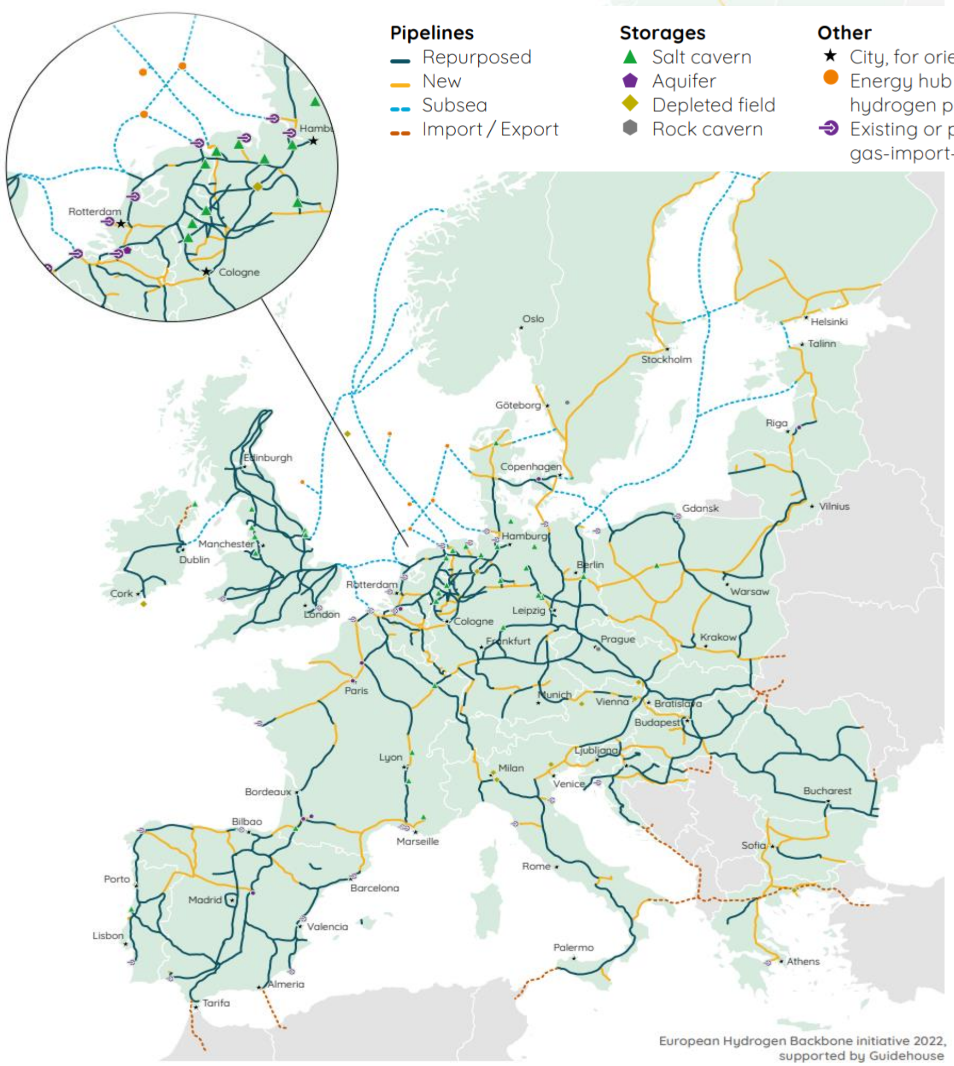
Agenda

Motivation - Strategy European Hydrogen Backbone 2022

Green Deal

REPowerEU

Fit for 55

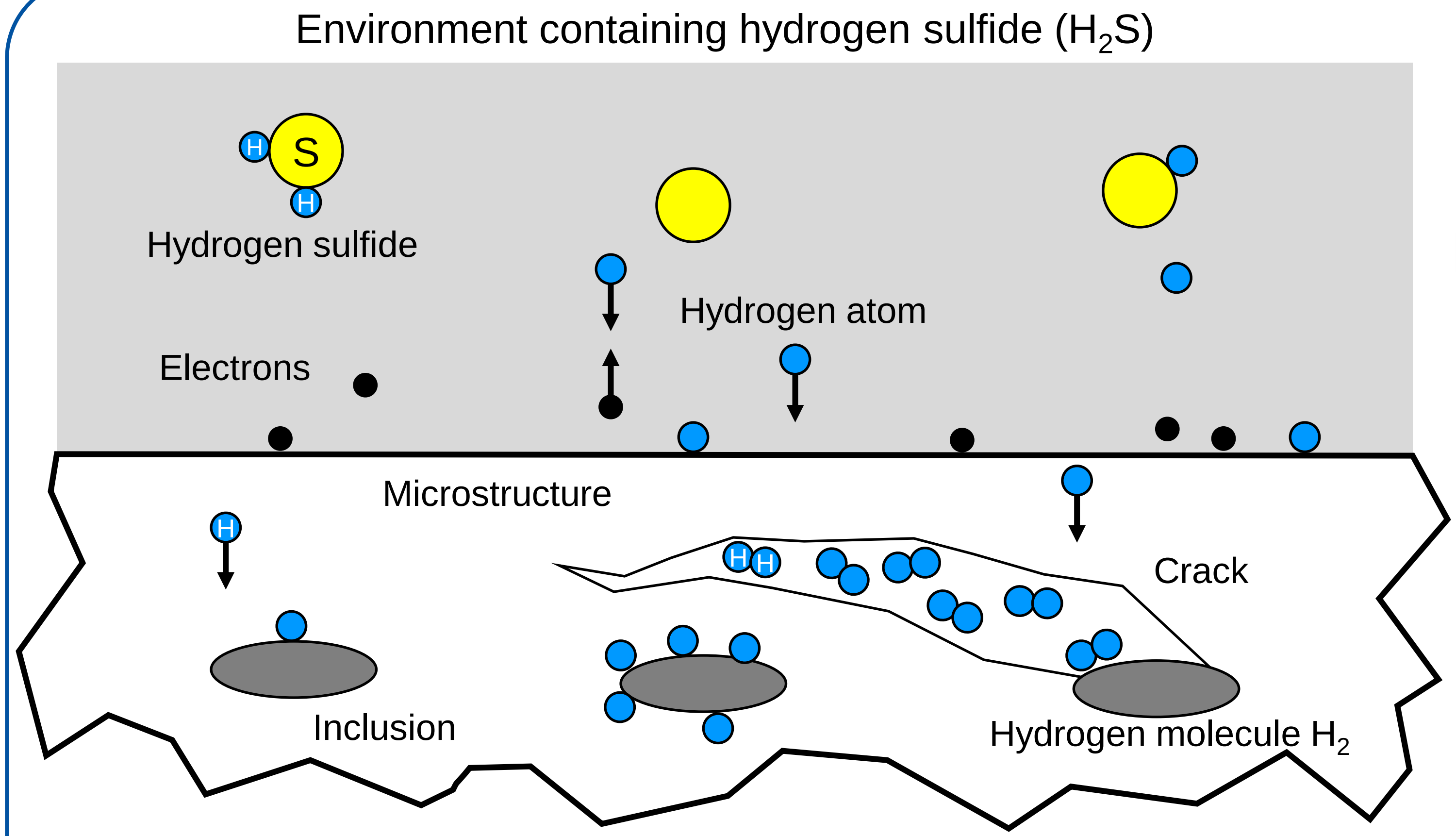


Until 2040:

- approx. 53.000 km pipeline network
- 60 % redesignated from pipelines for natural gas transport

Explosion craters Carlsbad 19.08.2000
(Source: NTSB/PAR-03/01)

Evolution of Hydrogen-Induced-Cracking (HIC) in Steels



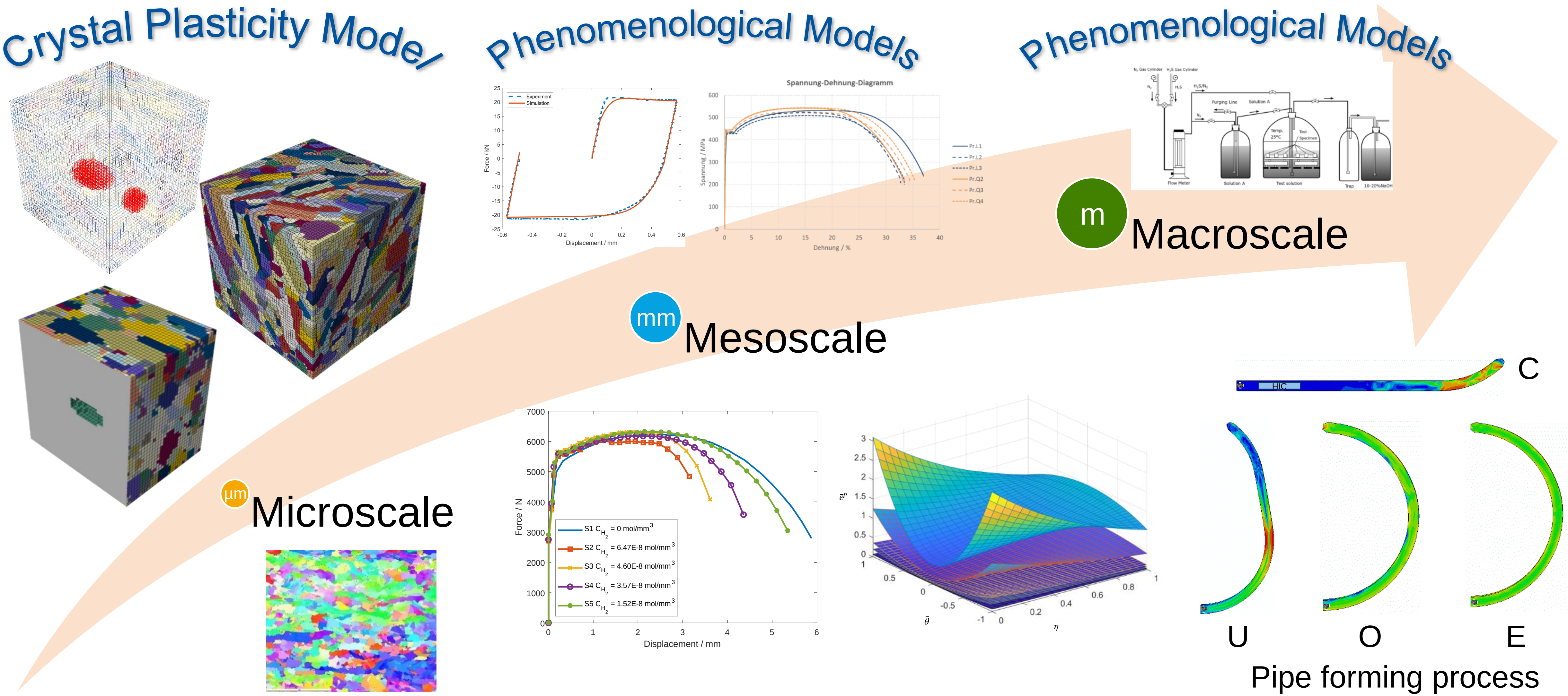
Dissociation:

$$H_2S \rightarrow H^+ + HS^-$$

$$2H_{\mathrm{Atom}} \rightarrow H_2$$

Are the natural gas pipelines suitable for the transition to hydrogen on the material side?

Multi-scale description of HIC resistance



Implementation of hydrogen diffusion according to Oriani (1970)

- Hydrogen diffusion can be described by Fick's laws
- Hydrogen atoms diffuse into areas of high elastic stress
- The hydrogen concentration is a function of hydrostatic stress and plastic strain
- Hydrogen atoms dissolved in the traps $\overset{!}{\Leftrightarrow}$ hydrogen atoms dissolved in the interstitial lattice sites.

Time Integration

Implicit

- **Degree of freedom**: Lattice concentration C_L

- Convergence problems when modelling damage
- Straight forward boundary conditions

Explicit

- **Degree of freedom**: Chemical potential μ_L
- Needs non-dimensional modelling
- Mass scaling

- Suitable for coupled damage modelling
- Complex boundary conditions

Implementation of hydrogen diffusion according to Oriani (1970)

Time Integration

Implicit

- **Degree of freedom**: Lattice concentration C_L

$$\underbrace{\frac{d\tilde{C}_L}{dt}\left[1+\frac{\partial \tilde{C}_T^d}{\partial \tilde{C}_L}+\frac{\partial \tilde{C}_T^{gb}}{\partial \tilde{C}_L}+\frac{\partial \tilde{C}_T^c}{\partial \tilde{C}_L}\right]}_{\text{Diffusion flux}} - \underbrace{\nabla_x \cdot \left[D_L \nabla_x \tilde{C}_L\right]}_{\text{Concentration difference over boundary}}$$

$$+ \underbrace{\nabla_x \cdot \left[\frac{D_L \tilde{C}_L V_H}{RT} \nabla_x \sigma_h\right]}_{\text{Hydrogen concentration as a function of hydrostatic stress}} + \underbrace{\sum_i^d \frac{\partial \tilde{C}_T^i}{\partial \tilde{N}_T^i} \cdot \frac{\partial \tilde{N}_T^i}{\partial \varepsilon^p} \cdot \frac{d\varepsilon^p}{dt}}_{\text{Hydrogen concentration as a function of plastic strain}} = 0$$

Explicit

- **Degree of freedom**: Chemical potential μ_L
- Needs non-dimensional modelling
- Mass scaling

$$D^* \bar{C}_L \frac{d\bar{\mu}_L}{dt} - \nabla_x \cdot \left[D_L \bar{C}_L \nabla_x \bar{\mu}_L\right] =$$

$$\underbrace{-D^* \bar{C}_L \frac{V_H}{\mu_L^r} \frac{d\sigma_h}{dt} - \frac{RT}{C_L^r\, \mu_L^r}\, \theta_T \frac{dN_T}{d\varepsilon^p} \frac{d\varepsilon^p}{dt}}_{\text{Hydrogen source}}$$

$$D^* = 1 + \frac{K_T\, N_T/N_L}{\left(1+K_T\, C_L\, C_L^r/N_L\right)^2}$$

Implementation of hydrogen diffusion into Abaqus/Standard

Start Increment
Inc = Inc+1

USER-Subroutine UMAT

- Calculation of equivalent plastic strain ε^p
- Calculation of damage D
- Save ε^p and D as SDV

USER-Subroutine USDFLD

- Read hydrostatic stress σ_h
- Save σ_h in COMMON Block
- Calculation of gradient of hydrostatic stress $\nabla\sigma_H$
- Save $\nabla\sigma_h$ as SDV

Heat equation	Mass diffusion equation
$\rho c_{\mathrm{p}} \frac{\partial T}{\partial t} + \nabla \cdot \boldsymbol{J}_{\mathrm{w}} + r_{\mathrm{w}} = 0$	$\frac{\partial \tilde{C}_{\mathrm{T}}}{\partial t} + \nabla \cdot \tilde{J}_{\mathrm{d}} + r_{\mathrm{d}} = 0$
Derivative of thermal energy per unit:	Derivative of total hydrogen concentration:
$\dot{U}_{\mathrm{w}} = c_{\mathrm{p}} \frac{\partial T}{\partial t}$	$\frac{\partial \tilde{C}_{\mathrm{T}}}{\partial t} = \frac{\partial(\tilde{C}_{\mathrm{L}} + \tilde{C}_{x})}{t}$
Degree of freedom: T	Degree of freedom: $\tilde{C}_{\mathrm{L}}$
Heat flux: $\tilde{J}_{\mathrm{w}}$	Hydrogen flux: $\tilde{J}_{\mathrm{d}} = -\frac{D_{\mathrm{L}} \tilde{C}_{\mathrm{L}} V_{\mathrm{H}}}{RT} \nabla_{\chi} \sigma_{\mathrm{h}} - D_{\mathrm{L}} \nabla_{\chi} \tilde{C}_{\mathrm{L}}$
Heat source: r_{w} (Assumption $r_{\mathrm{w}} = 0$)	Hydrogen source: r_{d} (Assumption $r_{\mathrm{d}} = 0$)
Density: ρ	1

Convergence?

No

Yes

End Increment

Implementation of hydrogen diffusion into Abaqus/Explicit

Start Increment
Inc = Inc+1

USER-Subroutine VUMAT

- Calculation of equivalent plastic strain ε^p
- Calculation of hydrostatic stress σ_h
- Calculation of damage D
- Calculation of hydrogen source via dissipated inelastic sp. energy
- Save σ_h, ε^p and D as SDV

Heat equation	Mass diffusion equation
$\rho\, c_p \frac{dT}{dt} + \nabla \cdot \boldsymbol{J}_w + r_w = 0$	$D^*\, \bar{C}_L \frac{d\bar{\mu}_L}{dt} + \nabla \cdot \boldsymbol{J}_{H^+} + r_{H^+} = 0$
Degree of freedom: T	$\bar{\mu}_L$
Heat flux: $\boldsymbol{J}_w$	Hydrogen flux: $\boldsymbol{J}_{H^+} = D^*\, \bar{C}_L \nabla \bar{\mu}_L$
Heat source: r_w	Hydrogen source: $r_{H^+} = D^*\, \bar{C}_L \frac{V_H}{\mu_L^r} \frac{\partial \sigma_h}{\partial t} - \frac{RT}{C_L^r\, \mu_L^r}\, \theta_T \frac{dN_T}{d\varepsilon^p} \frac{d\varepsilon^p}{dt}$
Specific heat: c_p	$D^*\, \bar{C}_L$
Conductivity: k_e	$D_L\, \bar{C}_L$
Internal energy: U	$U = U + \frac{D^* \bar{C}_L}{\rho} \Delta \bar{\mu}_L$
Density: ρ	Mass scaling factor

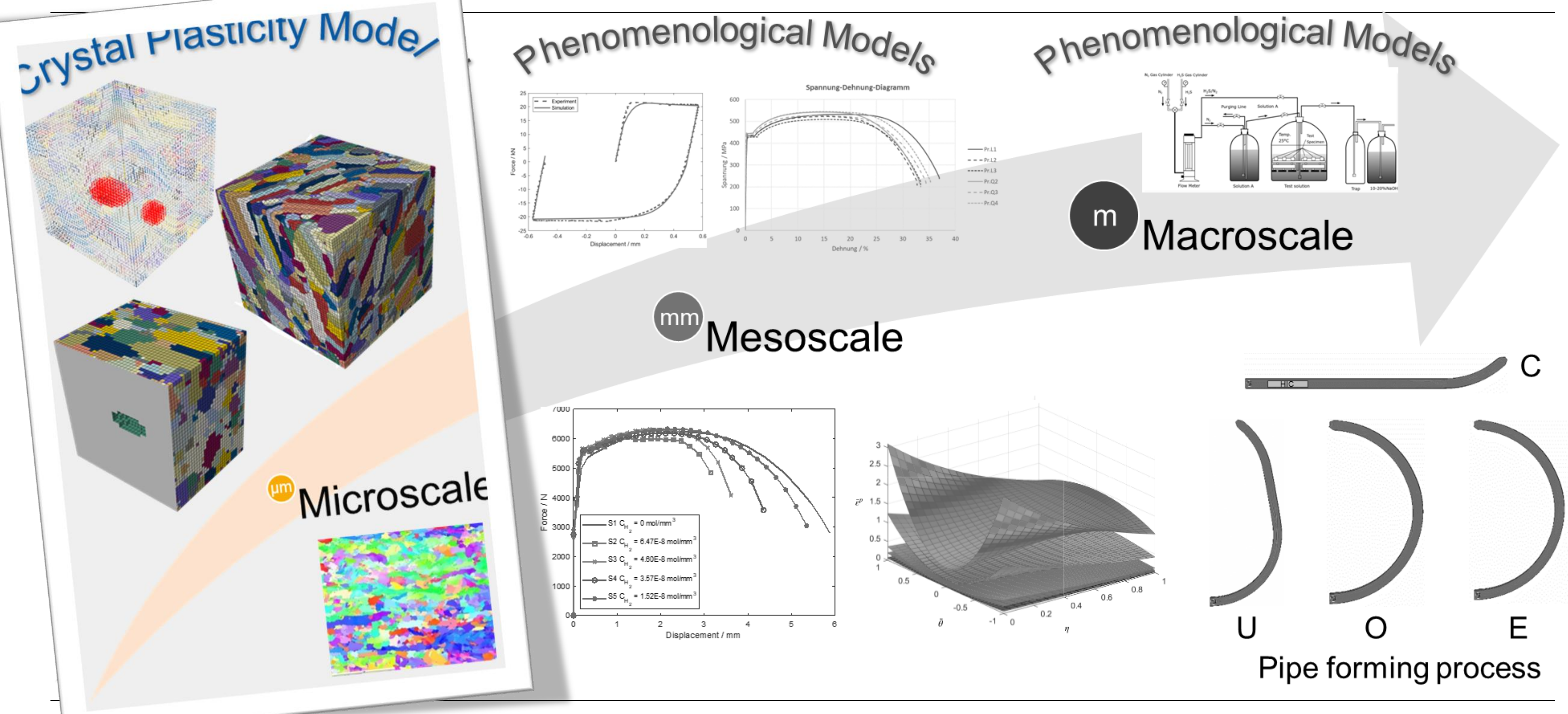
Convergence?

No

Yes

End Increment

Multi-scale description of the HIC resistance



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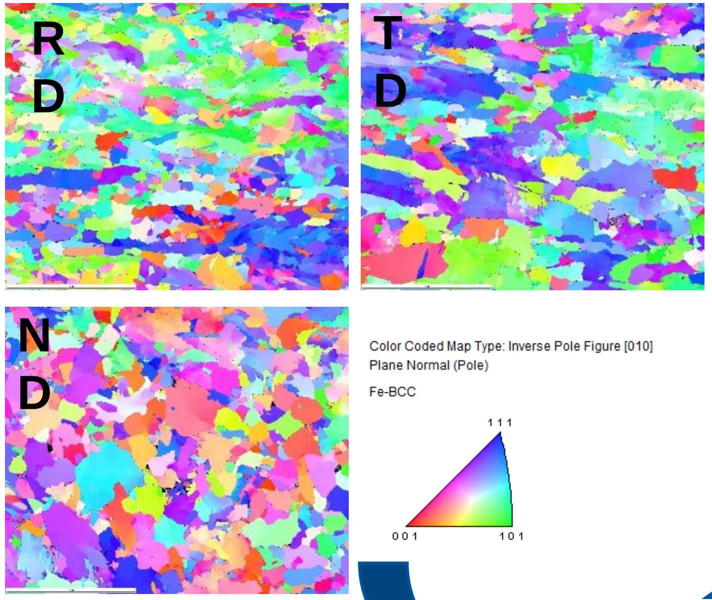
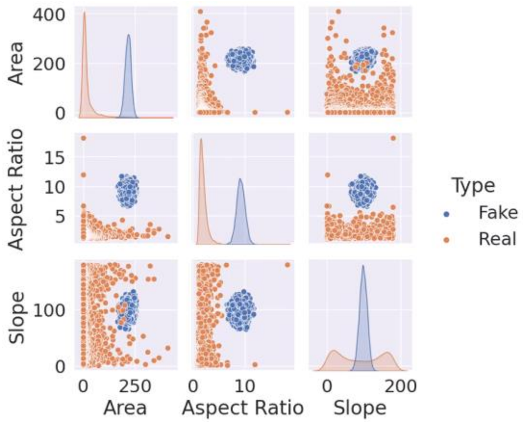
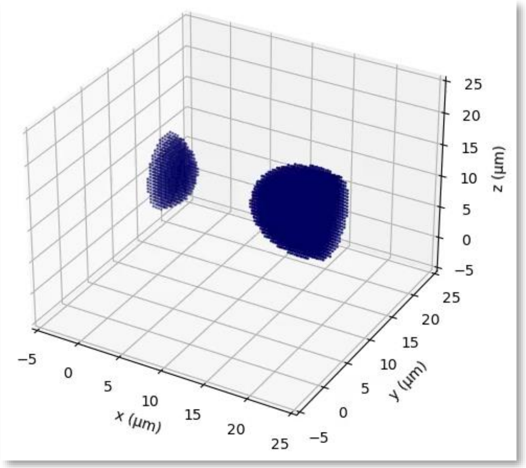
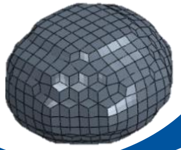
RVE Generation via DRAGen (in-house open-source software)









Microstructural measurements
- ➢ LOM
- ➢ SEM
- ➢ EBSD

Statistical analysis
- ➢ Grain size
- ➢ Aspect ratio
- ➢ Misorientation angle
- ➢ …

Grain placement & Volume filling
- ➢ Discrete Packing-Algorithm (RSA)
- ➢ Discrete Tessellation (Voronoi)
- ➢ Assignment of crystallographic orientation

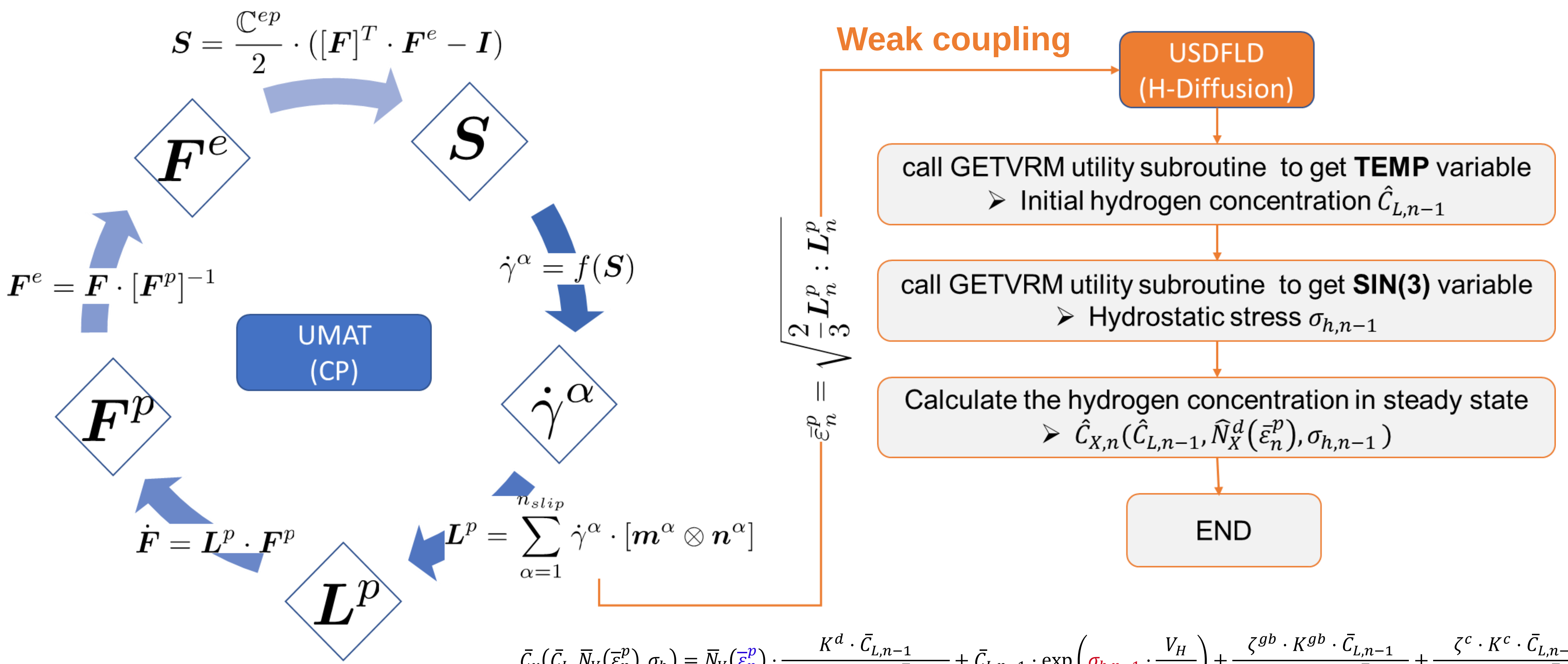
Generation of substructures
- ➢ Packets
- ➢ Blocks
- ➢ Assignment of Block orientation

Generation of inclusions
- ➢ Al_2O_3
- ➢ MnS
- ➢ MgO
- ➢ CaO

Generation of voids

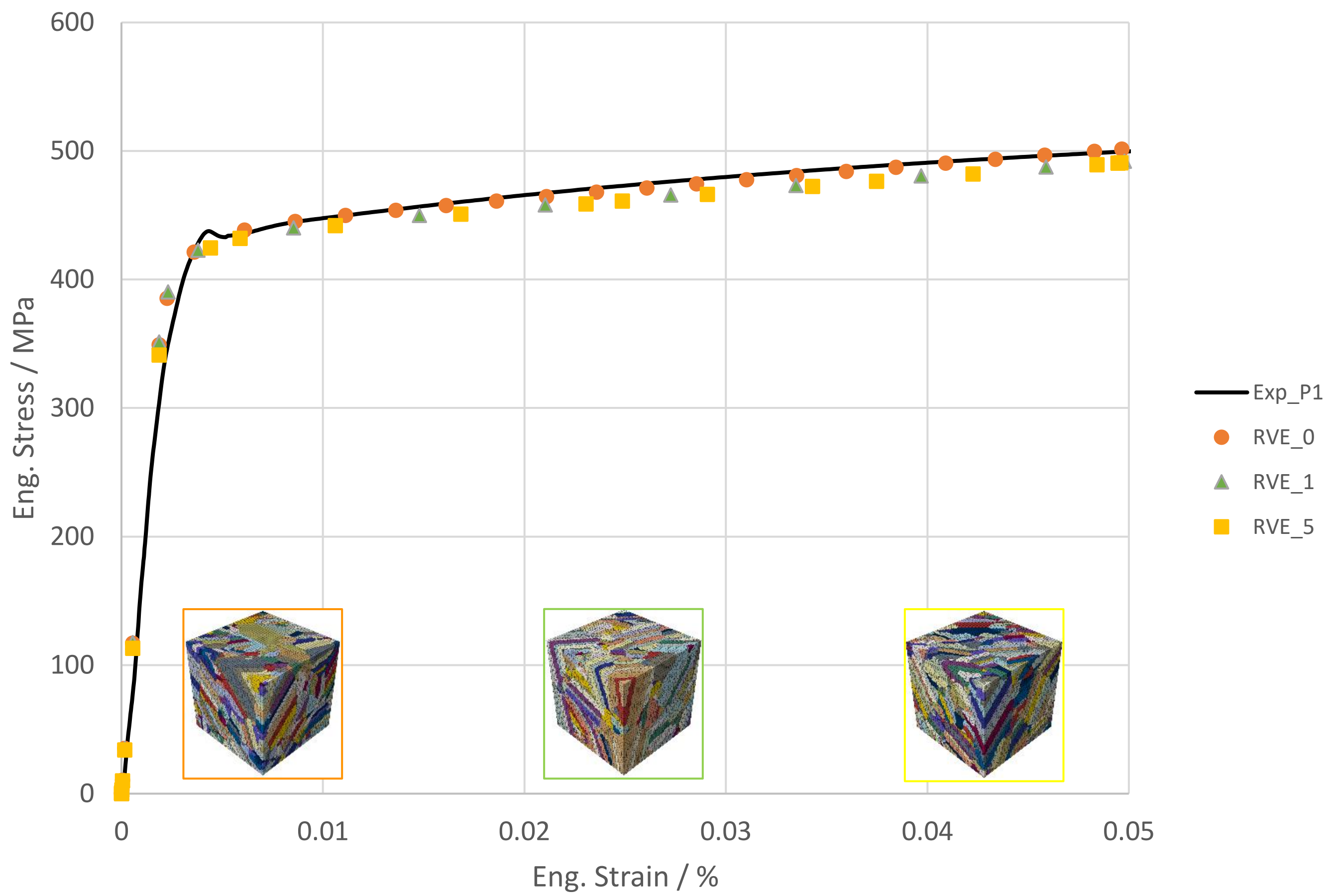
Finite-Element-Model
- ➢ Creation of the geometry
- ➢ Meshing the geometry

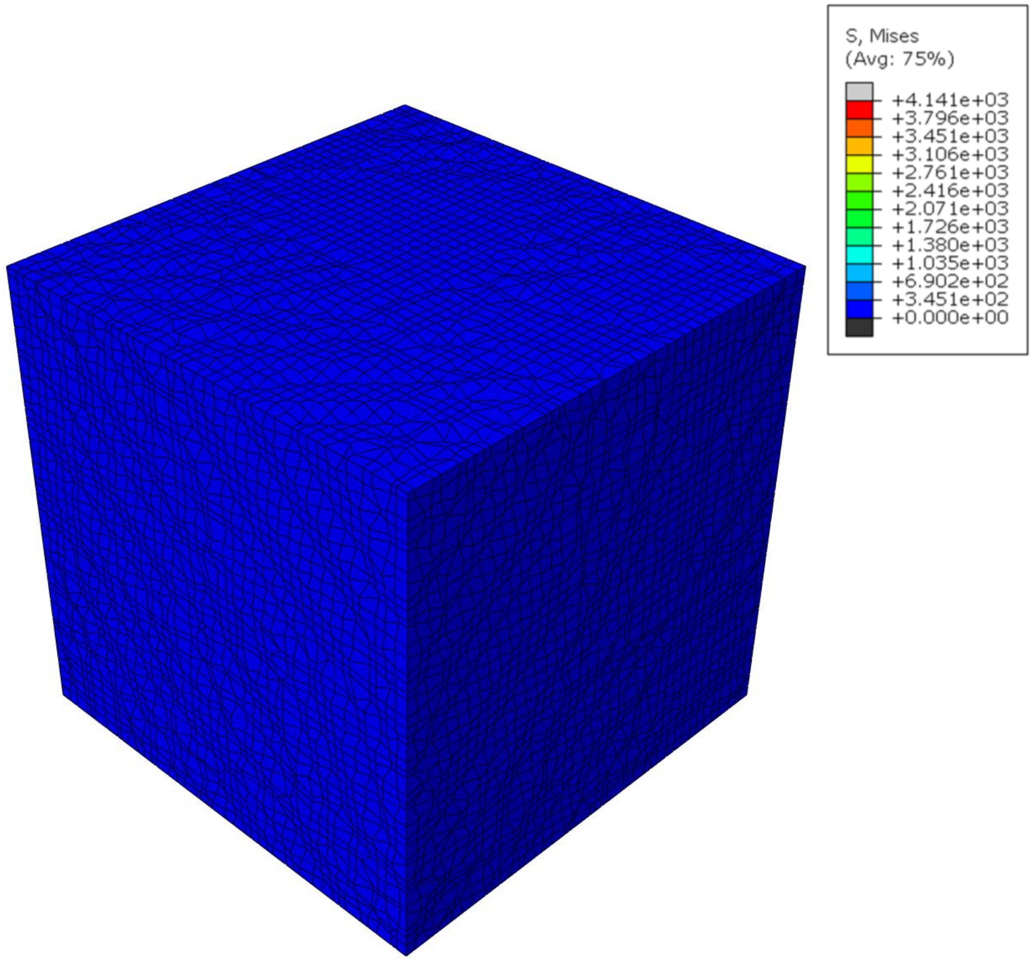
Weak coupling of crystal plasticity (CP) model with hydrogen transport



$$\bar{C}_x(\bar{C}_L,\bar{N}_V(\bar{\varepsilon}_n^p),\sigma_h) = \underbrace{\bar{N}_V(\bar{\varepsilon}_n^p)\cdot\frac{K^d\cdot\bar{C}_{L,n-1}}{\beta\cdot\bar{N}_L+K^d\cdot\bar{C}_{L,n-1}}}_{\text{plastic strain}} + \underbrace{\bar{C}_{L,n-1}\cdot\exp\left(\sigma_{h,n-1}\cdot\frac{V_H}{R\cdot T}\right)}_{\text{hydrostatic stress}} + \underbrace{\frac{\zeta^{gb}\cdot K^{gb}\cdot\bar{C}_{L,n-1}}{\beta\cdot\bar{N}_L+K^{gb}\cdot\bar{C}_{L,n-1}}}_{\text{grain boundary}} + \underbrace{\frac{\zeta^{c}\cdot K^{c}\cdot\bar{C}_{L,n-1}}{\beta\cdot\bar{N}_L+K^{c}\cdot\bar{C}_{L,n-1}}}_{\text{carbide}}$$

Calibration of crystal plasticity model with a uniaxial tensile test





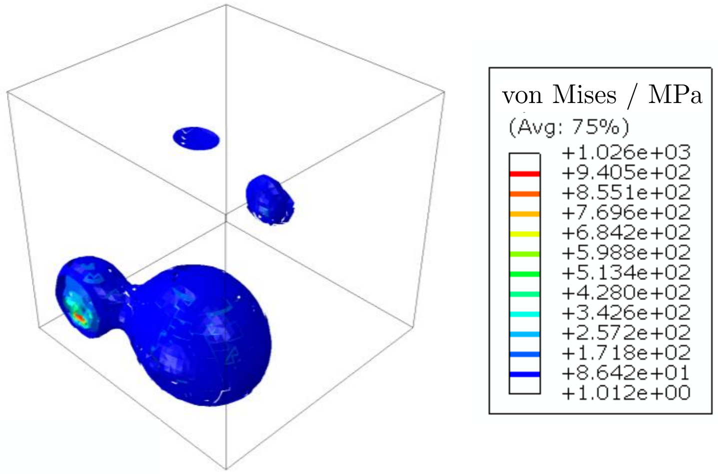
$$\bar{\sigma}_{RVE} = \sum_{i}^{grains} \bar{\sigma}^{i}_{22,grain} \cdot \frac{V^{i}_{grain}}{V_{RVE}} \quad ; \; \bar{\varepsilon}_{RVE} = \sum_{i}^{grains} \bar{\varepsilon}^{i}_{22,grain} \cdot \frac{V^{i}_{grain}}{V_{RVE}}$$

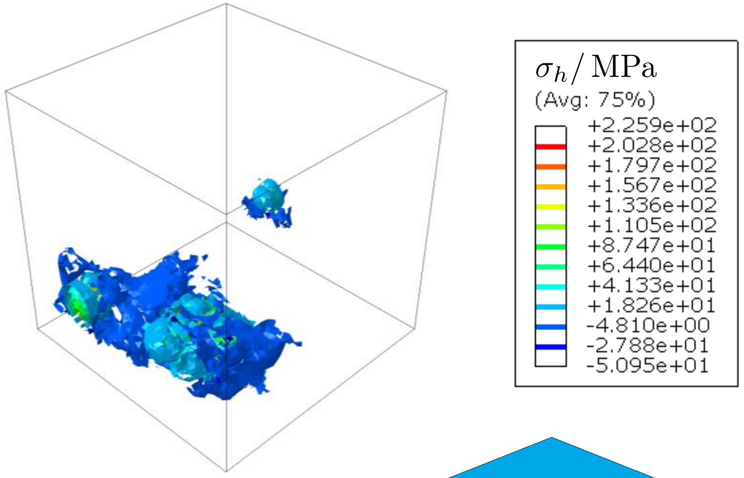
RVE edge length: 30 µm

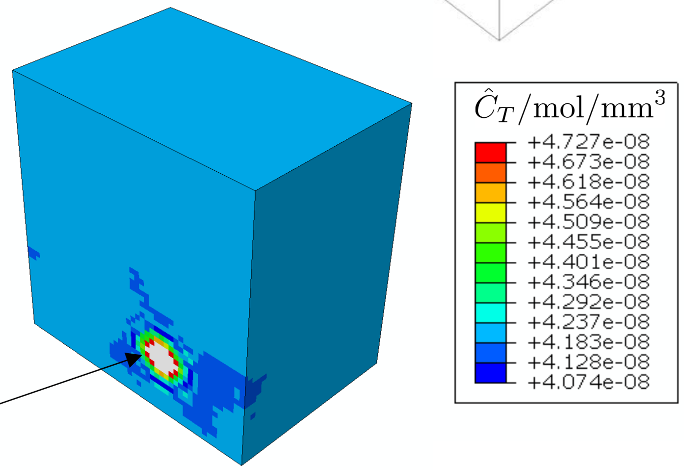
Periodic boundary conditions

Influence of non-metallic inclusions on local hydrogen concentration
Thermally-induced residual stresses

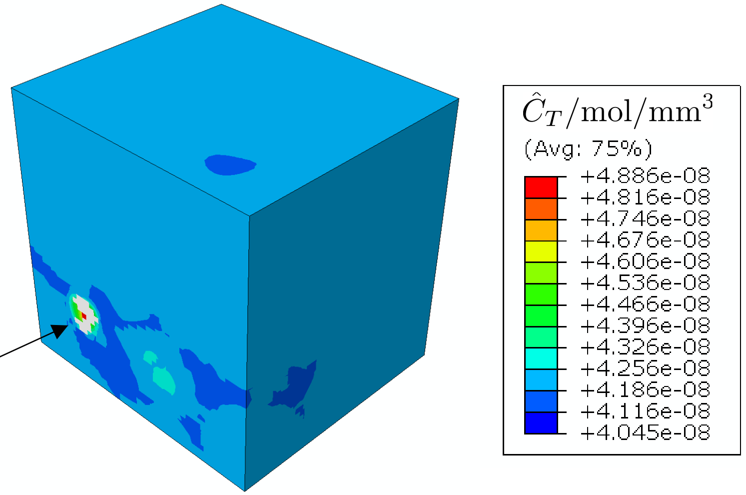
Step 1: Cooling (723°C-20°C) → Step 2: Model duplication → Step 3: Stress state assignment → Step 4: Hydrogen loading → Step 5: Hydrogen diffusion







Non-metallic inclusion



Non-metallic inclusion

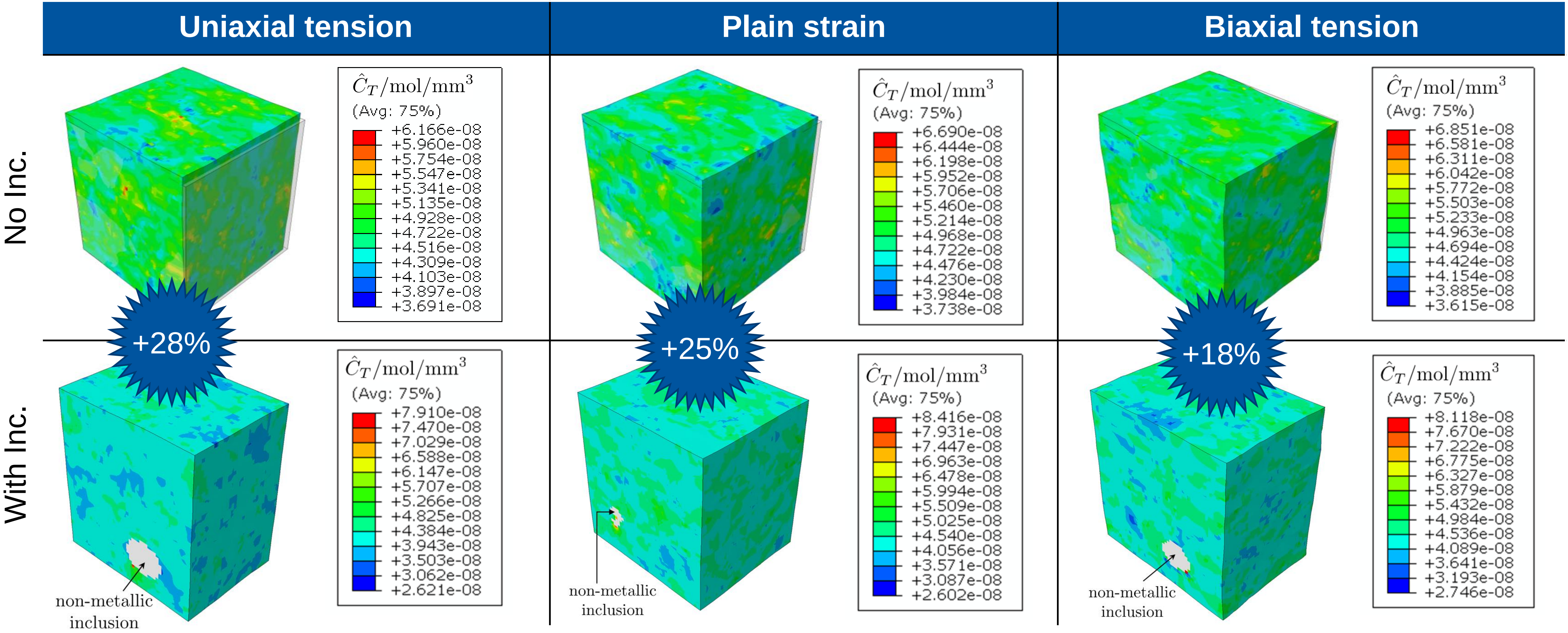
Initial hydrogen concentration: $3.57 \cdot 10^{-8}$ mol/mm^3

A multiscale approach to characterize the HIC resistance of pipeline steels| Berk Tekkaya | Workshop Aalto | Chair of Material Modelling in Forming Technology, RWTH Aachen University | 03-04.09.2024

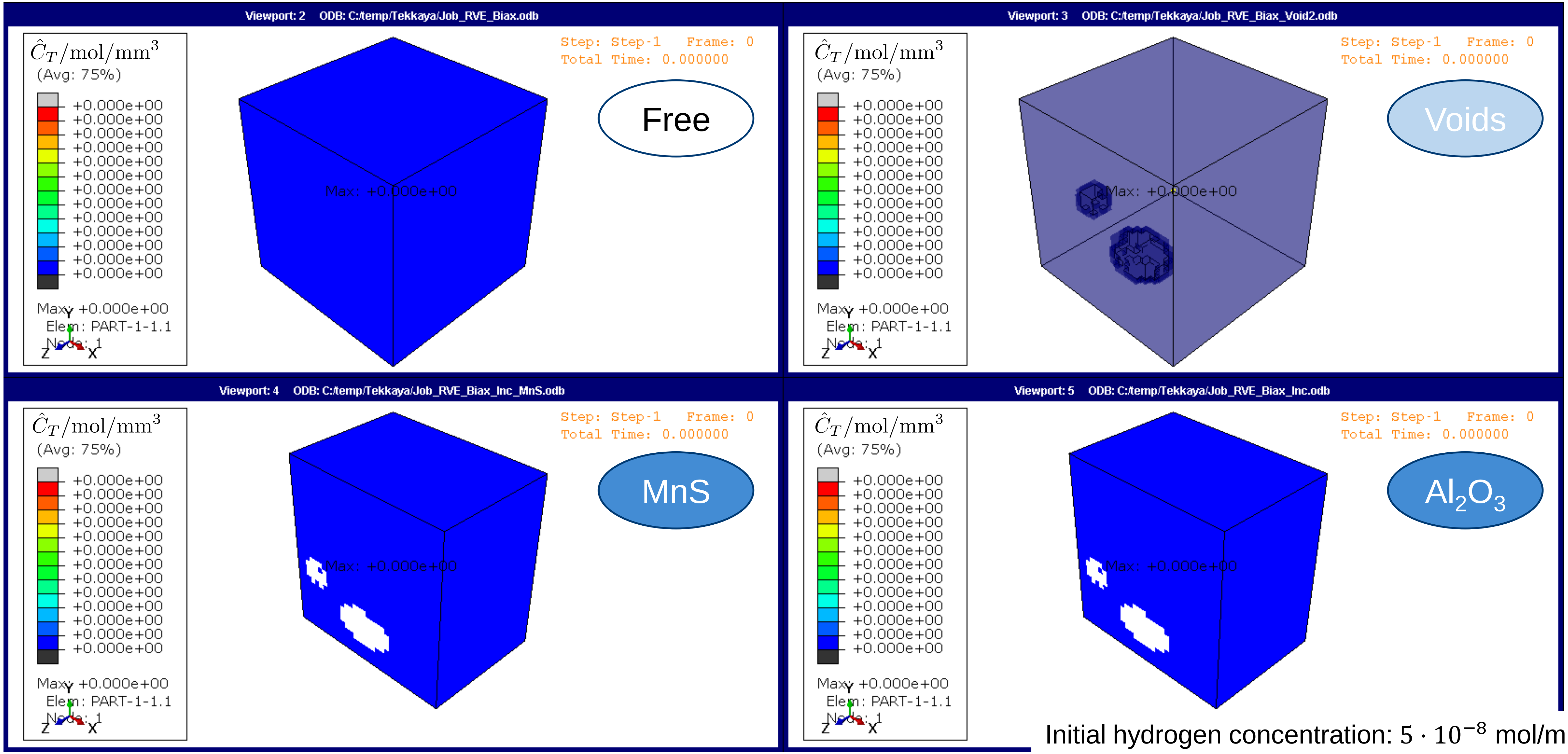
Influence of non-metallic inclusions on local hydrogen concentration
Mechanical loading

Initial hydrogen concentration: $3.57 \cdot 10^{-8}$ mol/mm^3

Step 1: Mechanical loading | Step 2: Hydrogen loading | Step 3: Hydrogen diffusion

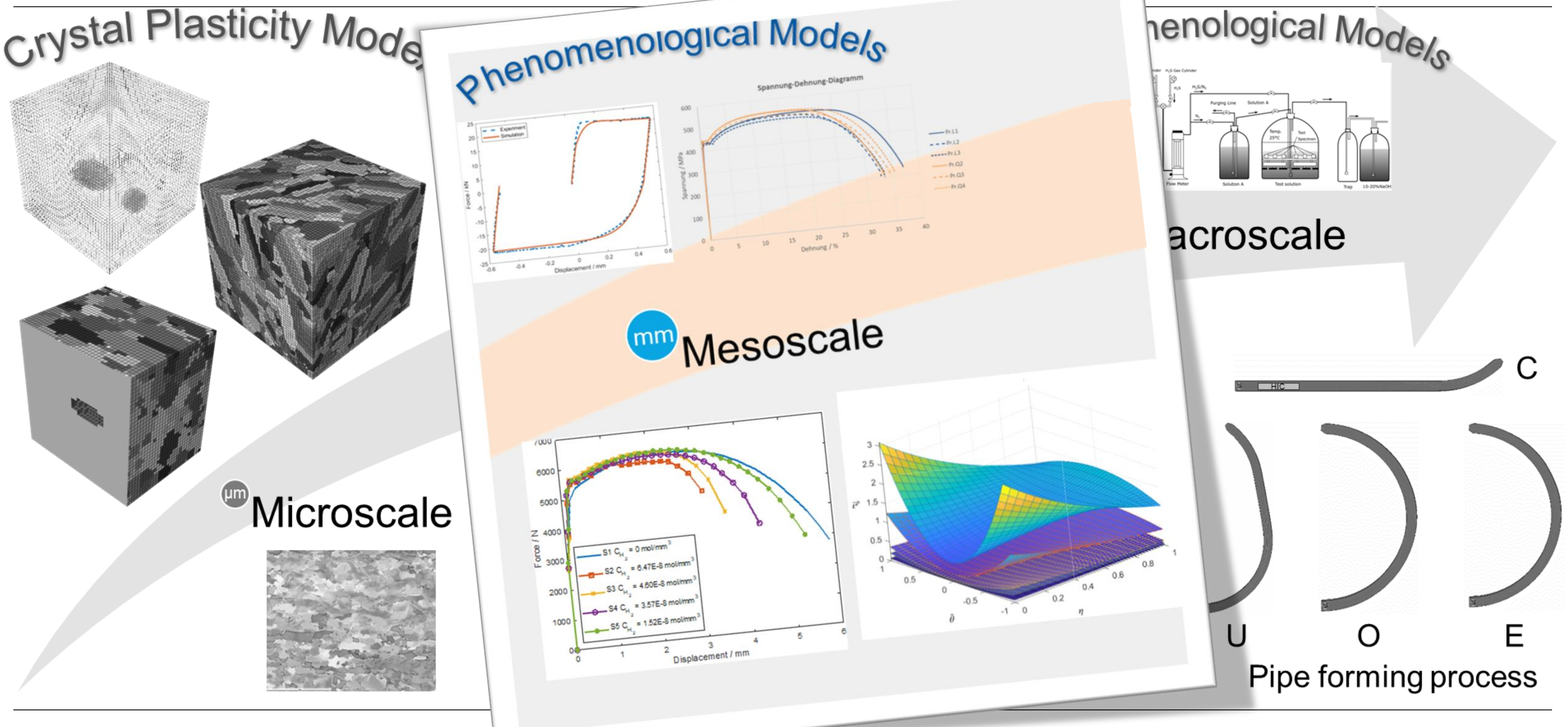


General influence of voids, soft and hard non-metallic inclusions on local hydrogen concentration under *idealized* biaxial tension



Initial hydrogen concentration: $5 \cdot 10^{-8}$ mol/mm³

Multi-scale description of the HIC resistance



Material modeling:
Coupled damage model: Modified-Bai-Wierzbicki-Model (MBW)

- **Coupled damage:**

$$\phi^{MBW} = \sigma_{vM} - \left(1 - D(\eta, \bar{\theta}, C_{H^+})\right) \cdot \sigma_Y(\bar{\varepsilon}_p) \cdot f(\eta) \cdot f(\bar{\theta}) \cdot f(C_{H^+}) \leq 0$$

- **(Ductile) damage initiation:**

$$\bar{\varepsilon}_{ddi} = \left[\left(D_1^{ddi} \cdot e^{-D_2^{ddi} \cdot \eta_{avg}} - D_3^{ddi} \cdot e^{-D_4^{ddi} \cdot \eta_{avg}}\right) \bar{\theta}_{avg}^2 + D_3^{ddi} \cdot e^{-D_4^{ddi} \cdot \eta_{avg}}\right] \cdot f_{ddi}(C_{H^+})$$

$$I_{ddi} = I_{ddi} + \frac{\Delta\bar{\varepsilon}_p}{\bar{\varepsilon}_{ddi}(\eta_{avg}, \bar{\theta}_{avg}, C_{H^+})}$$

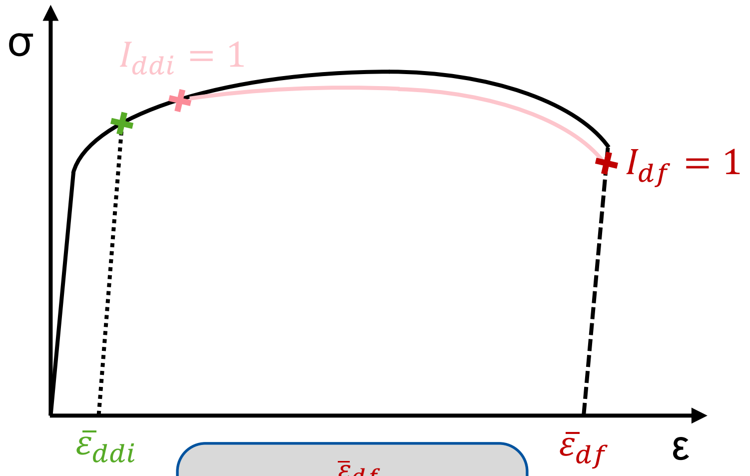
- **(Ductile) fracture:**

$$\bar{\varepsilon}_{df} = \left[\left(D_1^{df} \cdot e^{-D_2^{df} \cdot \eta_{avg}} - D_3^{df} \cdot e^{-D_4^{df} \cdot \eta_{avg}}\right) \bar{\theta}_{avg}^2 + D_3^{df} \cdot e^{-D_4^{df} \cdot \eta_{avg}}\right] \cdot f_{df}(C_{H^+})$$

$$I_{df} = I_{df} + \frac{\Delta\bar{\varepsilon}_p}{\bar{\varepsilon}_{df}(\eta_{avg}, \bar{\theta}_{avg}, C_{H^+})}$$

- **Damage evolution law:**

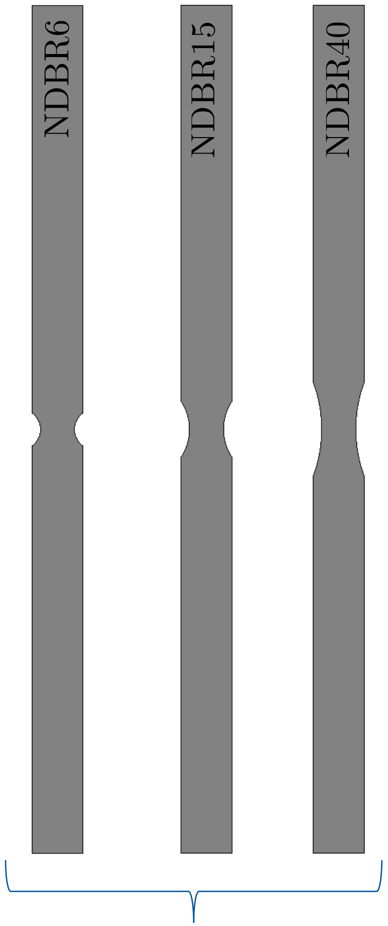
$$D = D + D_{cr} \cdot \frac{\Delta\bar{\varepsilon}_p}{\bar{\varepsilon}_{df}(\eta_{avg}, \bar{\theta}_{avg}, C_{H^+})}$$



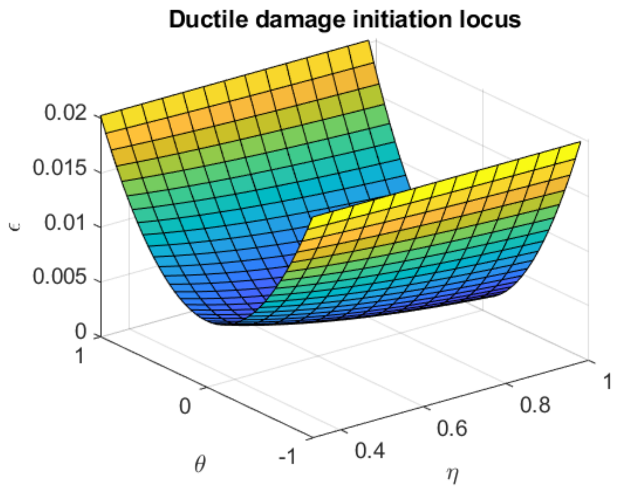
$$D_{cr} = \int_{\bar{\varepsilon}_{ddi}}^{\bar{\varepsilon}_{df}} \frac{\sigma_{y0}}{G_f} d\bar{\varepsilon}$$

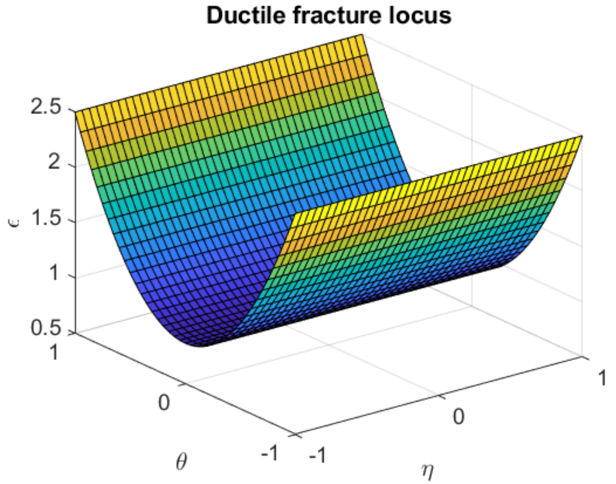
$$D(\bar{\varepsilon}_p, \eta, \bar{\theta}, C_{H^+}) = \begin{cases} \text{update } I_{ddi}, I_{ddi} < 1 \bigwedge \eta > -\frac{1}{3} \\ \text{update } I_{df}, I_{ddi} \geq 1 \bigwedge \eta > -\frac{1}{3} \\ \text{update } D, I_{df} < 1 \bigwedge \eta > -\frac{1}{3} \\ D = 1, I_{df} \geq 1 \bigwedge \eta > -\frac{1}{3} \end{cases}$$

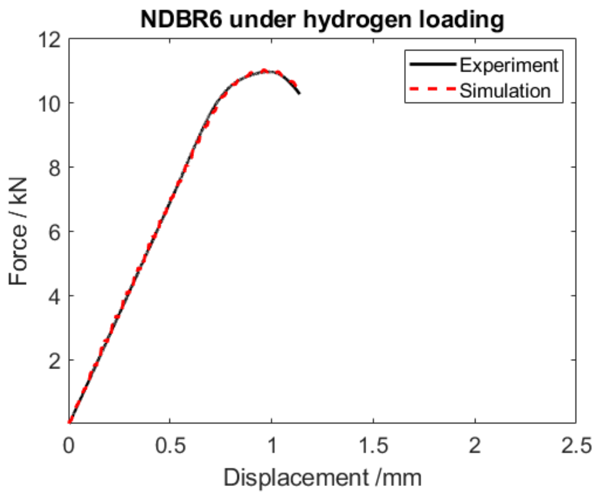
Model calibration for CP1000 based on in-situ SSRT @Aalto

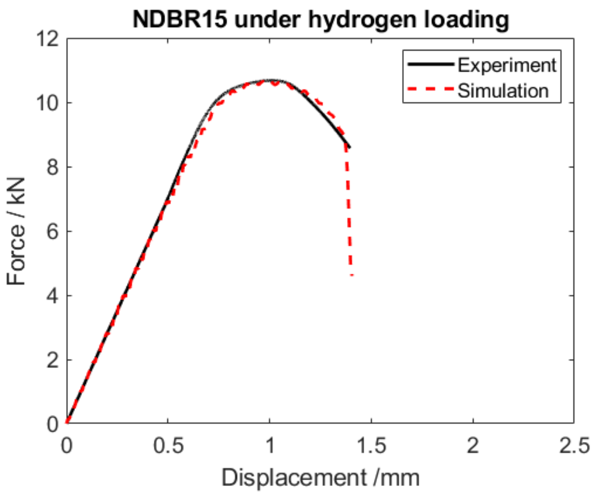


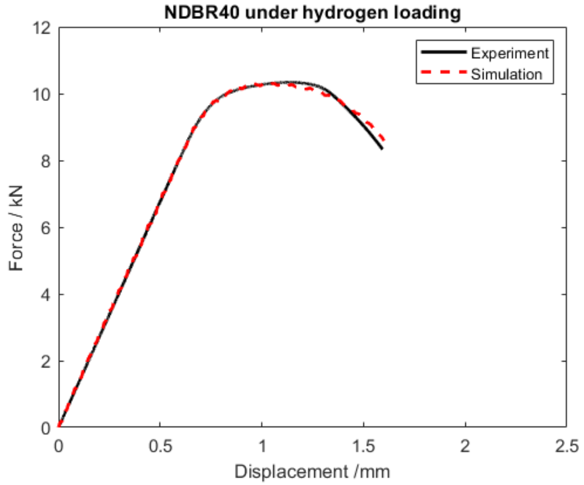
Pre-charged
up to saturation

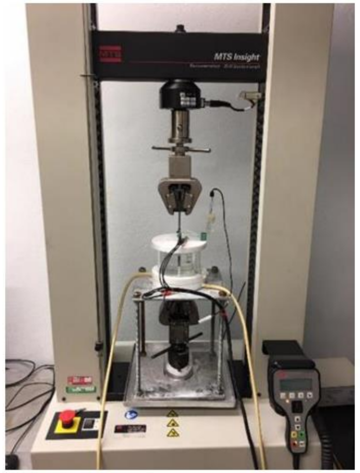




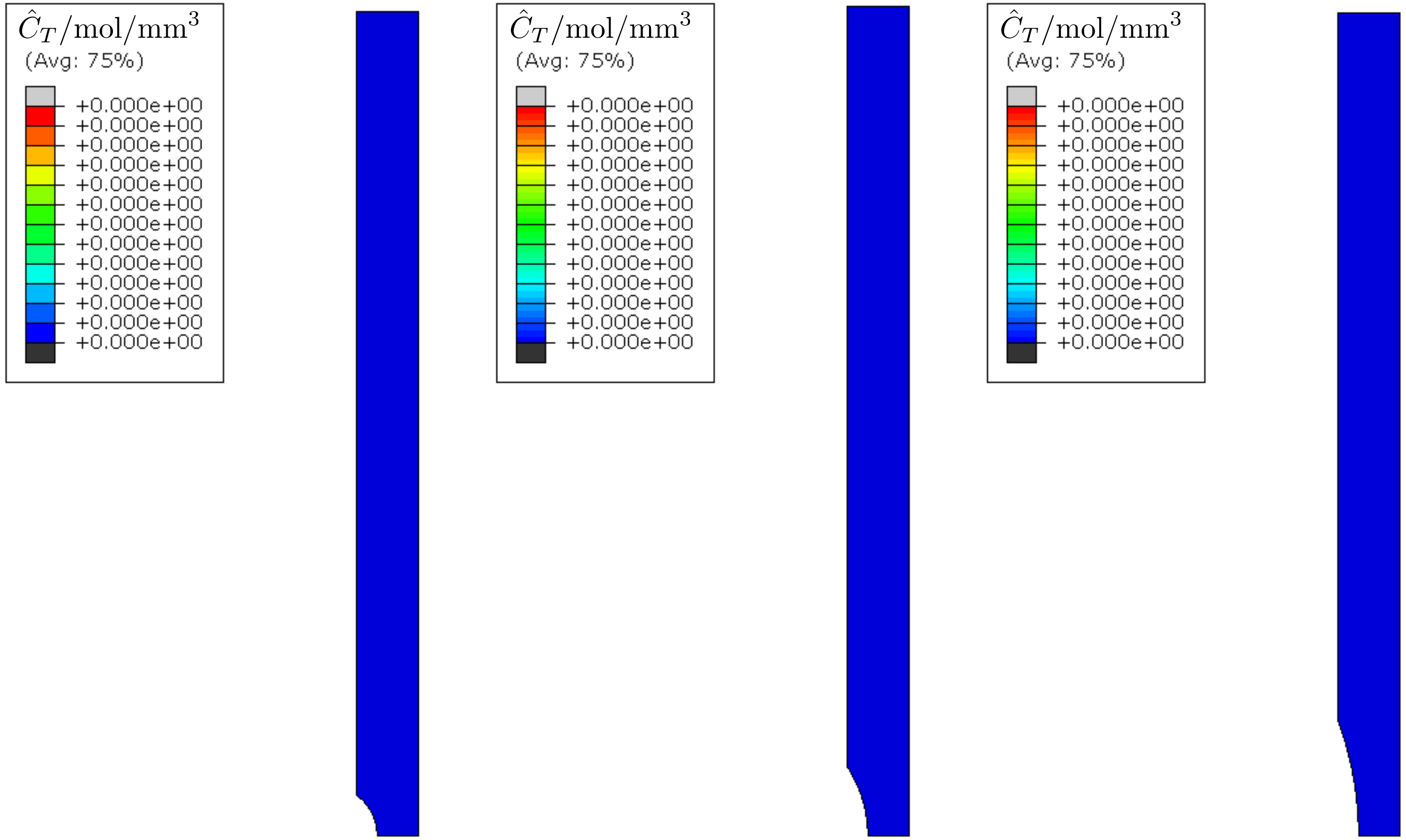




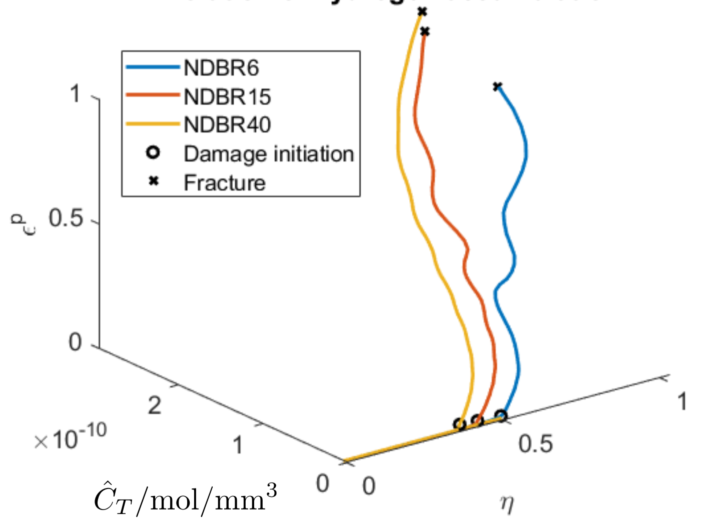


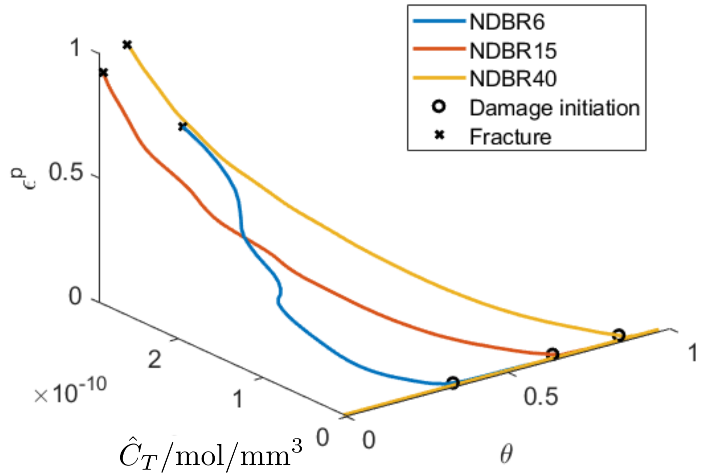


Hydrogen-induced damage modelling on mesoscale under in-situ SSRT conditions



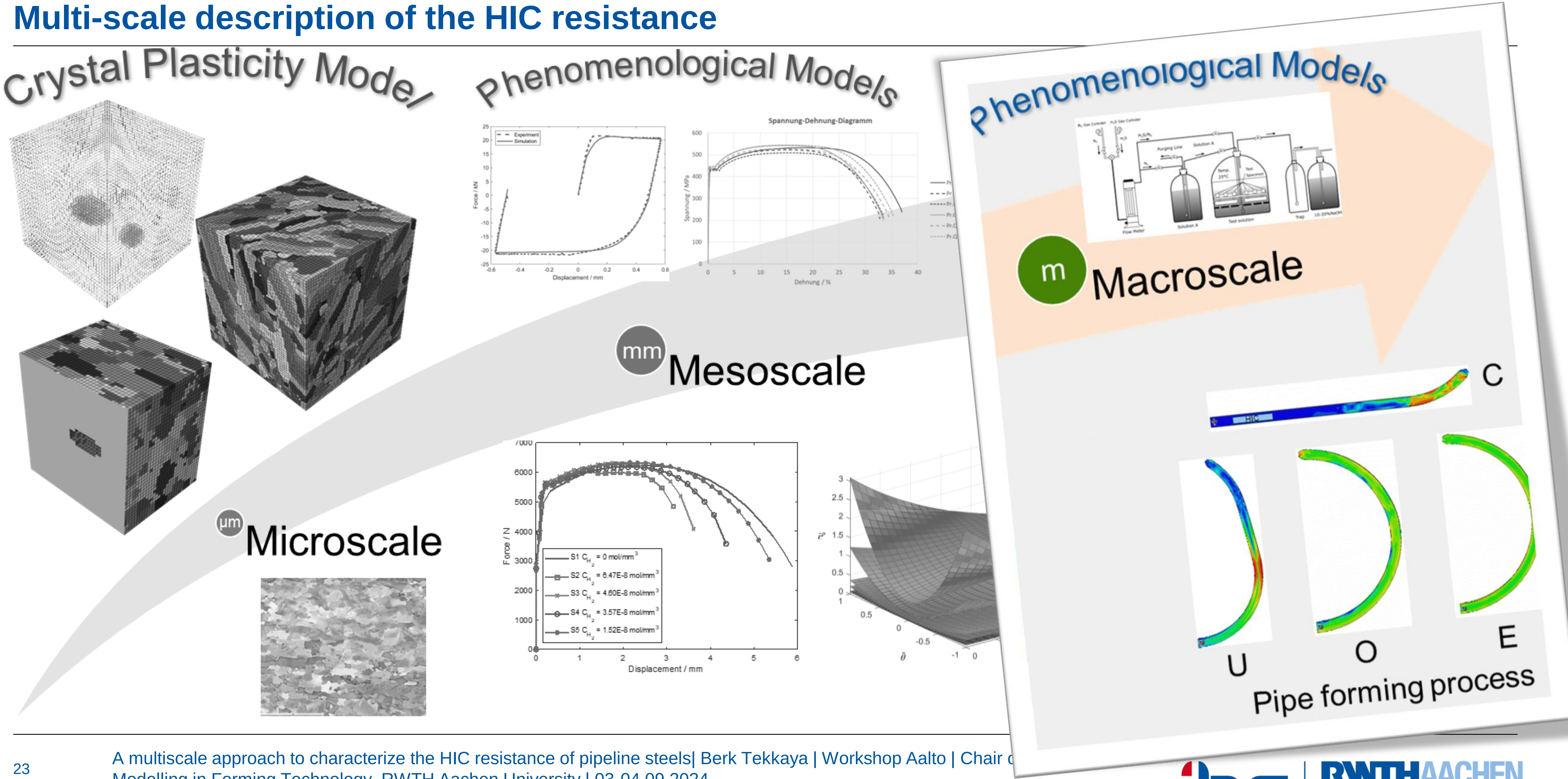
Evolution of hydrogen accumulation





Element type: C3D8RT   Mesh size: 0.1 mm

Multi-scale description of the HIC resistance



Implicit material model for coupled isotropic-kinematic hardening

- **Yield function:**

$$\phi = \left\|\boldsymbol{\sigma}^{dev} - \boldsymbol{\alpha}\right\| - \sigma_y(\bar{\varepsilon}^p) \leq 0$$

- **Isotropic hardening:**

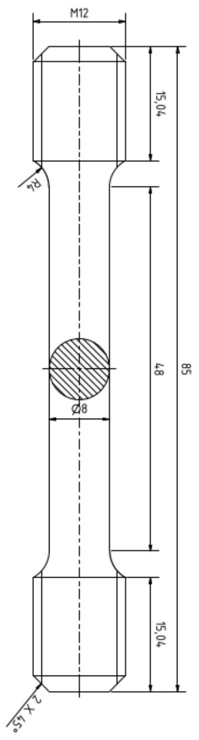
$$\sigma_y(\bar{\varepsilon}^p) = \sigma_{y0} + A\left[1 - \exp(-B\,\bar{\varepsilon}^p)\right]$$

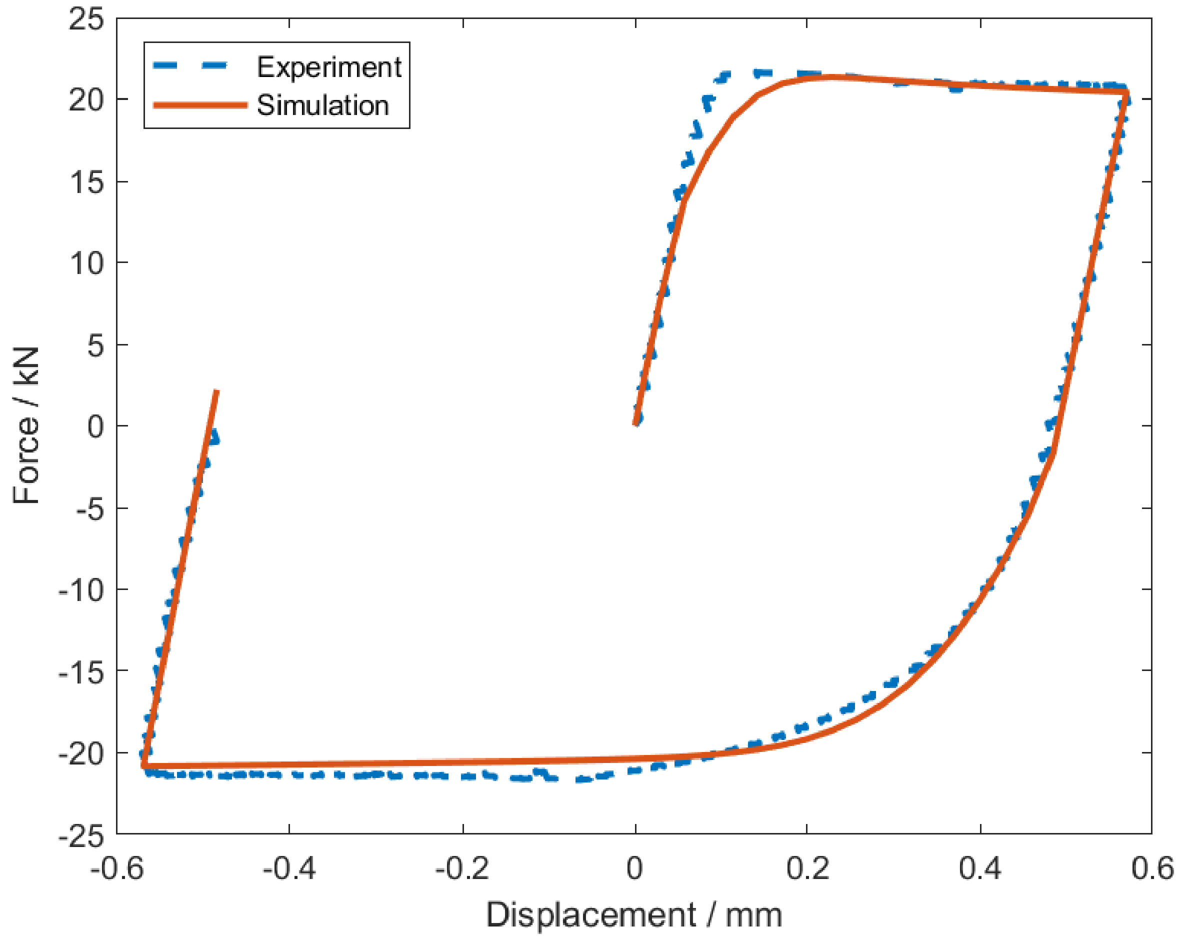
- **Evolution law for back stress**

$$\dot{\boldsymbol{\alpha}} = Q(\bar{\varepsilon}^p)\,\dot{\varepsilon}^p - \Omega\,\boldsymbol{\alpha}\,\dot{\bar{\varepsilon}}^p$$

$$Q(\bar{\varepsilon}^p) = Q_0 + Q_b\left[1 - \exp(-Q_c\,\bar{\varepsilon}^p)\right]$$

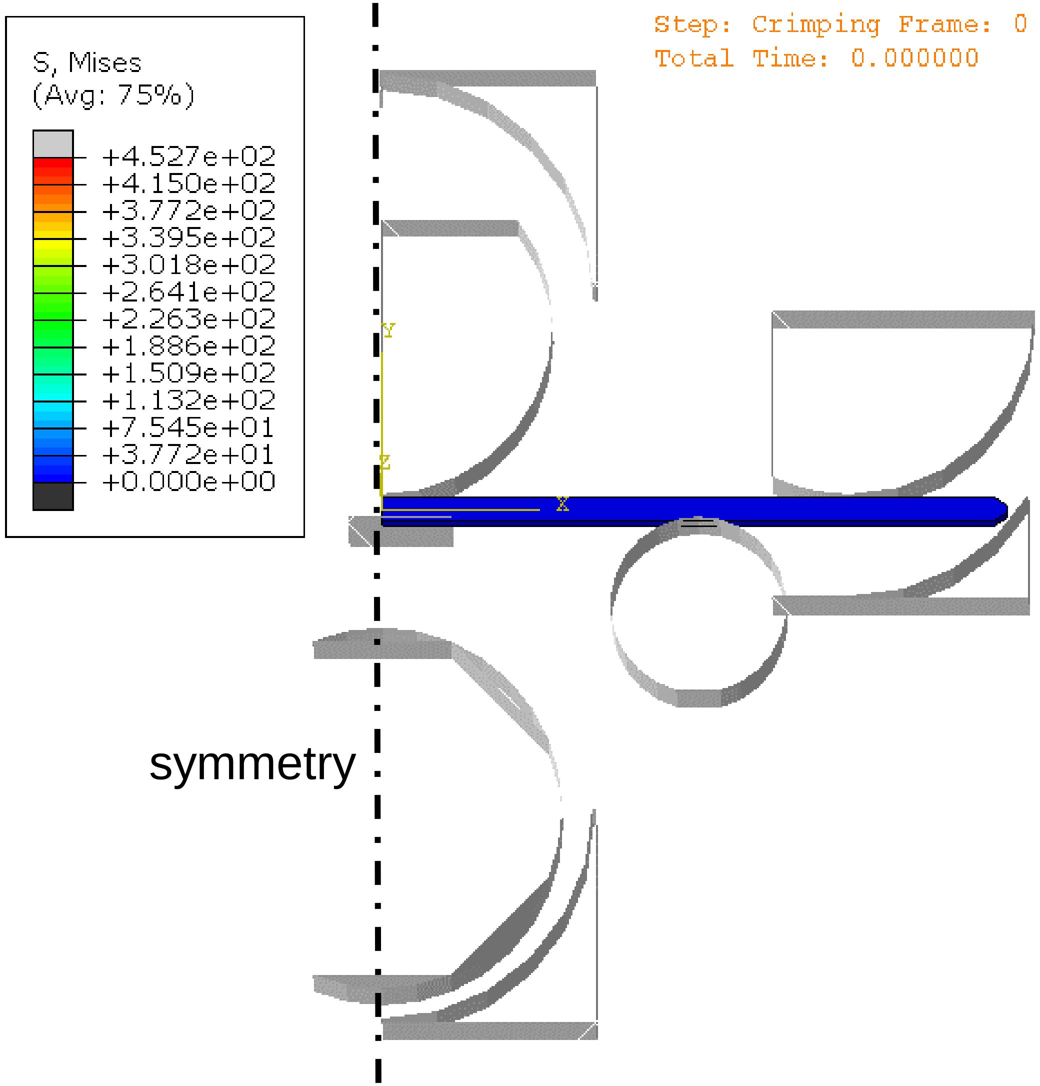
B8x40





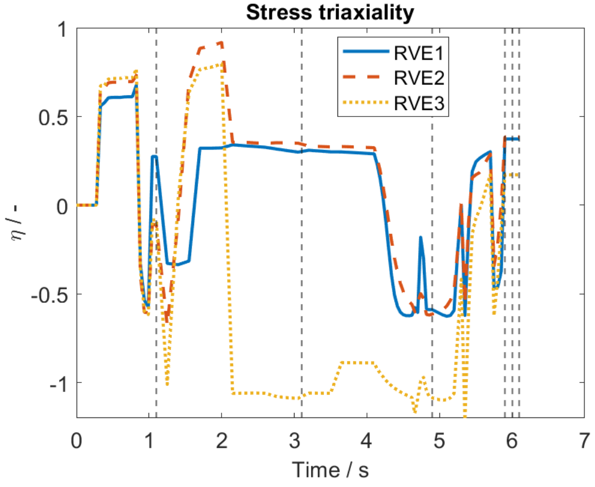
σ_y	A	B	Q_0	Q_b	Q_c	Ω
250 MPa	−30 MPa	70 MPa	190000 MPa	−65000 MPa	1000 MPa	500 MPa

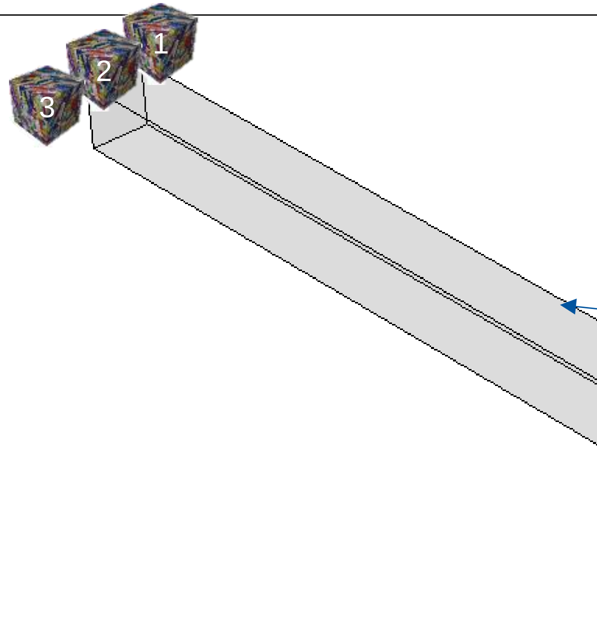
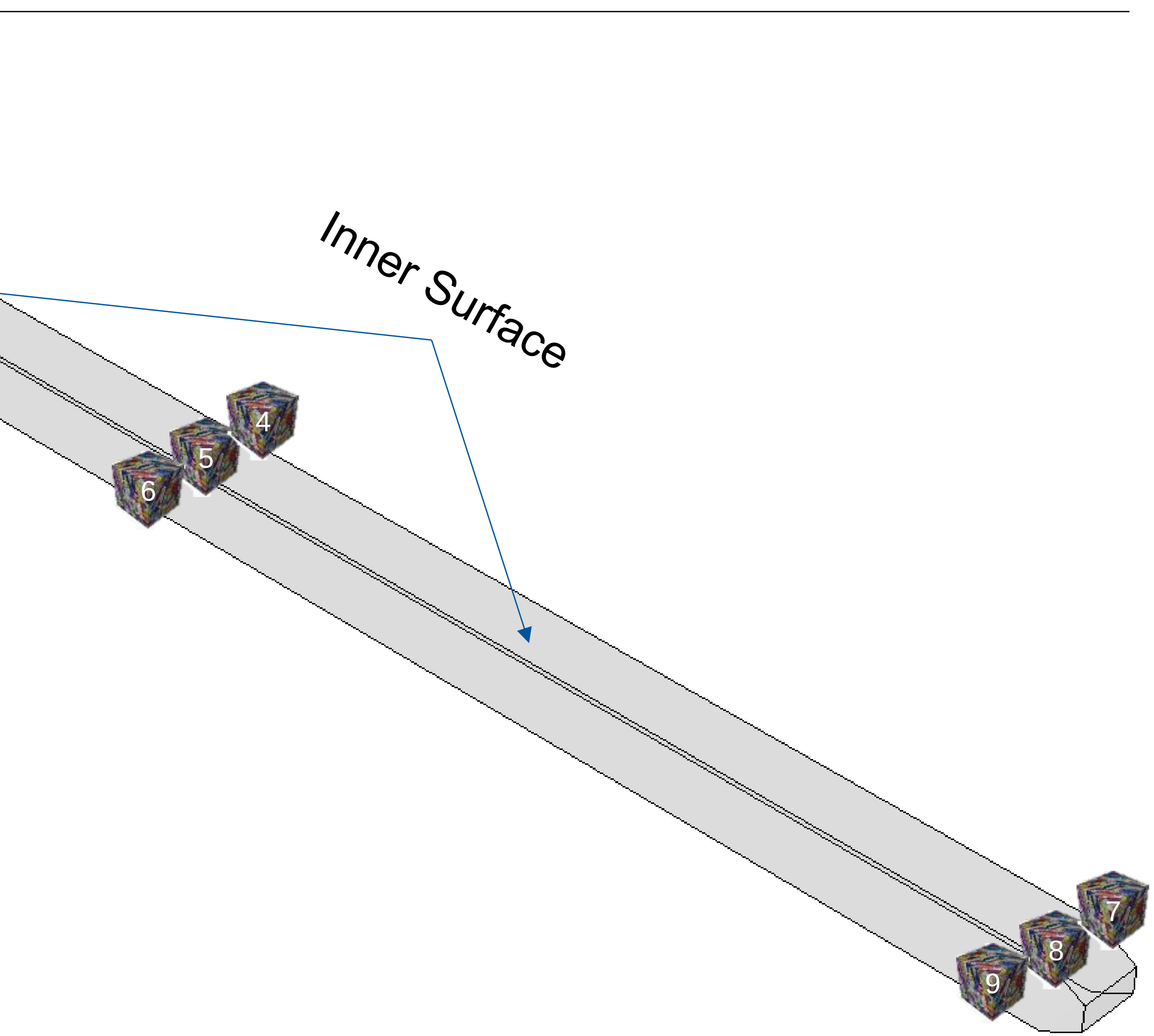
Step 1:
3D (C)UOE pipe forming simulation on macroscale

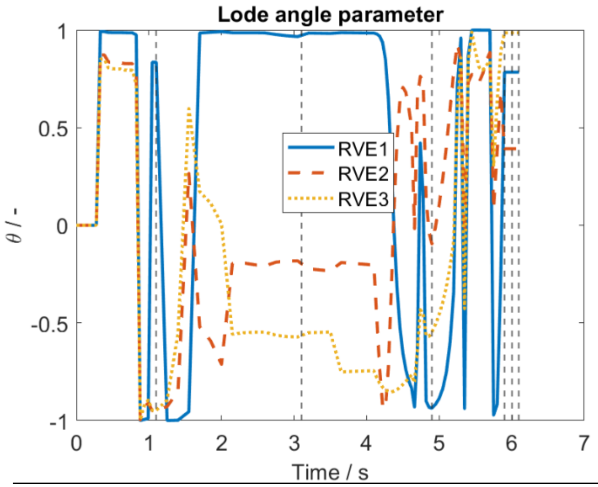


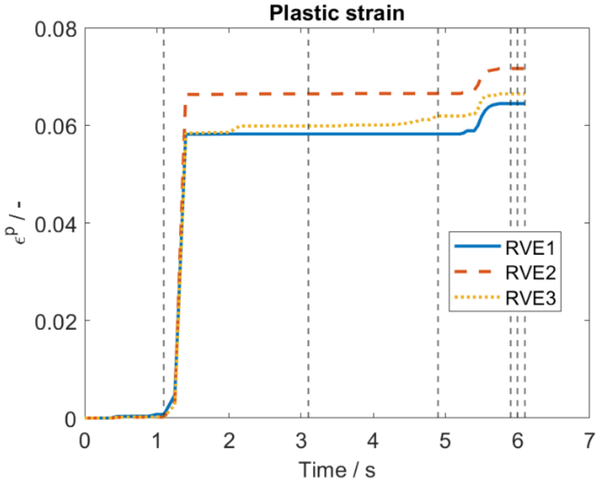
Step 2:
3D Pipe forming simulation on microscale via submodeling

C U O E

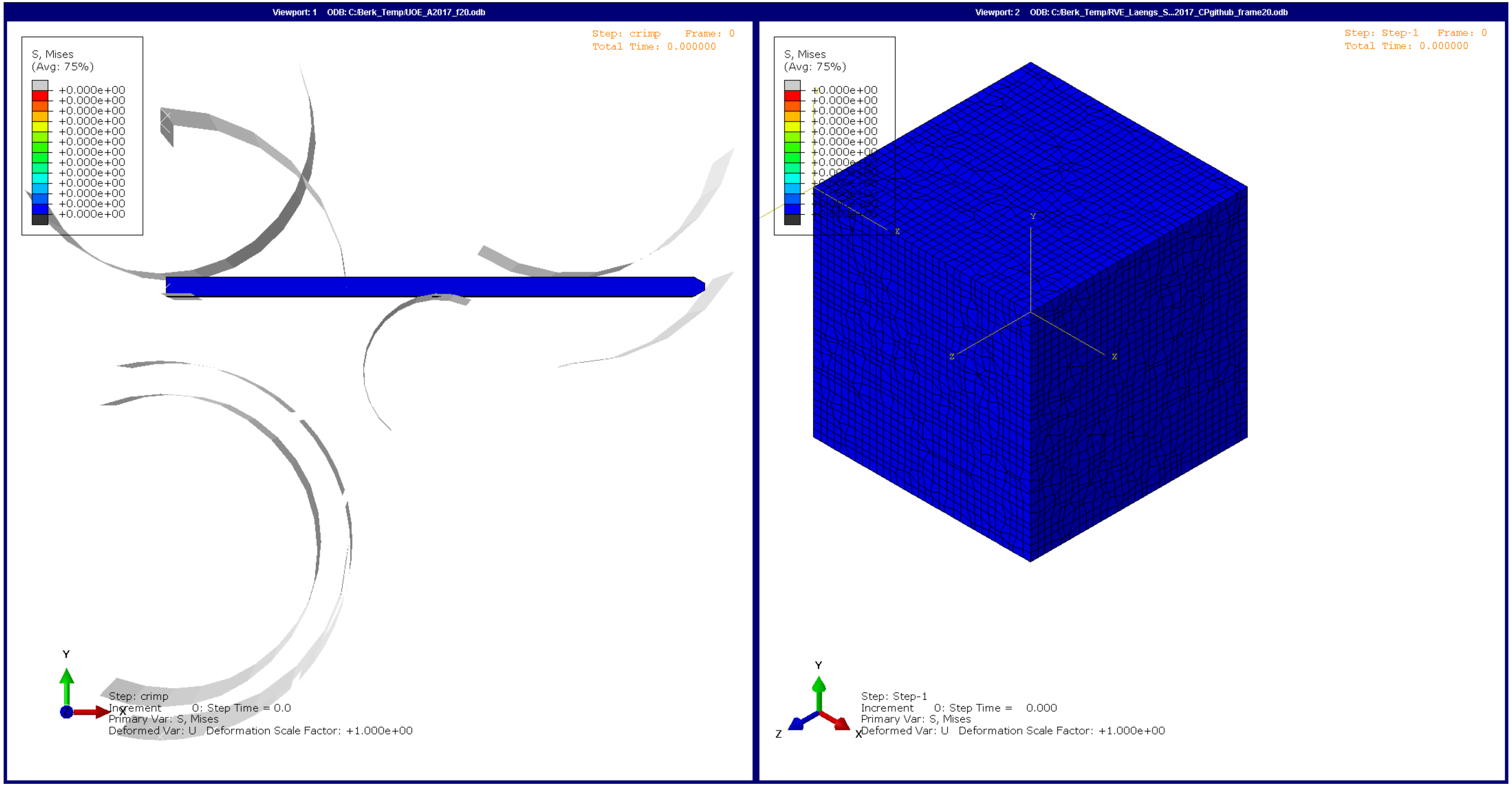




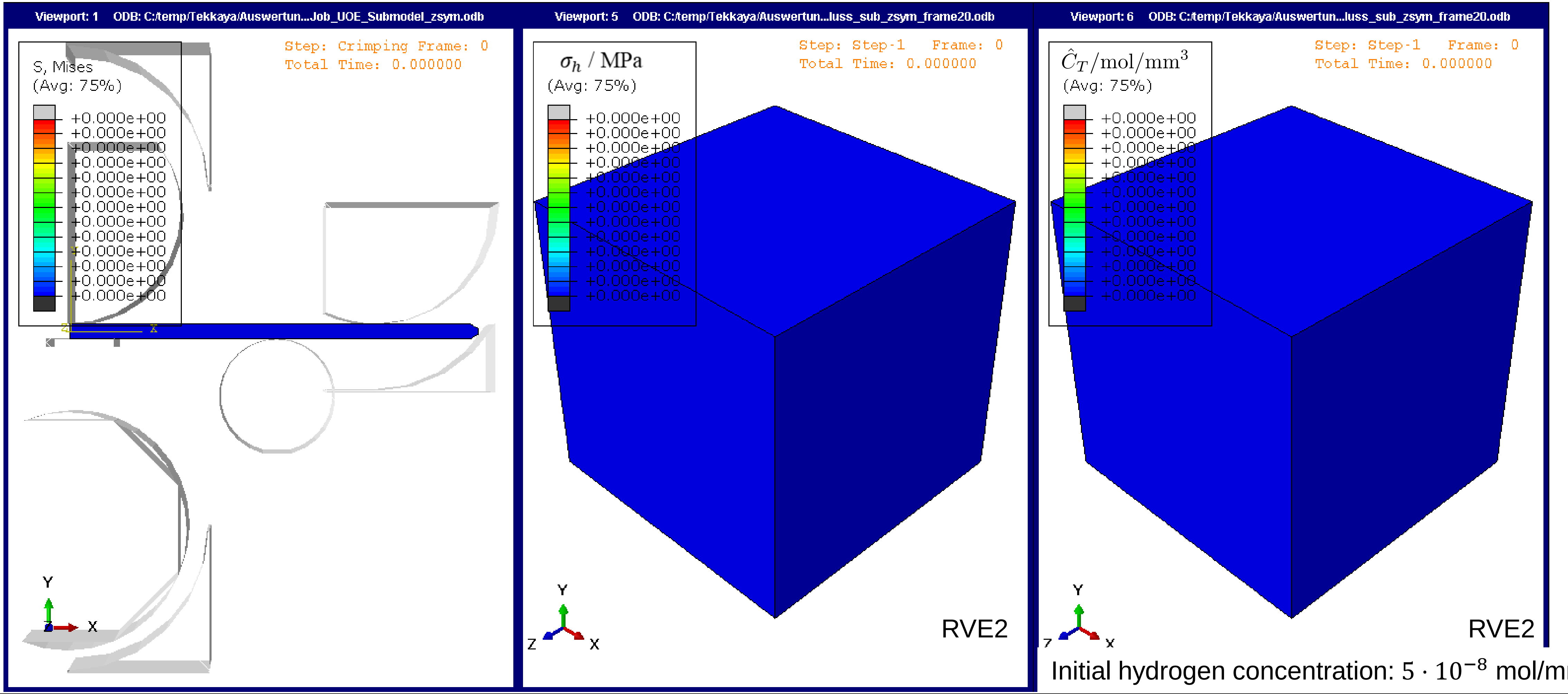


Step 2:
3D Pipe forming simulation on microscale via submodeling



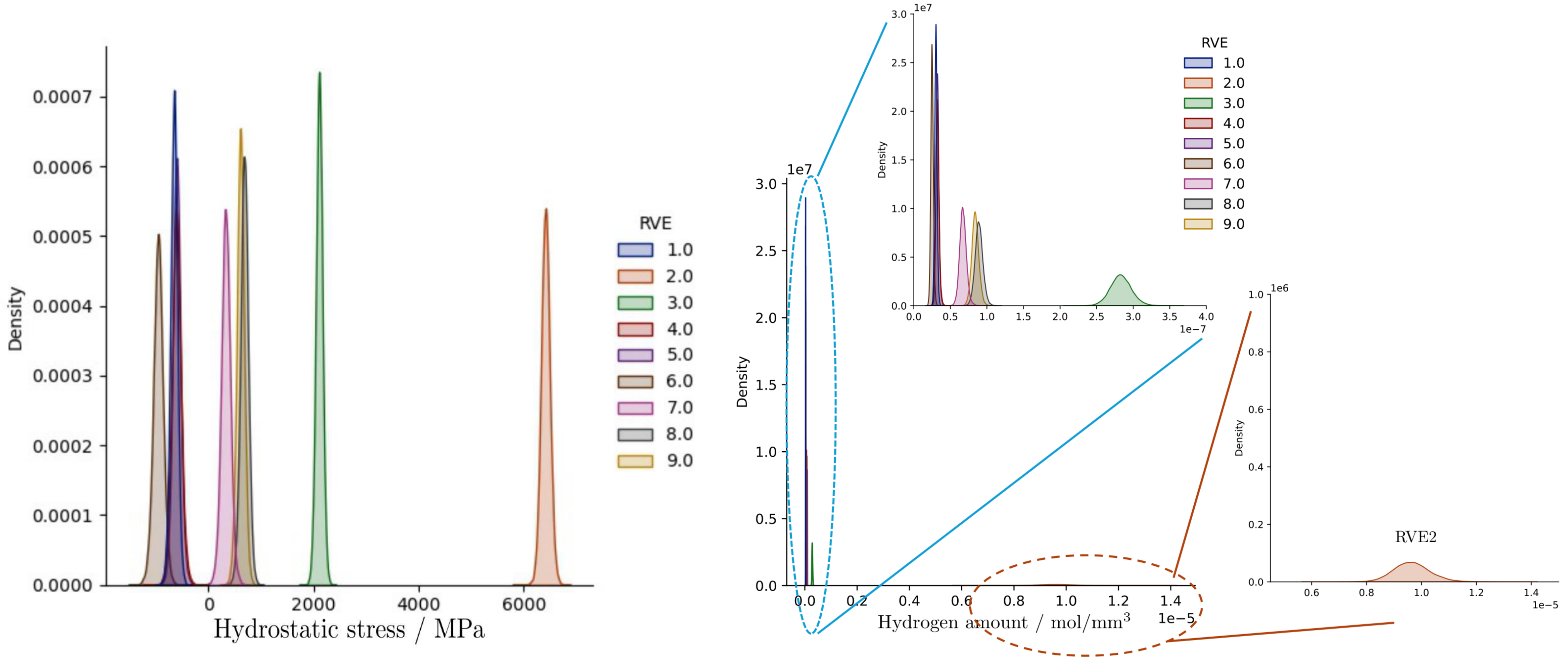
Step 3:
3D Pipe forming simulation on microscale with hydrogen diffusion via submodeling

C → U → O → E → Mechanical Unloading → H^+ Loading → Hydrogen Diffusion



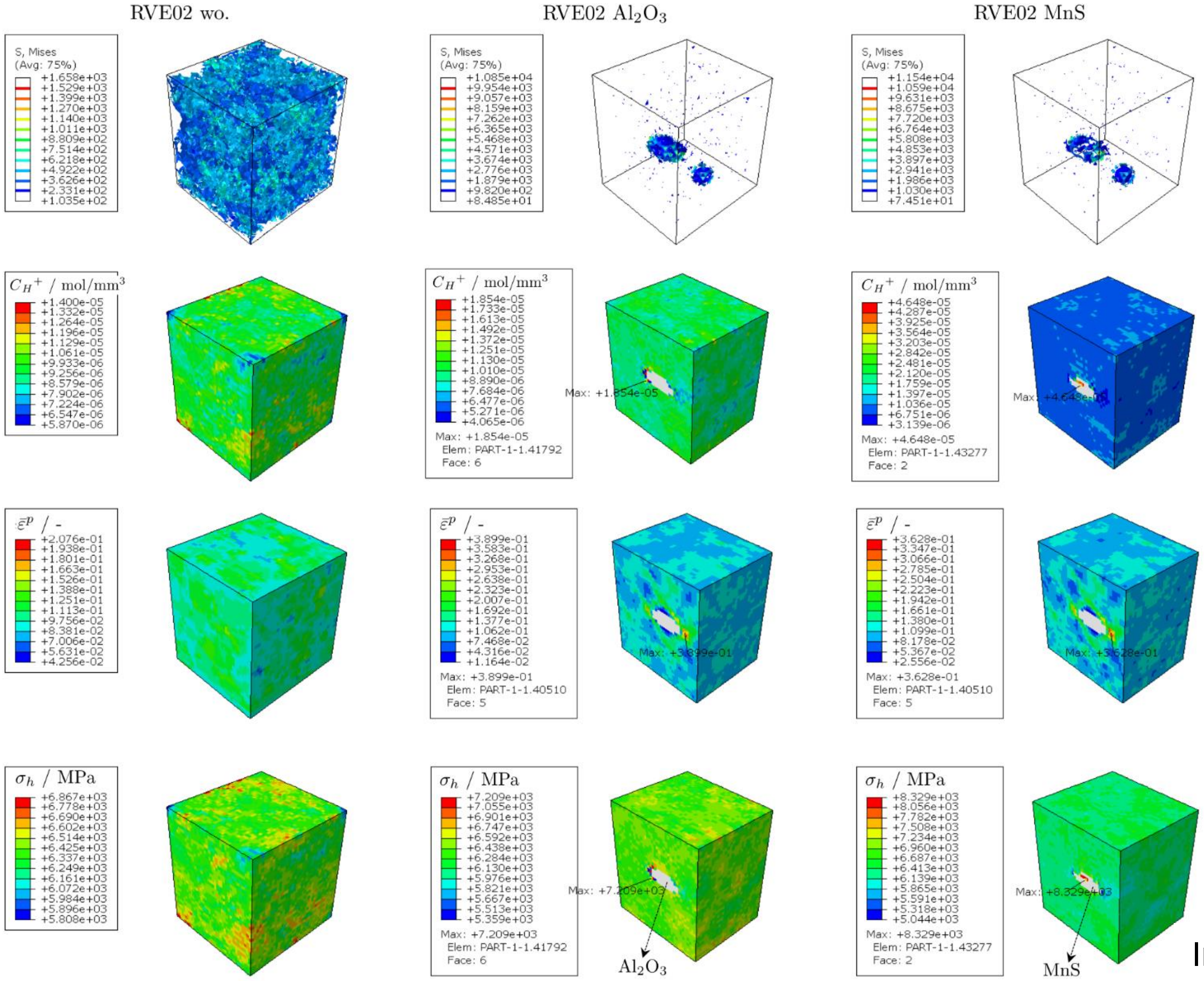
Initial hydrogen concentration: $5 \cdot 10^{-8}$ mol/mm³

Identification of HIC susceptible regions in the pipe based on the microstructural characteristics



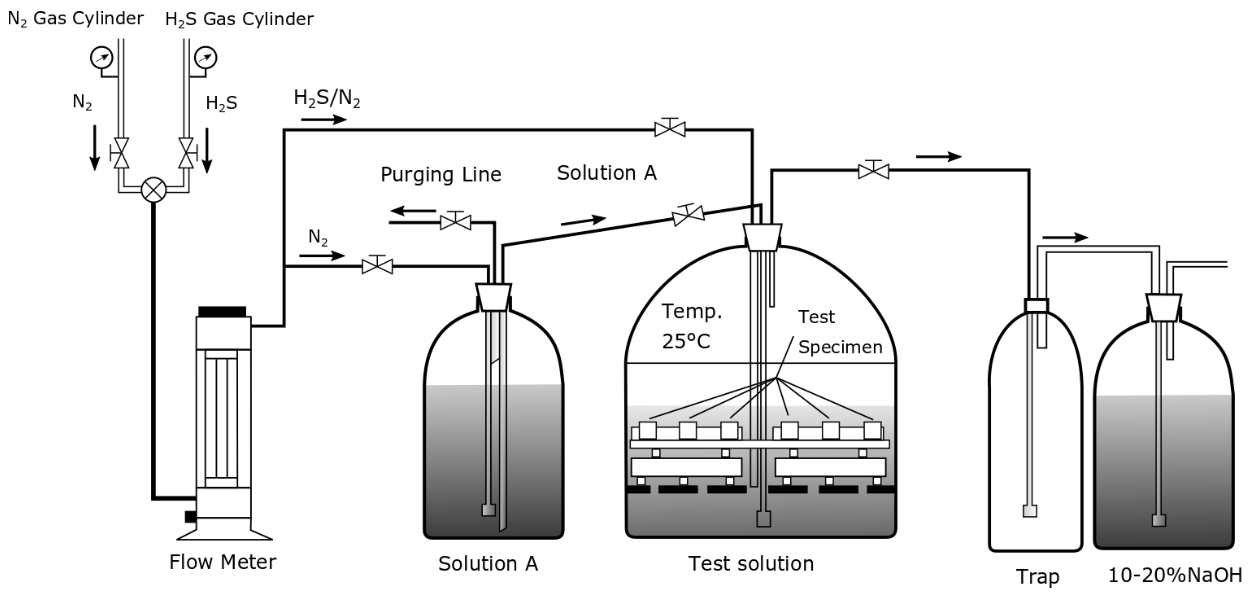
Initial hydrogen concentration: $5 \cdot 10^{-8}$ mol/mm³

Influence of hard and soft non-metallic inclusions based on the UOE loading history

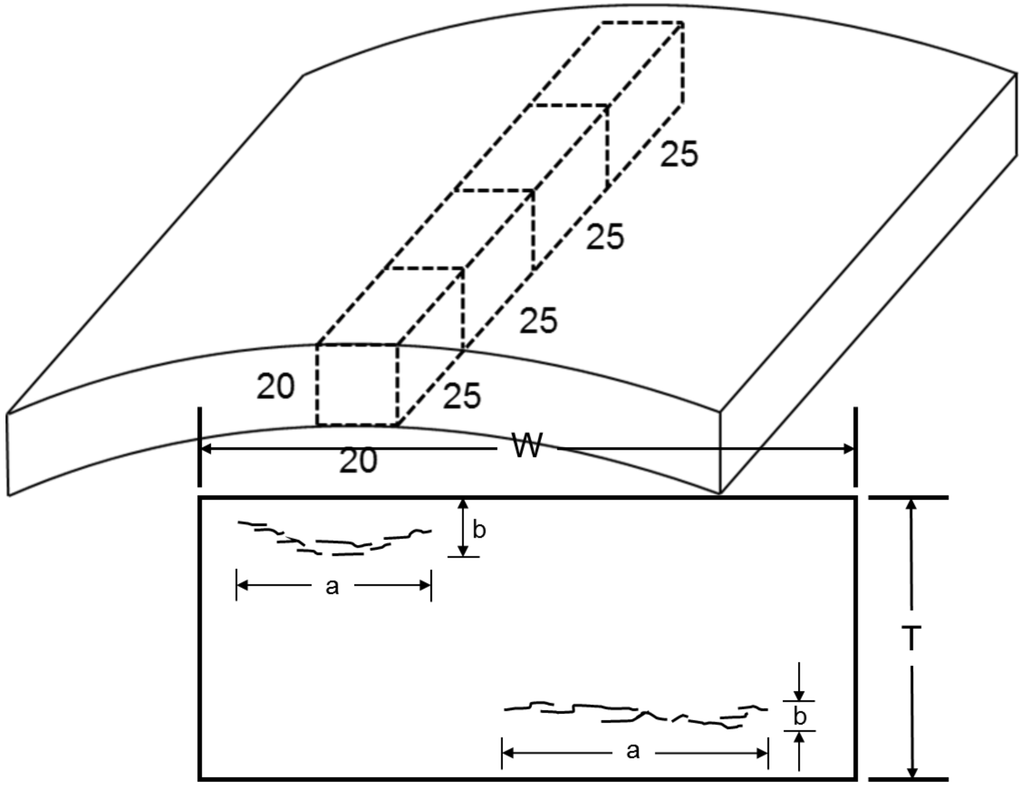


Initial hydrogen concentration: $5 \cdot 10^{-8}$ mol/mm^3

HIC-Test



Norm: NACE TM0284-2016

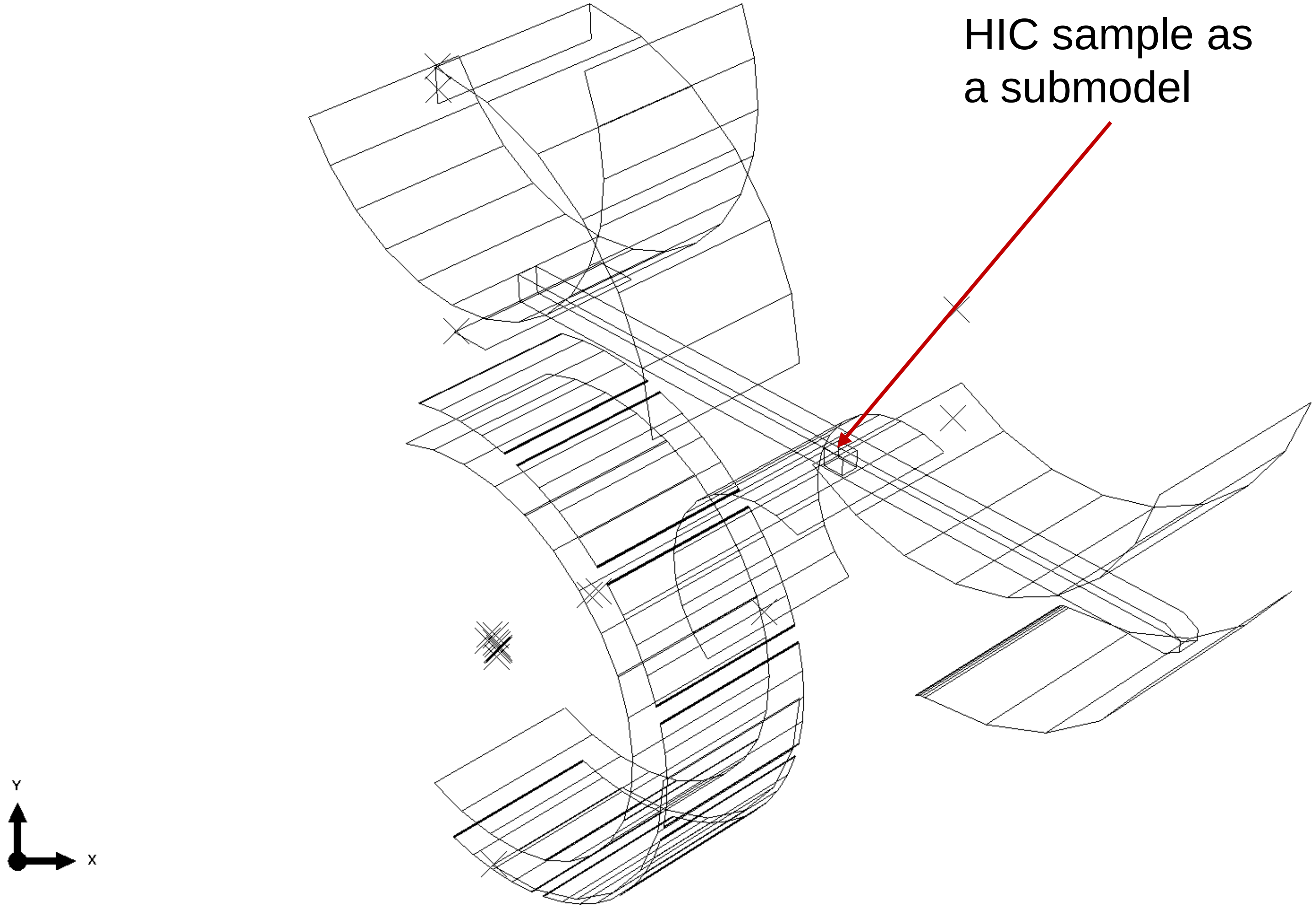


Crack Sensitivity Ratio, CSR = $\frac{\sum(a \cdot b)}{W \cdot T} \cdot 100\%$

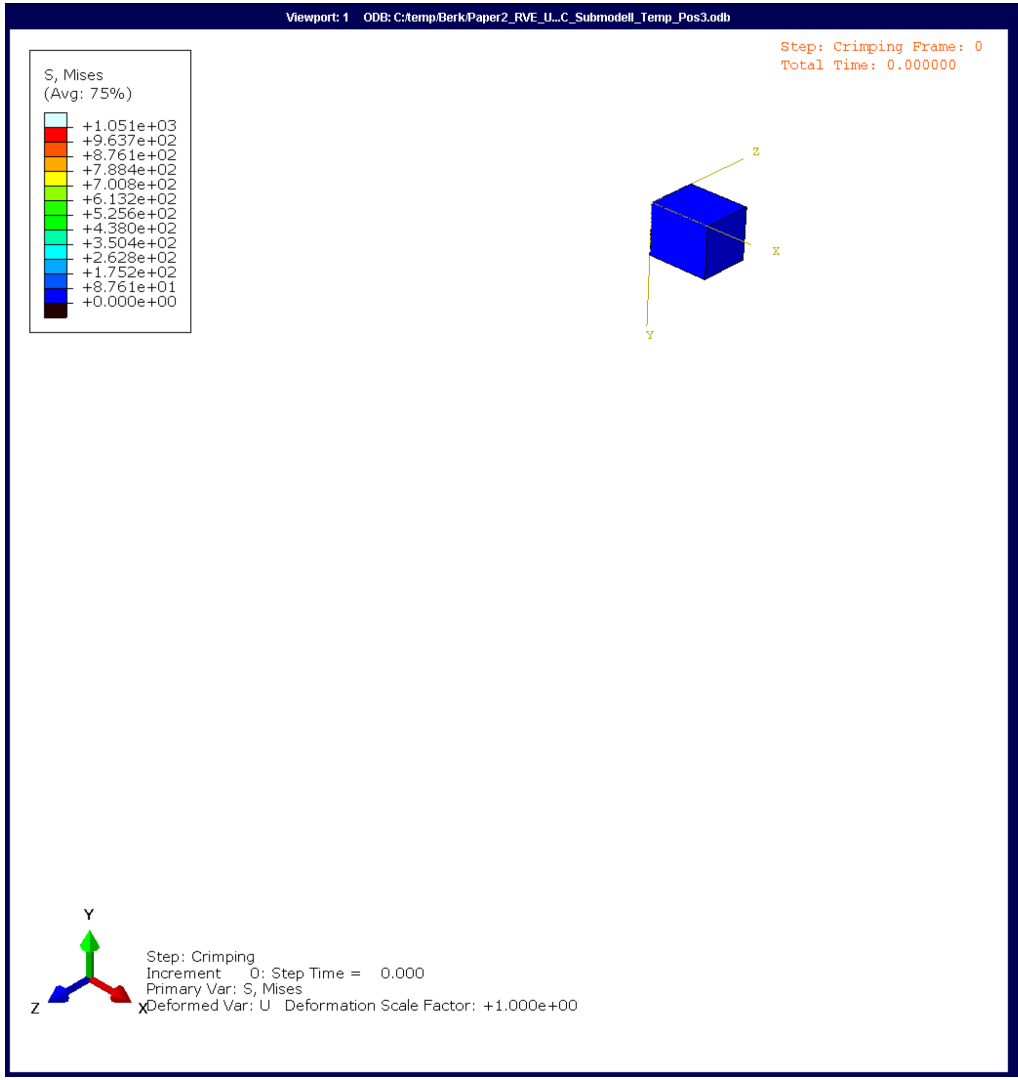
Crack Length Ratio, CLR = $\frac{\sum a}{W} \cdot 100\%$

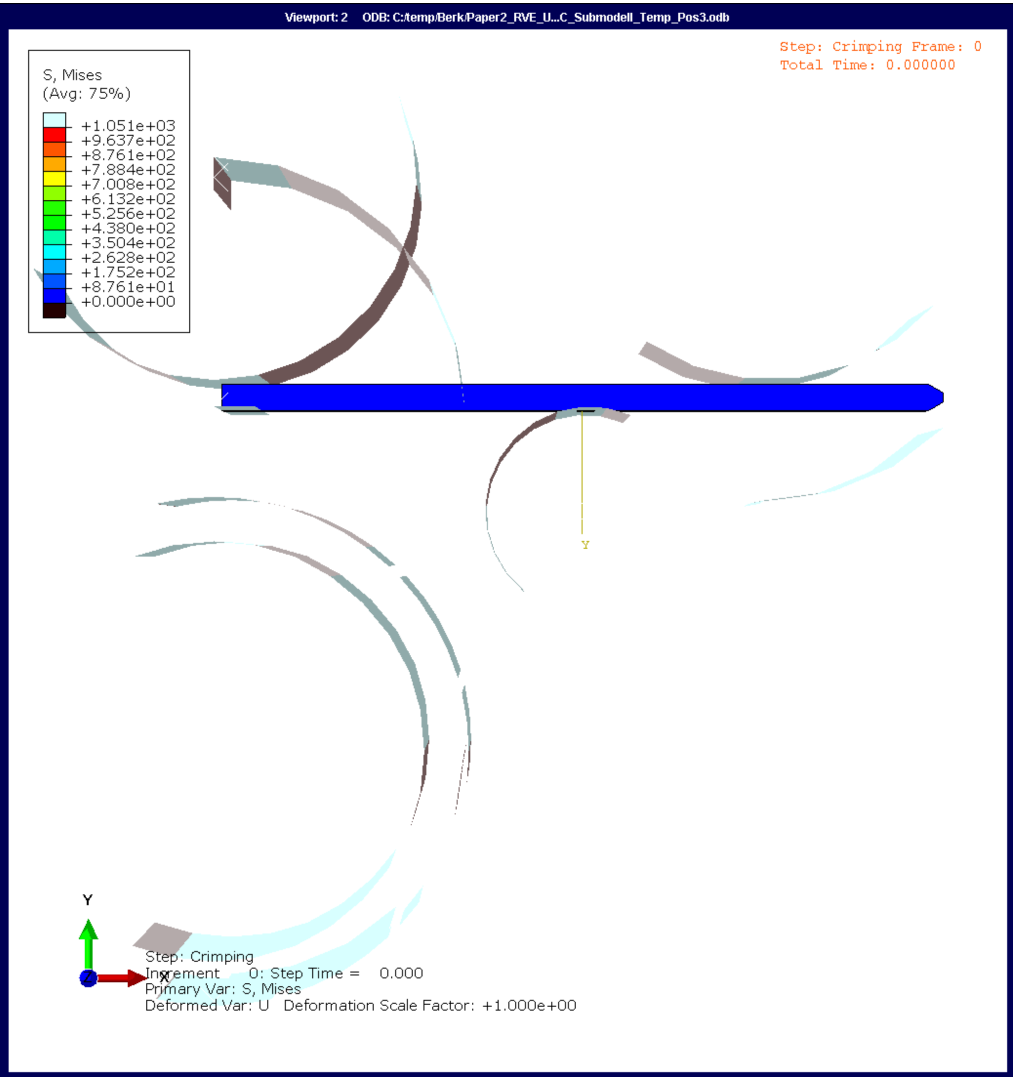
Crack Thickness Ratio, CTR = $\frac{\sum b}{W} \cdot 100\%$

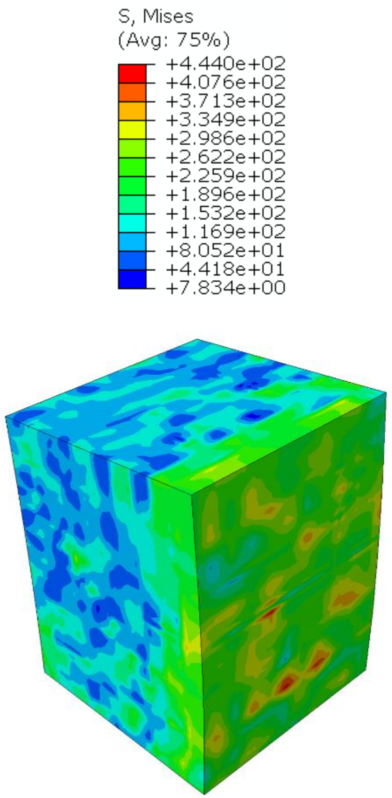
HIC sample as submodel



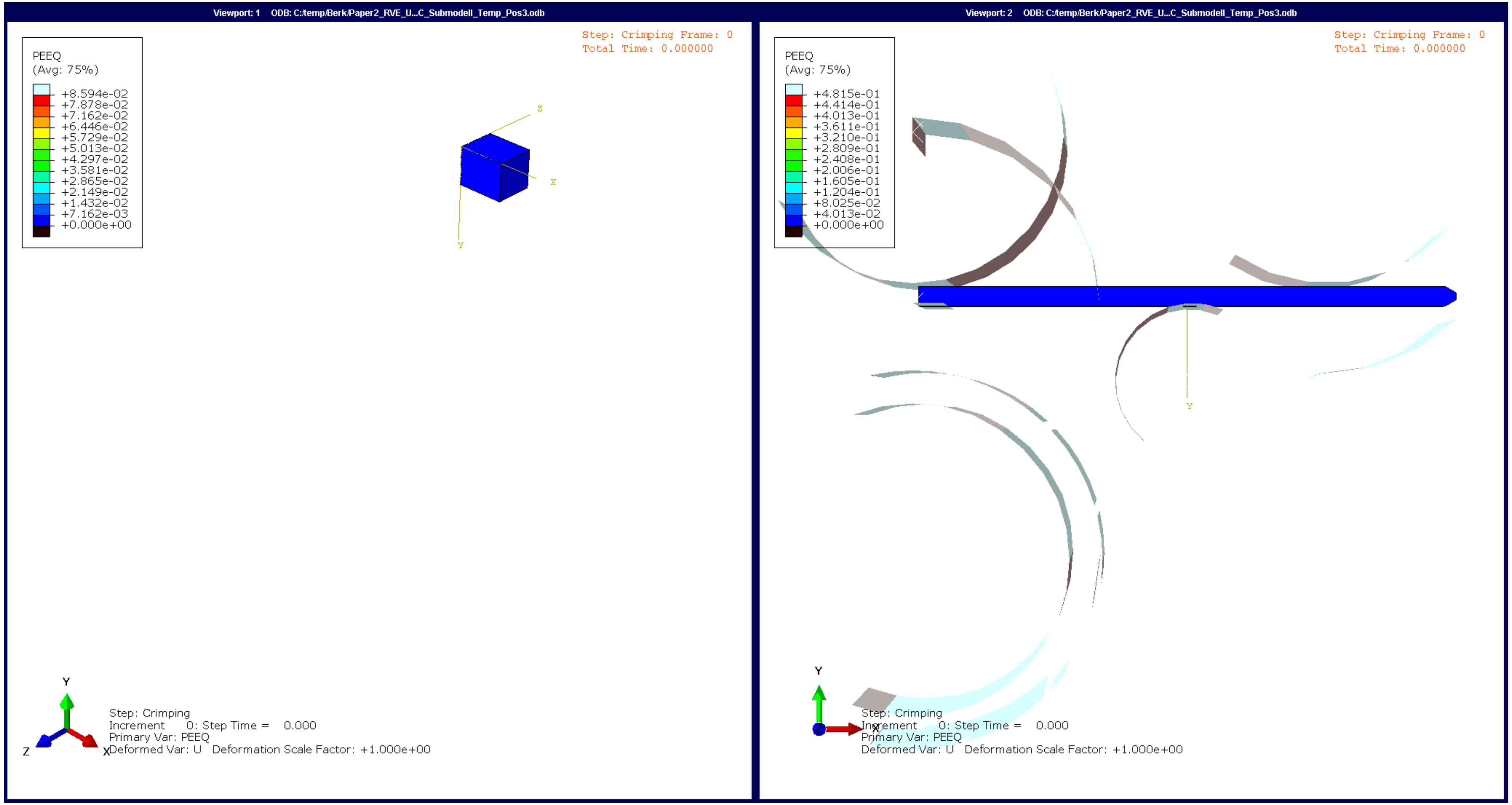
HIC sample as submodel

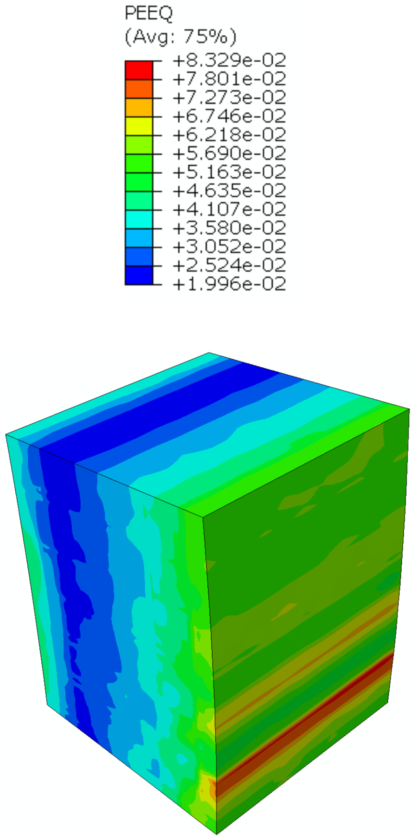






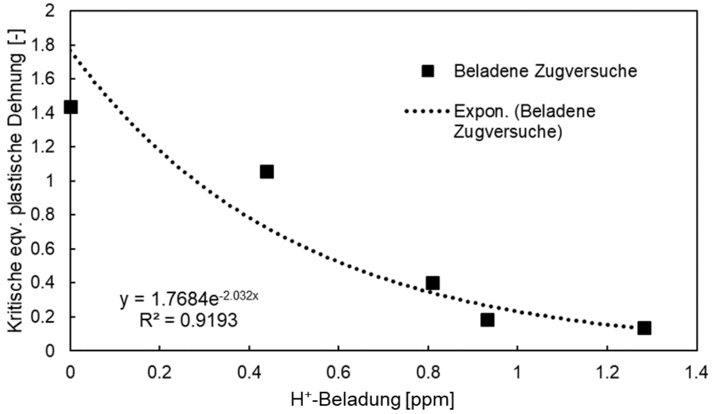
HIC sample as submodel





Result: HIC Test
Strain based (uncoupled) damage criterion

Strain based (uncoupled) damage criterion

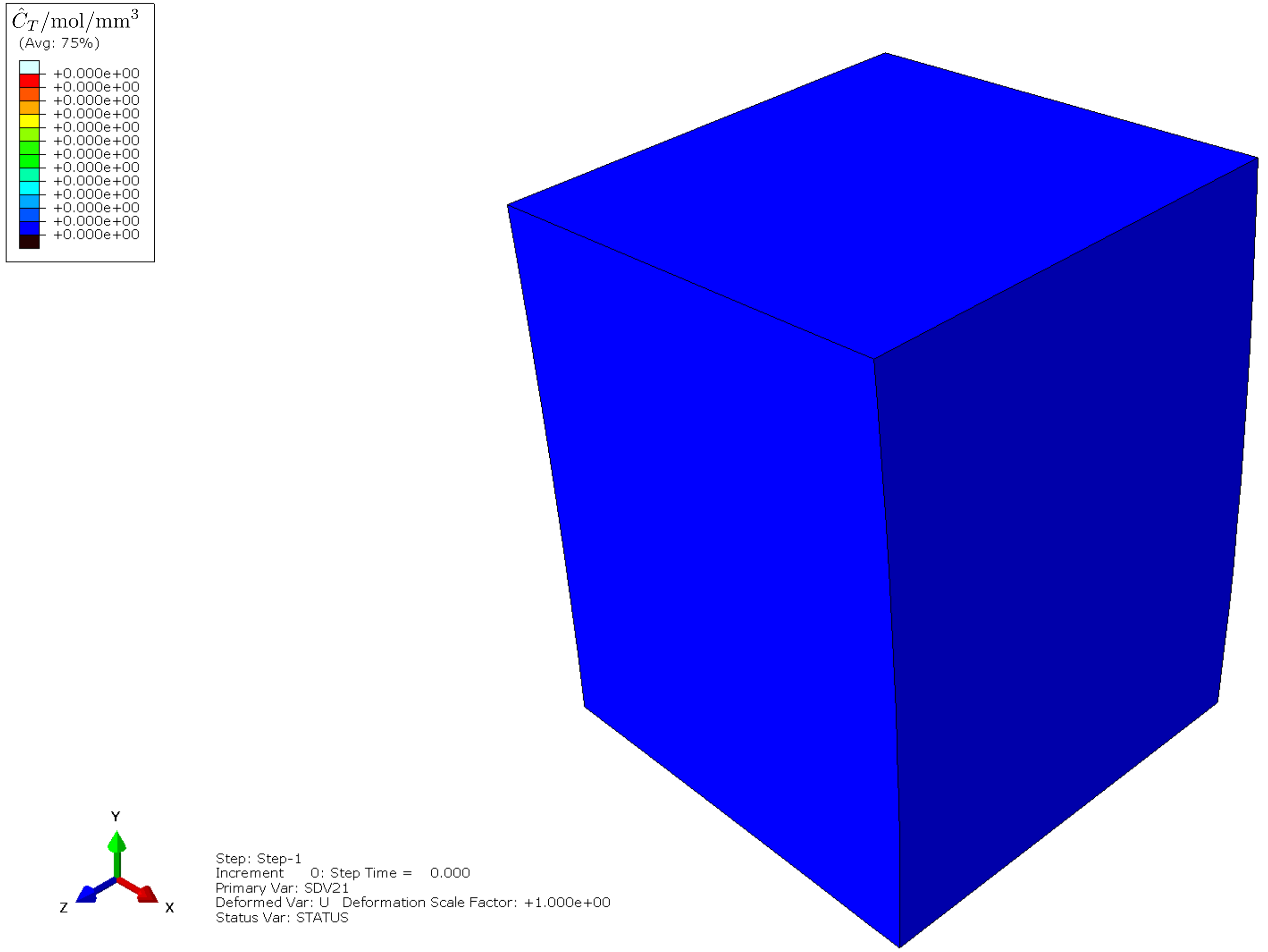


HELP Mechanism

$$f_{df}(\mathrm{C_{H^+}}) = 1{,}7684 \cdot \exp(-4 \cdot 10^7 \cdot C_{H^+})$$

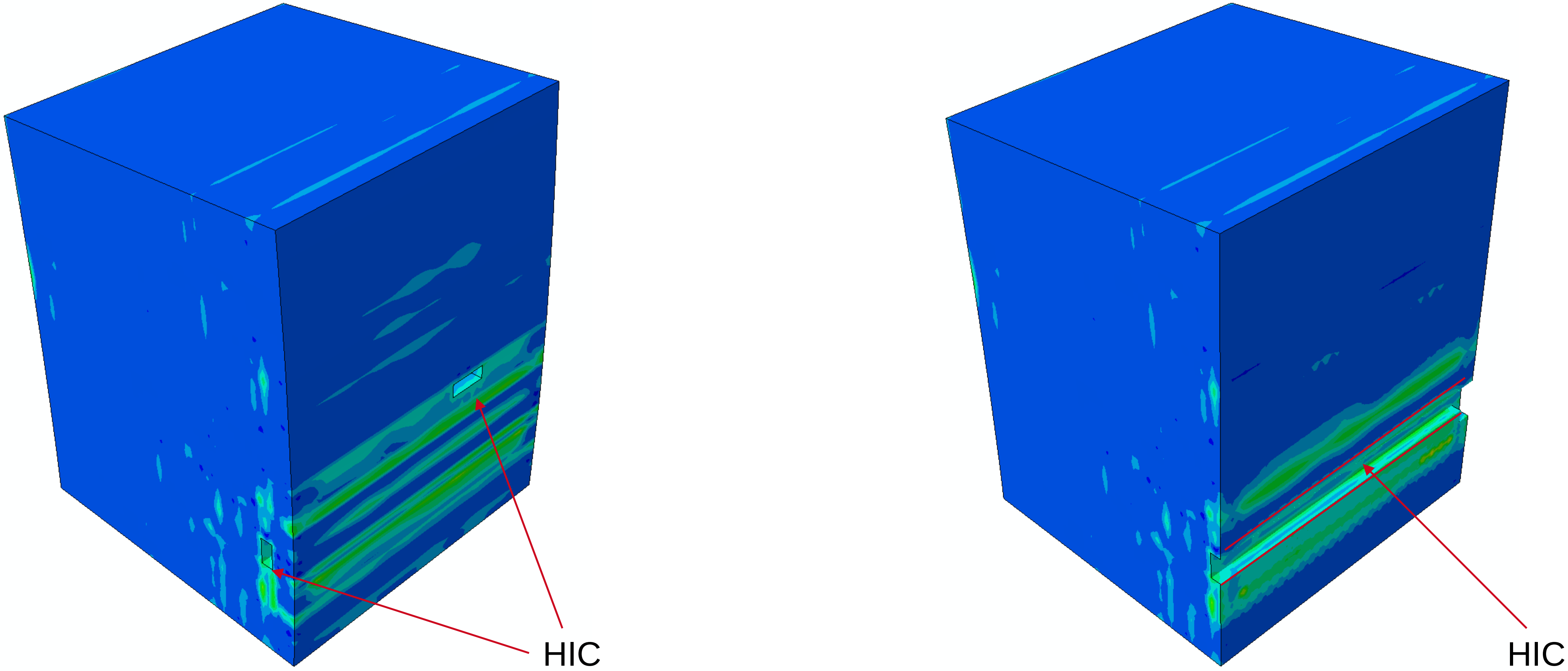
$$\bar{\varepsilon}_f \geq f_{df}(\mathrm{C_{H^+}})$$

$\mathrm{mol/mm^3}$



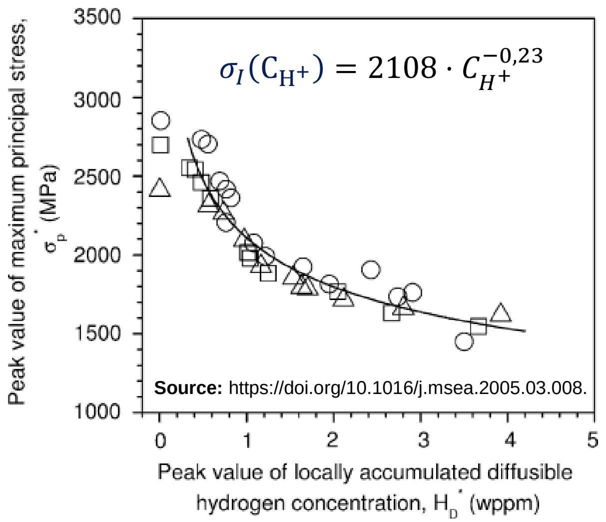
Initial hydrogen concentration: $1{,}7 \cdot 10^{-7}$ mol/mm³

Result: HIC Test
Strain based (uncoupled) damage criterion



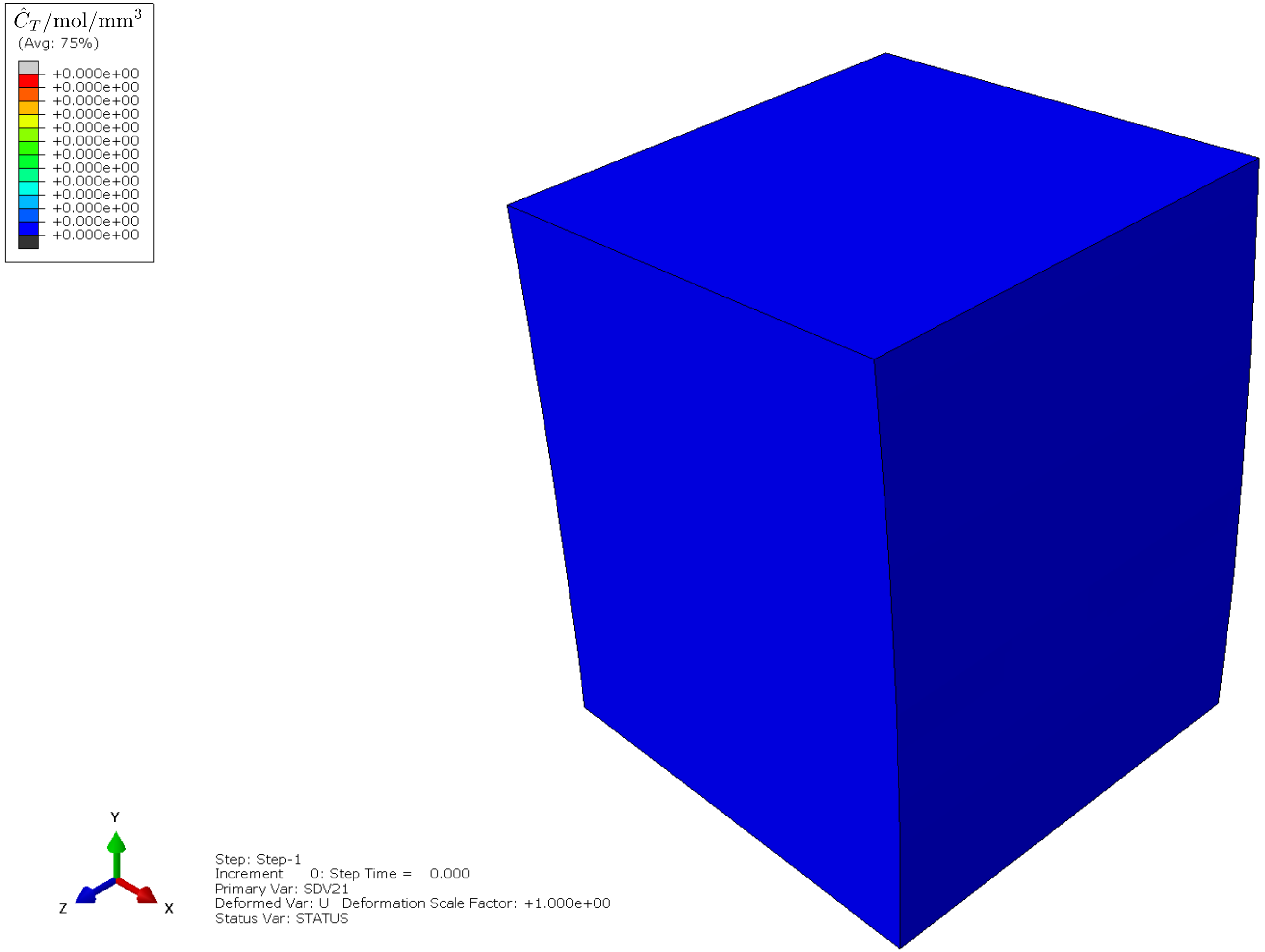
Result: HIC Test
Stress based (uncoupled) damage criterion

Stress based (uncoupled) damage criterion



HEDE Mechanism

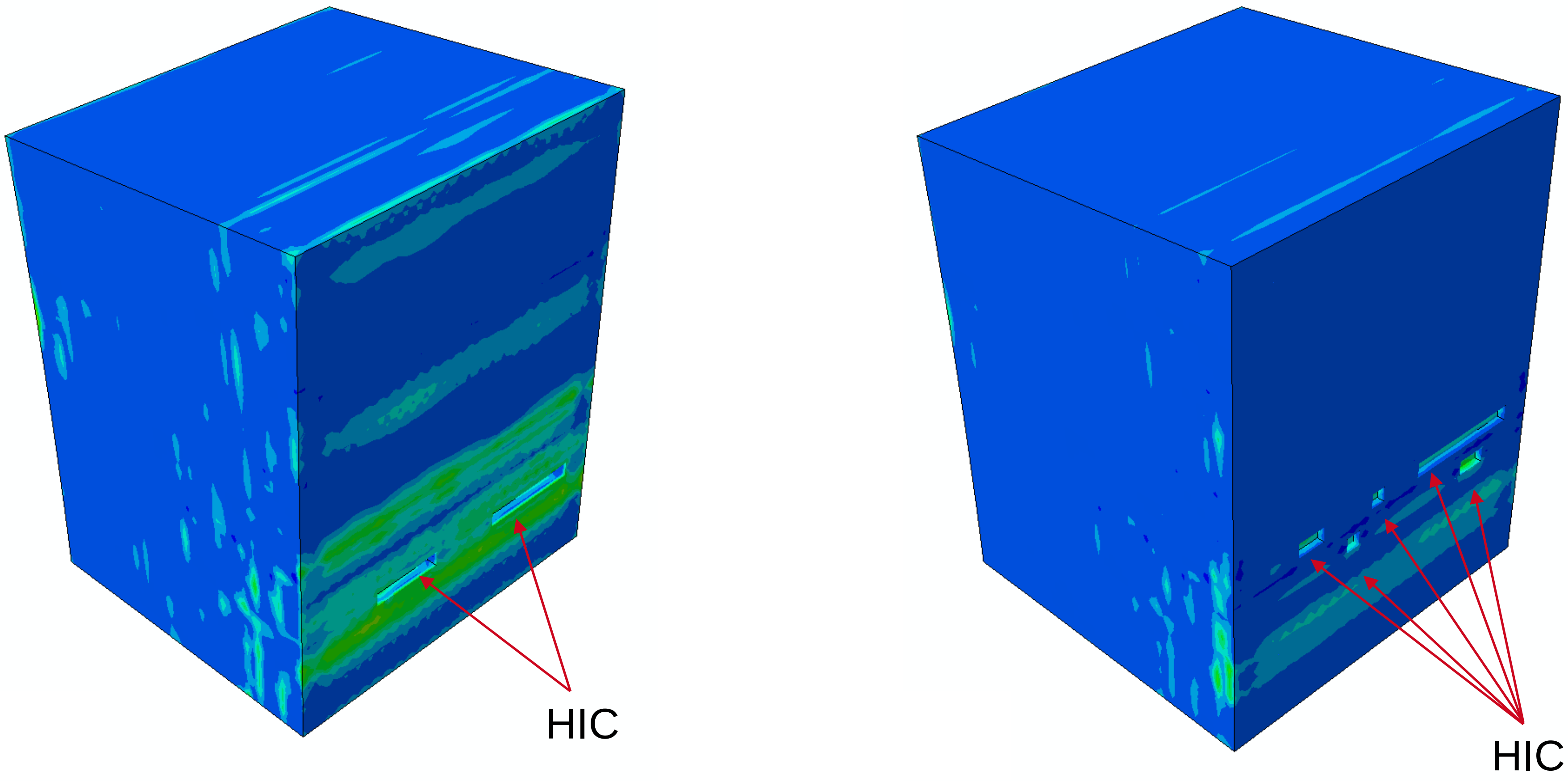
$$\max(|\sigma_I|, |\sigma_{II}|, |\sigma_{III}|) \geq \sigma_I(C_{H^+})$$



$1 \text{ wppm} \approx 7{,}8 \cdot 10^{-9} \text{ mol/mm}^3$

Initial hydrogen concentration: $5 \cdot 10^{-8}$ mol/mm³

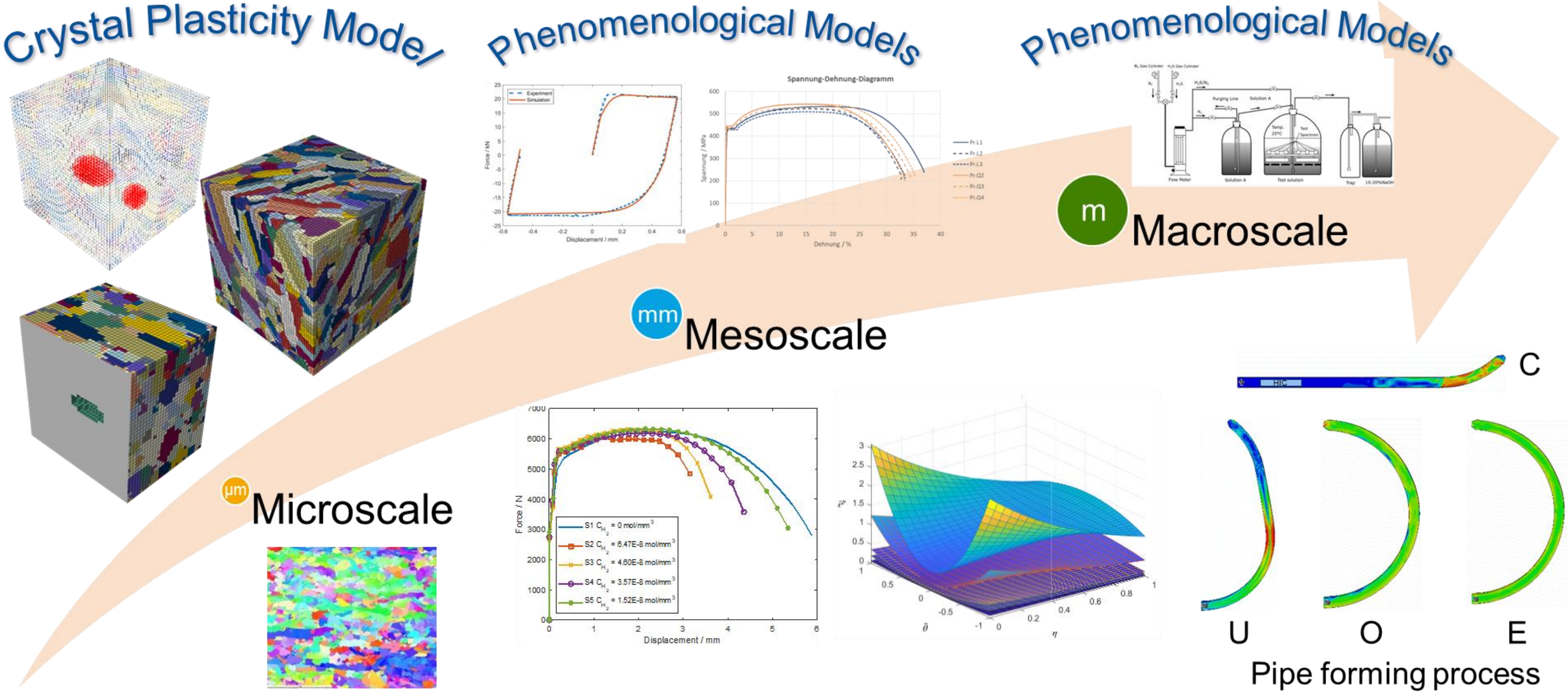
Result: HIC Test
Stress based (uncoupled) damage criterion



Agenda

1	Motivation
2	Microscale
3	Mesoscale
4	Macroscale
5	Conclusion

Conclusion:
Multi-scale description of HIC resistance



Thank you for your attention!