Modelling coupled chemo-mechanical fracture in DAMASK

Project No: T17019e
Project title: Multi-Field RVE simulation
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Institute: Max Planck Institute für Eisenforschung, Germany

materials innovation institute

Aim of the project

- Develop a framework to perform efficient multi-field simulations
- Complex interactions at the grain scale
- Multiple-fields are involved in describing a physical phenomenon
- Example: To study phenomenon like hydrogen embrittlement which is important given the focus on hydrogen economy

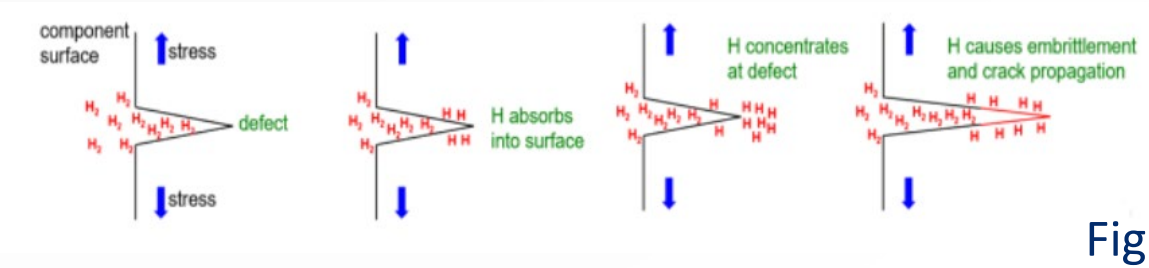


Fig.1 : HEDE schematic[1]

[1] *Gaseous hydrogen embrittlement of materials in energy technologies: the problem, its characterisation and effects on particular alloy classes*. Elsevier, 2012.

Application: Chemo-Mechanics-Damage

- Modelling Hydrogen embrittlement would require the coupling of chemistry, mechanics and damage fields.
- Interaction of fields at the constitutive level because of inter-dependent parameters

Scientific Tasks:

- Framework development
- Implementation of diffusion and damage solver
- Model development
- Model validation

Framework development

- **Standardization**:
  - YAML input
  - HDF5 output

- **Python based pre- & post- processing library:**
  - Integration with Neper/DREAM 3D
  - Paraview visualisation

- **Source code refactoring:**
  - Modularization of the code
  - Interaction of different physical fields

Diffusion theory

- Diffusion of a component can be defined as:

$$\dot{c}_{\mathrm{H}} = -\nabla.\mathbf{j}_{\mathrm{H}} + f_{\mathrm{H}}$$

- Formulating flux in terms of chemical potential:

$$\mathbf{j}_{\mathrm{H}} = -M\nabla\mu$$

where, M is the atomic mobility

- Chemical potential is the change in the free energy when an infinitesimal amount of solute is added to the system:

$$\mu = \frac{\partial G}{\partial c}$$

Thermodynamic models

- **Quadratic approximation:**

$$G = A + B(x - x_0) + C((x - x_0)^2)$$

where **x** is the concentration and x_0 is the equilibrium concentration

- **Substitutional regular solution model:**

$$G = \sum_i x_i G_i + RT \sum_i x_i \ln x_i + G^{xs}$$

The excess Gibbs free energy can been modelled using different approaches but Redlich-Kister formulation will be used in our case.

Chemo-mechanics coupling

- Region of high hydrostatic stress act as a sink for solutes
- Presence of solutes expands or contracts the lattice leading to eigen strains
- This is captured using the Vegard coefficient

$$G = G_{\text{mech}} + G_{\text{chem}}$$

$$G_{\text{mech}} = -\omega v_{\text{m}} (F_{\text{i}}^{T} S).I$$ → Elastic contribution

Brittle Damage

- Used a brittle damage phase field model already implemented in DAMASK[2]

$$\mu\dot{\phi} = f_\phi - \nabla \cdot \mathbf{f}_\phi$$

- Damage occurs when a critical energy value is reached

- The ratio of the elastic energy over the critical energy drives the damage

$$\mu\dot{\phi} = 1 - \frac{\phi\tilde{\psi}_E}{\frac{G_c}{l_c}} + \nabla \cdot l_c^2 \nabla\phi$$

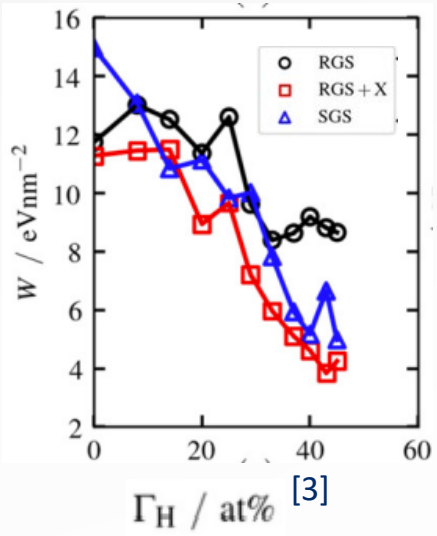
- Stiffness degradation is present as the damage phase field variable evolves

[2] Roters, et al. "DAMASK – The Düsseldorf Advanced Material Simulation Kit for modeling multi-physics crystal plasticity, thermal, and damage phenomena from the single crystal up to the component scale", *Computational Materials Science* (2019): 158, 420-478.

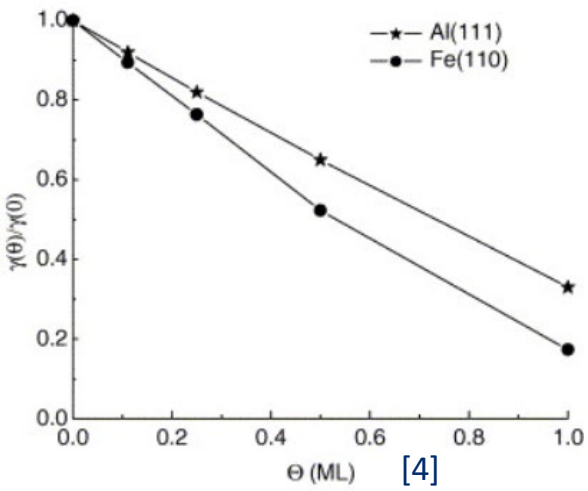
Chemical-Damage coupling

- Solute (Hydrogen) is said to decrease the surface energy creation at interfaces/GBs

$$W_{\mathrm{crit}} = W_{\mathrm{crit0}} + \frac{\partial W_{\mathrm{crit}}}{\partial c} * \left(c - c_{\mathrm{ref}}\right)$$



[3]



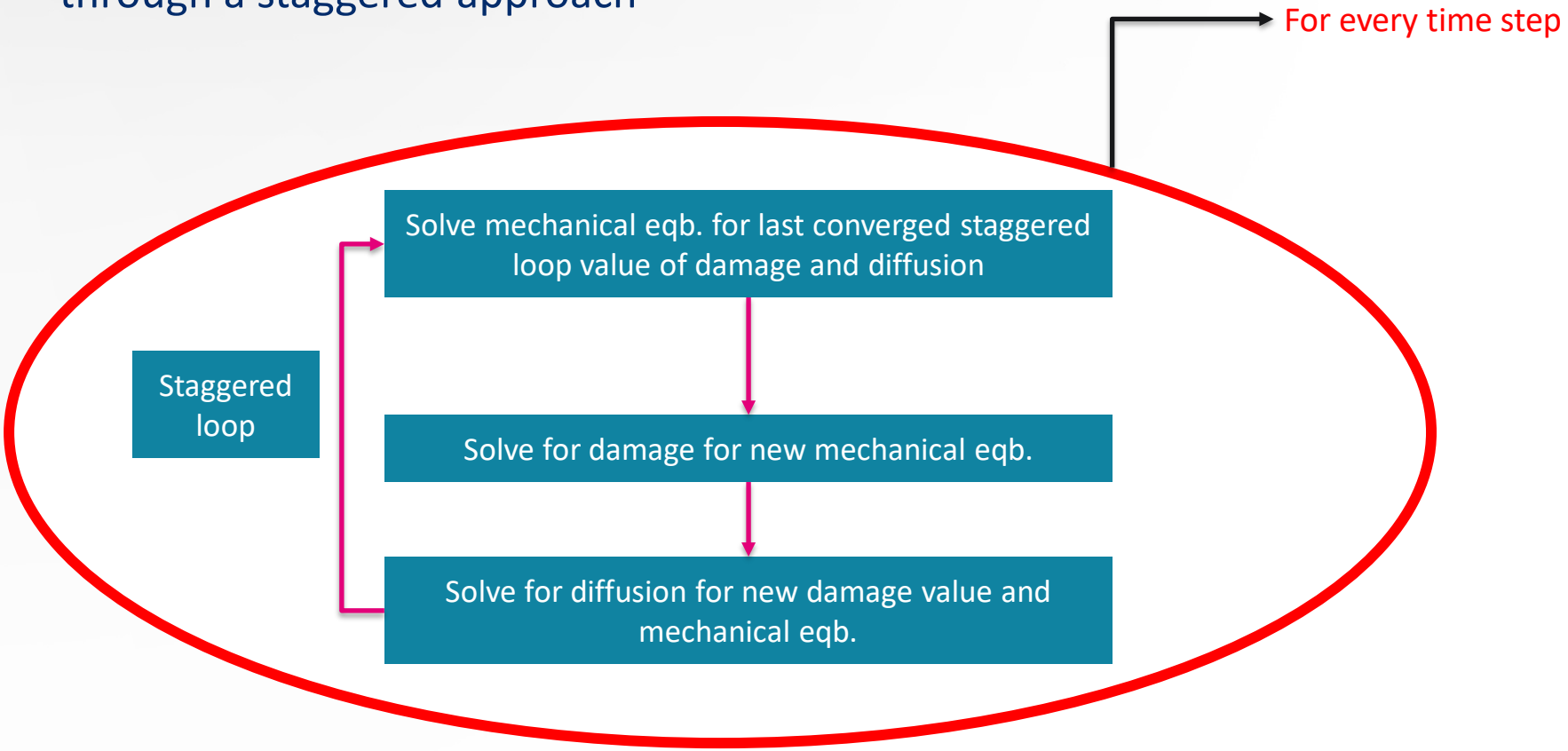
[4]

[3] Benjamin T Wilson *et al* 2022 *Modelling Simul. Mater. Sci. Eng.* **30** 035009

[4] Jiang, D. E., and Emily A. Carter. "First principles assessment of ideal fracture energies of materials with mobile impurities: implications for hydrogen embrittlement of metals." *Acta materialia* 52.16 (2004): 4801-4807.

Solving method

- Coupling between multiple fields is achieved in a self consistent manner through a staggered approach



Simulation setup

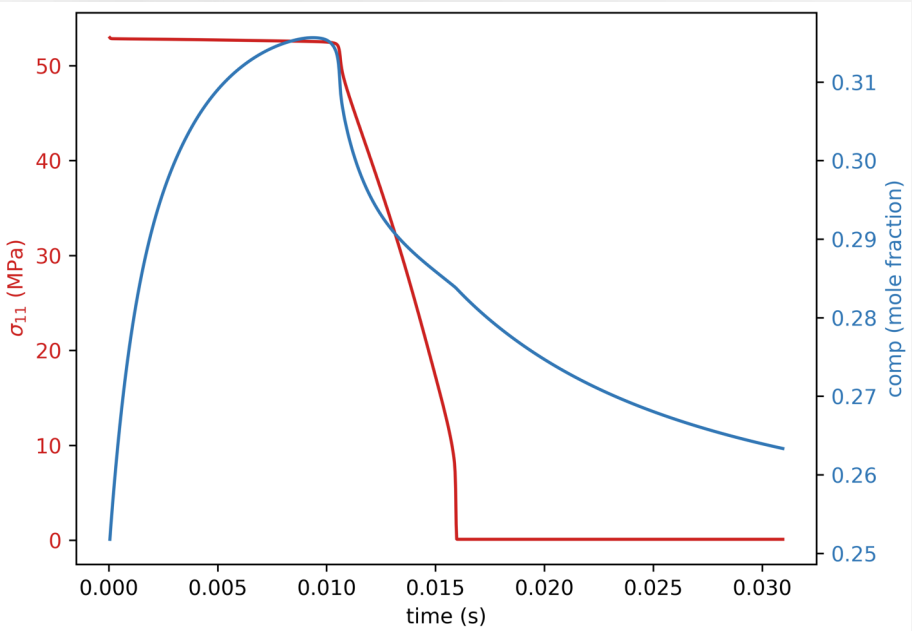
```
...
homogenization:
  SX:
    N_constituents: 1
    mechanical: {type: pass}
    damage:
      type: pass
      output: ['phi', 'f_phi']
    chemical:
      N_components: 2
      type: pass
      output: ['comp','mu']
phase:
  Aluminum_1:
    lattice: cF
    mechanical:
      elastic: {type: Hooke, C_11: 106.75e9, C_12: 60.41e9, C_44: 28.34e9}
      plastic:
        type: phenopowerlaw
        N_sl: [12]
        a_sl: 2.25
        atol_xi: 1.0
        dot_gamma_0_sl: 0.001
        h_0_sl-sl: 75000000.0
        h_sl-sl: [1, 1, 1.4, 1.4, 1.4, 1.4, 1.4]
        n_sl: 20
        output: [xi_sl]
        xi_0_sl: [31000000.0]
        xi_inf_sl: [63000000.0]
      eigen:
        - type: solutestrain
          epsilon_solute: [0.01]
    damage:
      - {type: isobrittle, G_crit: 1.65, G_crit,c: -5.0, c_ref: 0.20, l_c: 1.0e-6, mu: 1.0e-5}
    chemical:
      V_m: 1.0e-03
      energy_type: quadEnergy
      components:
        H: {M: 1.0e-14, c_0: 0.20, c_eq: 0.0, 'G,c': 0.0, 'G,c^2': 5000}
        Fe: {M: 0.0, c_0: 0.80}
  Air:
    lattice: cF
    mechanical:
      elastic: {type: Hooke, C_11: 106.75e9, C_12: 60.41e9, C_44: 28.34e9}
      plastic:
        type: none
    damage:
      - {type: isobrittle, G_crit: 1.65, c_ref: 0.20, l_c: 1.0e-6,mu: 1.0e-5}
    chemical:
      V_m: 1.0e-03
      energy_type: quadEnergy
      components:
        H: {M: 1.0e-14, c_0: 0.001, c_eq: 0.001, 'G,c': 2000.0, 'G,c^2': 50000}
        Fe: {M: 0.0, c_0: 0.999}
```

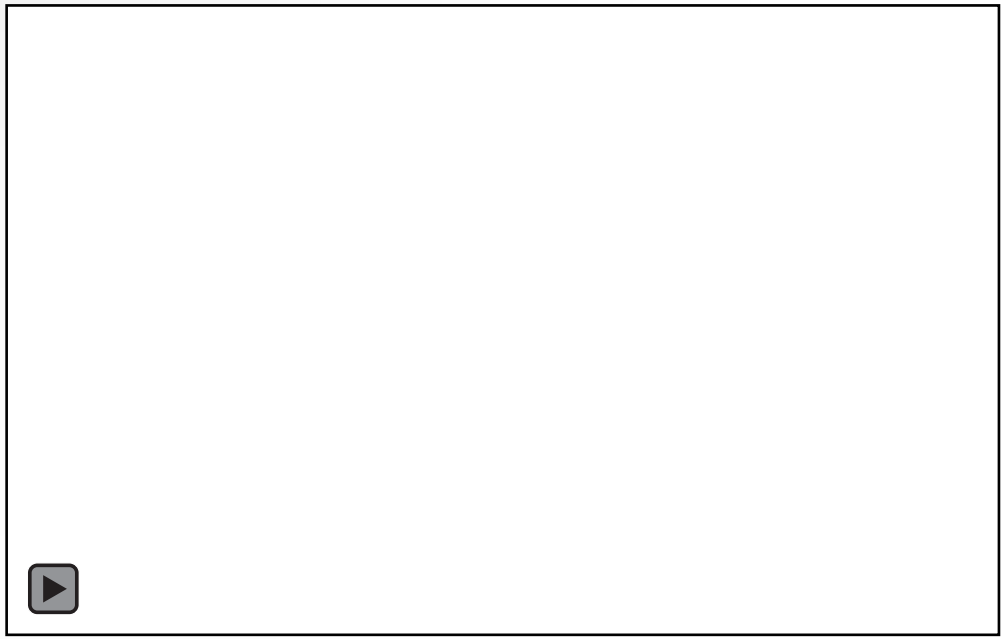
- **Two phases**: Matrix and notch with cube orientation.
- **Gibbs energy**: Quadratic potential
- **Damage**: brittle
- **Characteristic length**: 1 micron
- **W_crit**: Linear degradation
- **Plasticity**: phenomenological

Assumptions:

- High molar volume/or high lattice strain coefficient(to artificially increase concentration and speed up the process)

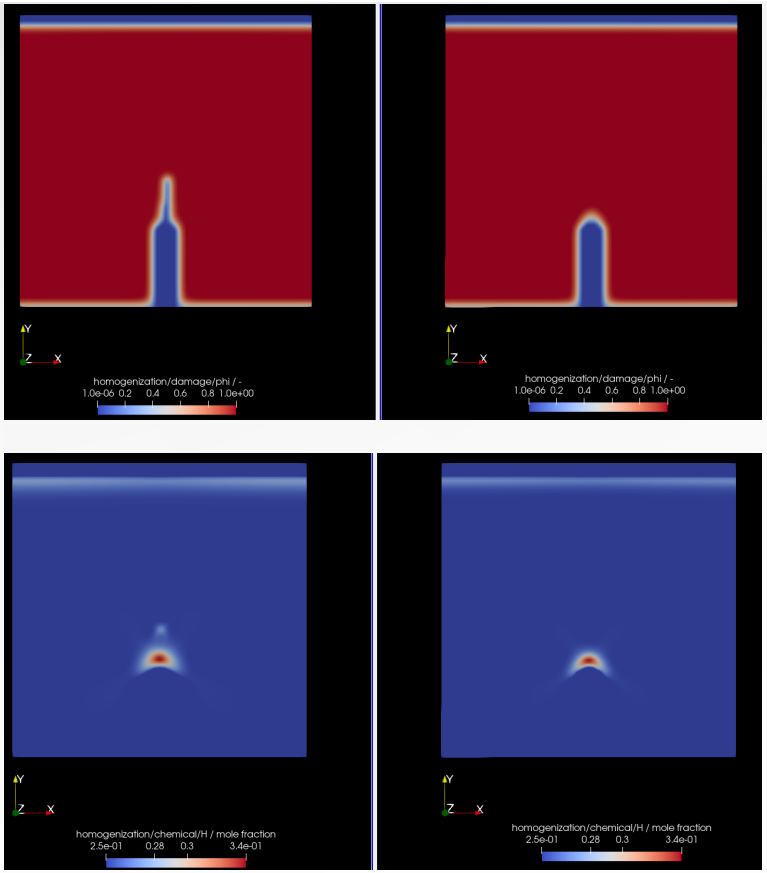
Application: Delayed Fracture



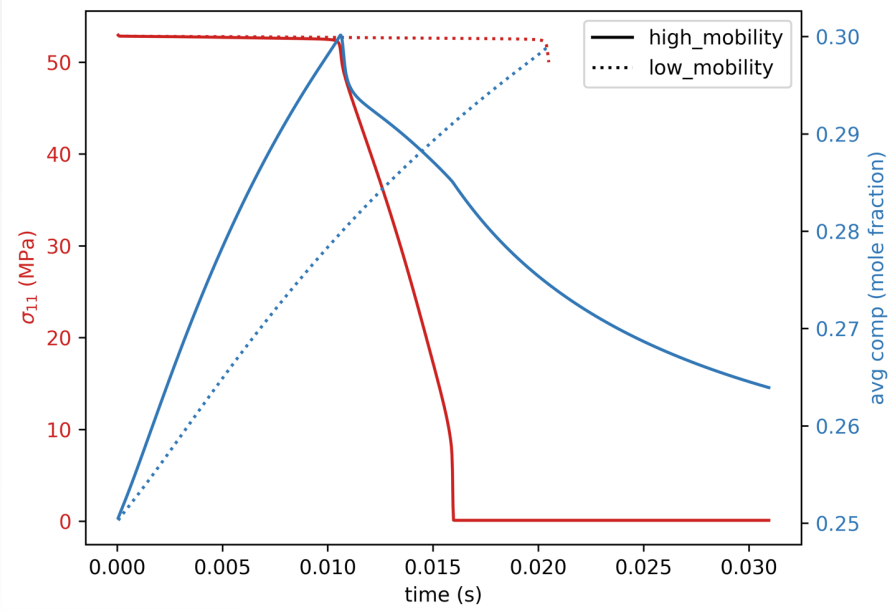


- Load the material in mode 1, close to its critical value at a high strain rate ($1000s^{-1}$) and hold at a constant stress
- Solute diffuses to the notch tip and lowers the critical energy for crack propagation

Effect of Mobility (The kinetics)



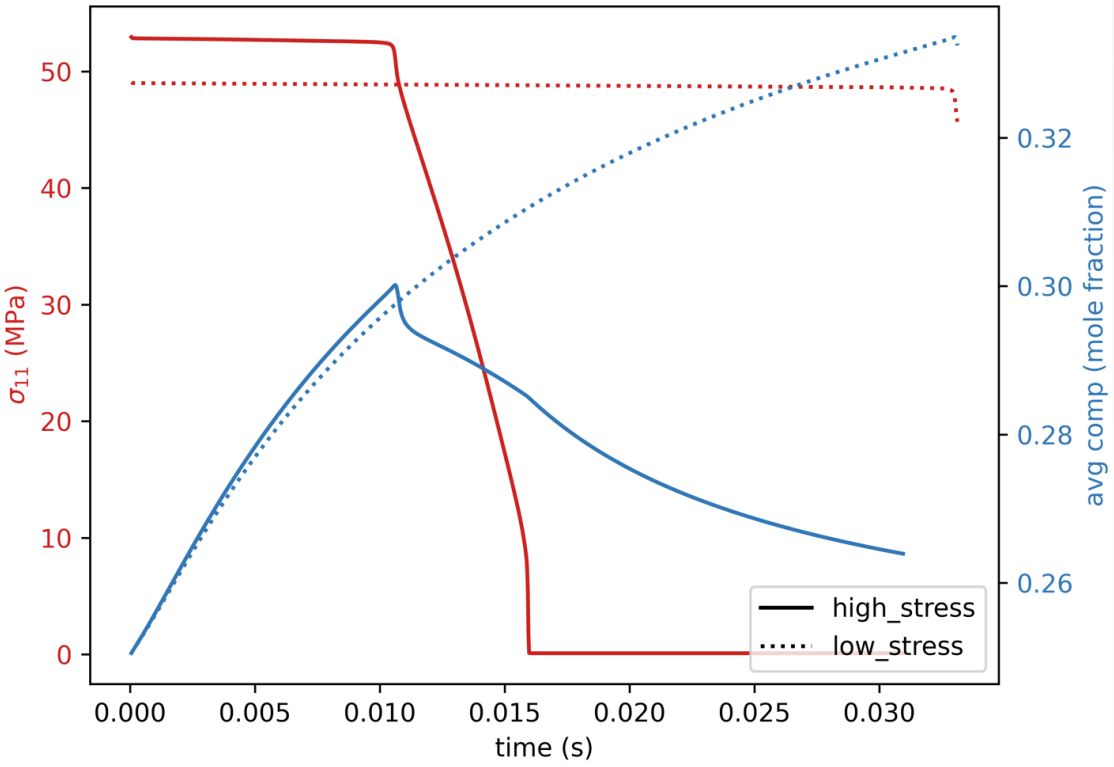
High mobility Low mobility



Higher mobility leads to faster crack propagation

$$t = 0.013s$$

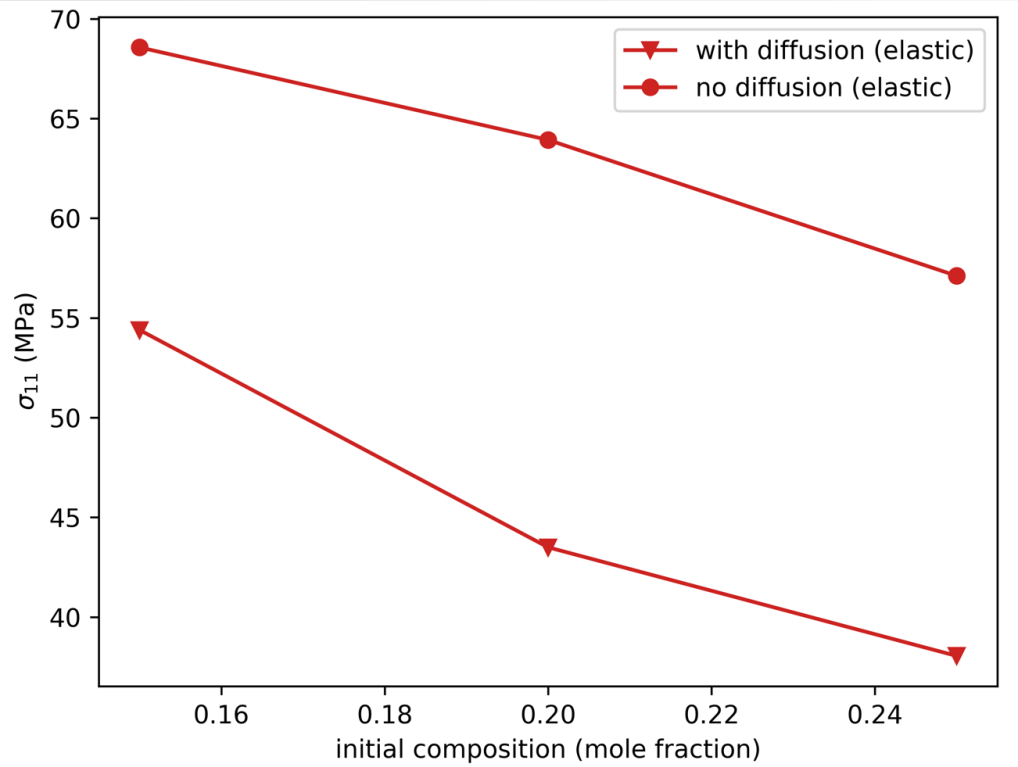
Effect of different residual stress



- Residual stress dictates how fast (given a constant mobility) the system is going to eventually fracture
- Lower residual stress would require higher solute concentration at the crack tip to allow its propagation

System loaded to different residual stress with other parameters remaining constant

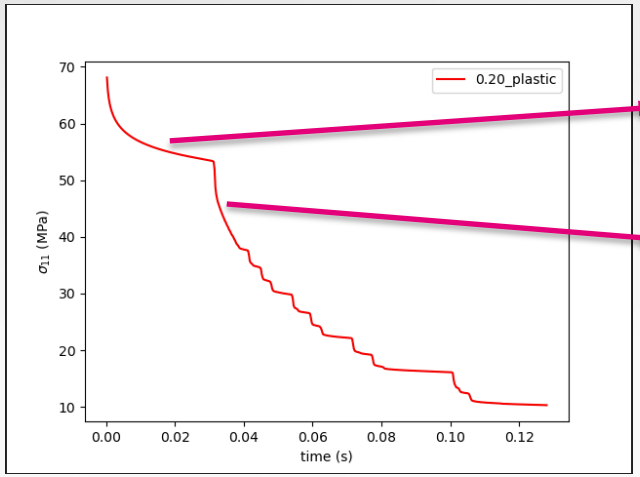
Max allowable stress vs composition



Maximum allowable elastic stress with and without diffusible solute for a given composition.

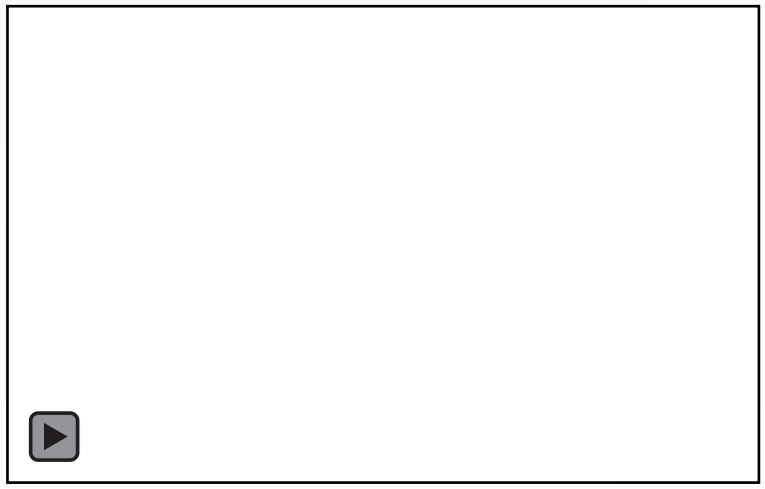
- Trapping all the solutes increases the max. allowed stress in a system
- Maybe given enough time for the solute to diffuse, it might eventually fail. But lower stress decreases the driving force for damage

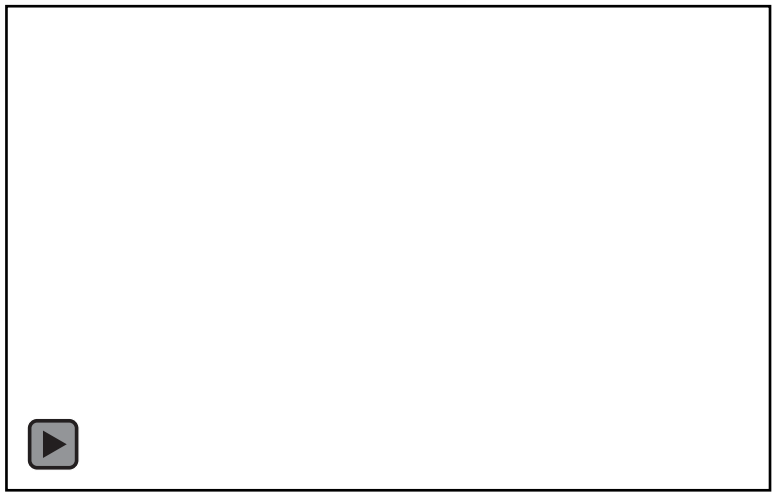
Plasticity helps reduce elastic strain



Plastic flow reducing Cauchy stress

Caused due to damage propagation





Dislocation and GB contribution

- Dislocation cores create an additional potential
- The binding energy dictate the composition inside the dislocation cores
- Similarly, grain boundaries (GB) create additional potential

- Calculate approximate dislocation density per slip system:

$$\rho = \left(\frac{\xi_{sl}}{0.5 * G * b}\right)^2 \tag{1}$$

- The total dislocation density in a material point:

$$\rho_{\text{total}} = \sum_{N=1}^{N_{sl}} \rho \tag{2}$$

- Volume fraction of dislocation cores:

$$f_\rho = \pi * r_c^2 * \rho_{\text{total}} \tag{3}$$

where, r_c is 2-4 times the burgers vector.

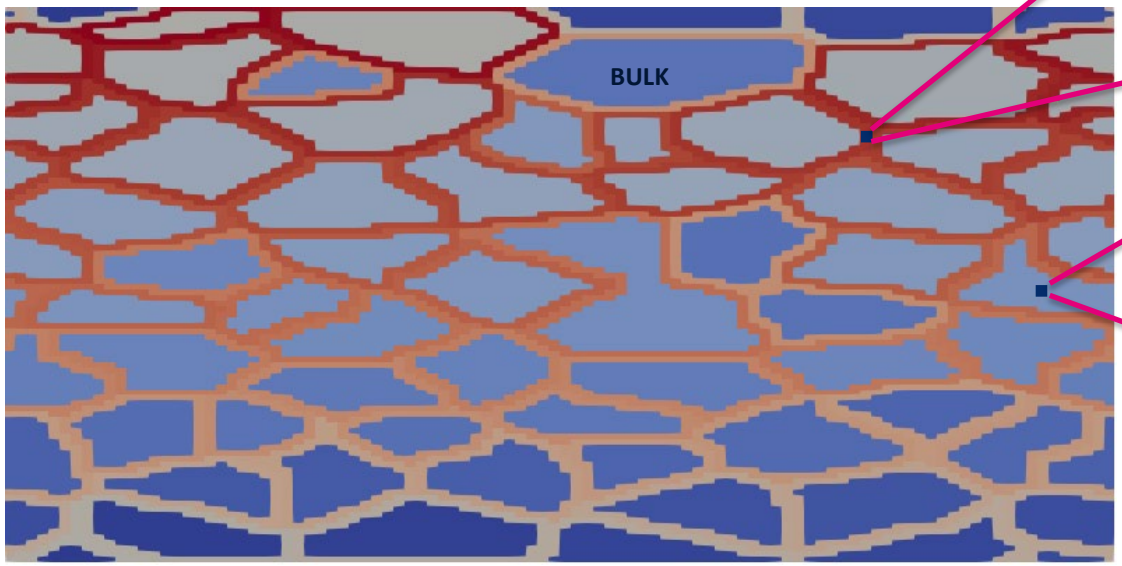
- Average composition in a voxel:

$$c_{\text{avg}} = \left(1 - f_\rho - f_{GB}\right) * c_{\text{bulk}} + f_\rho * c_\rho + f_{GB} * c_{GB} \tag{4}$$

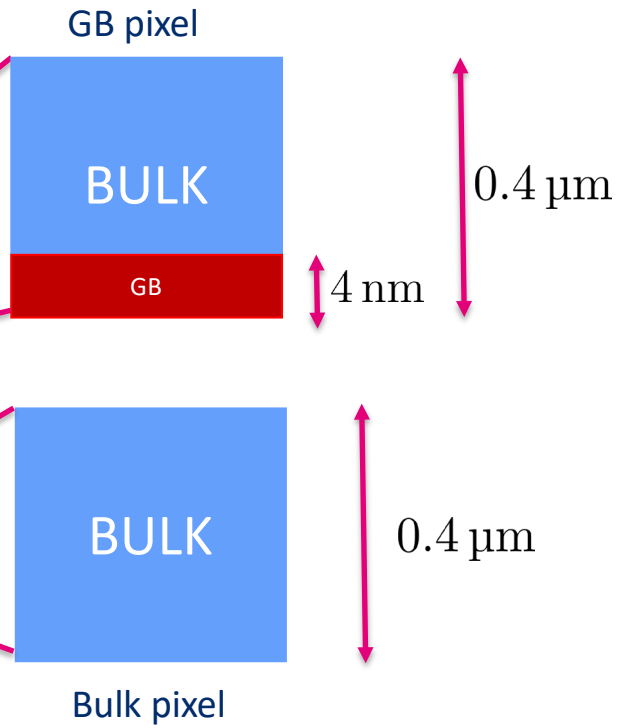
- The W_{crit} would be dependent on GB composition and not the bulk or average voxel composition. Therefore:

$$W_{\text{crit}} = f\left(c_{GB}\right) \tag{5}$$

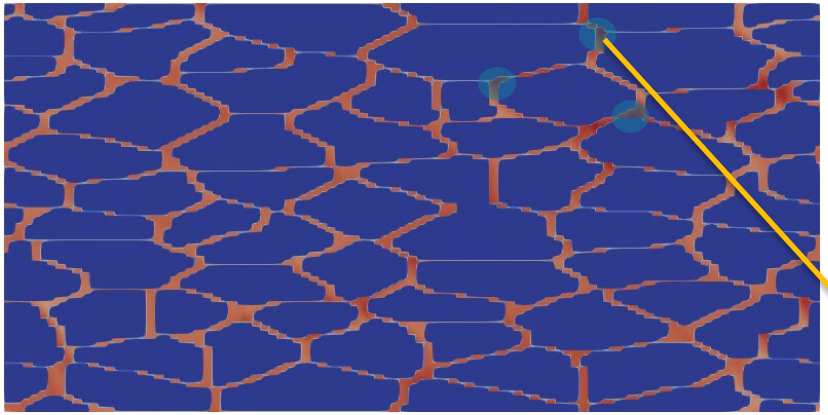
- Two different phase present:
  - Bulk
  - GB

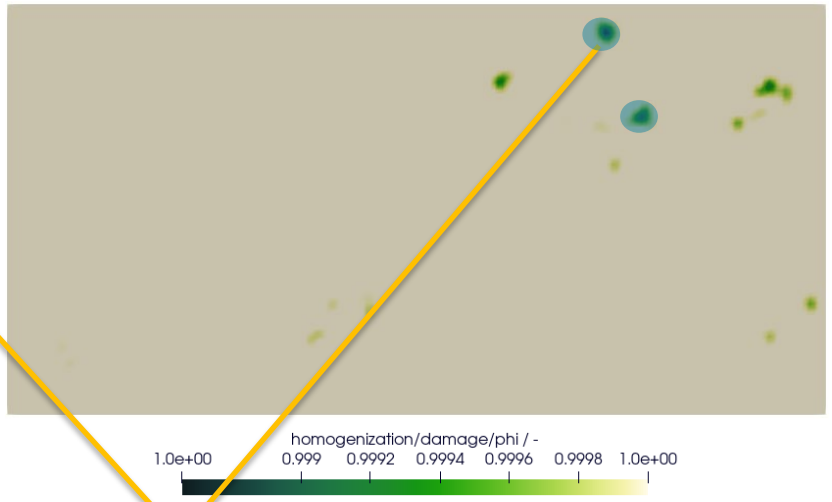


POLYCRYSTAL



- Not all of the GB pixel behaves as grain boundary
- 1% volume fraction of the pixel has grain boundary properties ~ 4nm GB width



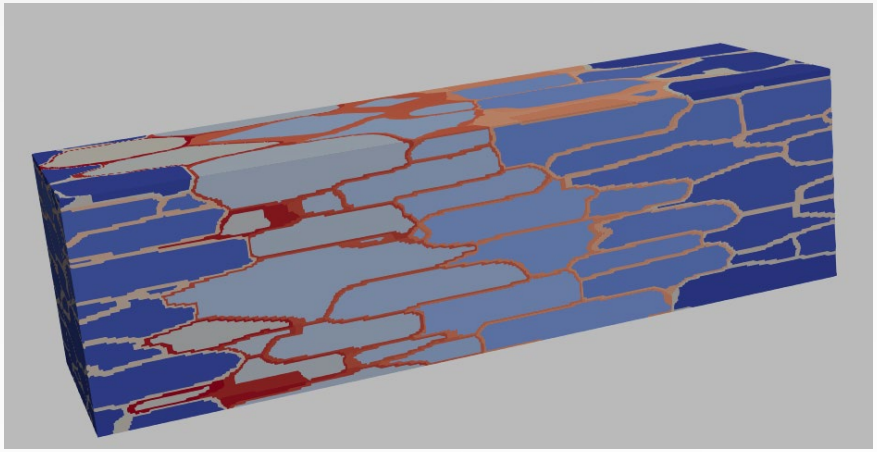


Damage initiation at GBs with high solute concentration

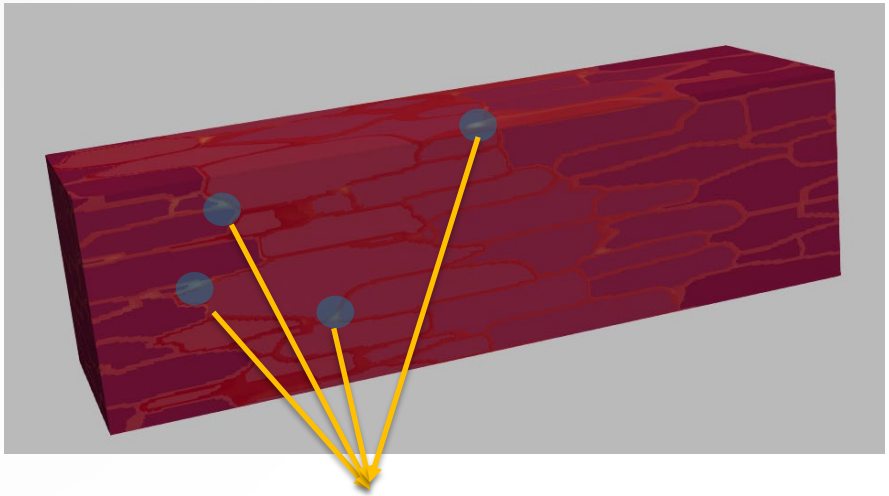
Intergranular crack propagation

Future work

- Effect of texture on delayed fracture
- Simulations on realistic microstructures and parameter set
- Source terms for hydrogen



Experimental microstructure



Damage initiation at GBs

Acknowledgments:

- F. Roters
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- V. Shah
- C. Bos
- J.S. Van Dokkum
- V. Rezazadeh

Thank you

TATA STEEL

DAMASK
Düsseldorf Advanced Material Simulation Kit

M2i materials innovation institute

MAX-PLANCK-INSTITUT FÜR EISENFORSCHUNG GmbH

Suggestions and Questions!!!

Thank You!

```yaml
phase:
Aluminium:
  lattice: cF
  mechanical:
    elastic: {type: Hooke, C_11: 106.75e9, C_12: 60.41e9, C_44: 28.34e9}
    plastic:
      type: phenopowerlaw
    eigen:
      - type: solutestrain
        epsilon_solute: [0.01]
  damage:
    - {type: isobrittle, G_crit: 1.1, G_crit,c: -4.5,
       c_ref: 0.1, l_c: 1.0e-06, mu: 0.001}
  chemical:
    V_m: 1.0e-05
    f_GB: 0.0
    energy_type: quadEnergy
    components:
      bulk:
        H: {M: 1.0e-14, c_0: 0.02, c_eq: 0.0, 'G,c': 0.0, 'G,c^2': 504.5}
      dislocation:
        H: {c_0: 0.0, c_eq: 0.0, 'G,c': 0.0, 'G,c^2': 250.0}
GB:
  lattice: cF
  mechanical:
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    plastic:
      type: phenopowerlaw
  damage:
    - {type: isobrittle, G_crit: 1.1, G_crit,c: -4.5,
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    f_GB: 0.01
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      GB:
        H: {c_0: 0.2137, c_eq: 0.0, 'G,c': 0.0, 'G,c^2': 45.0}
```
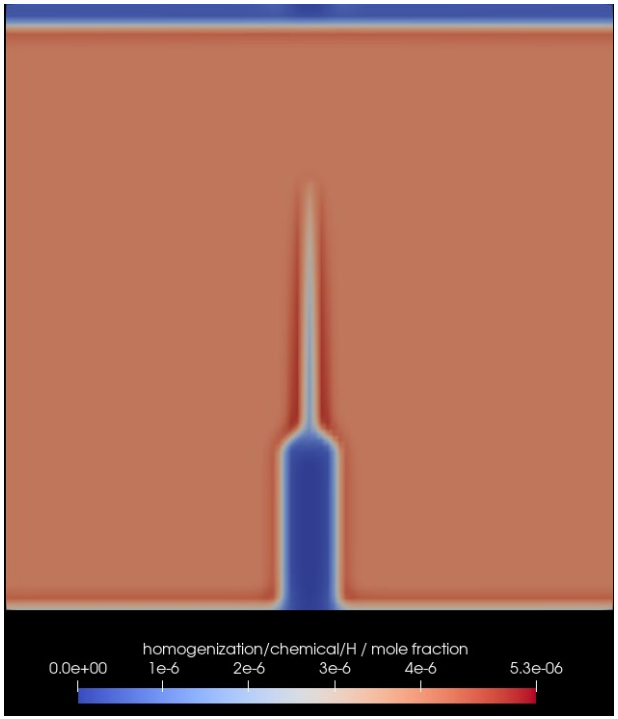

Solution - Multiphase field?

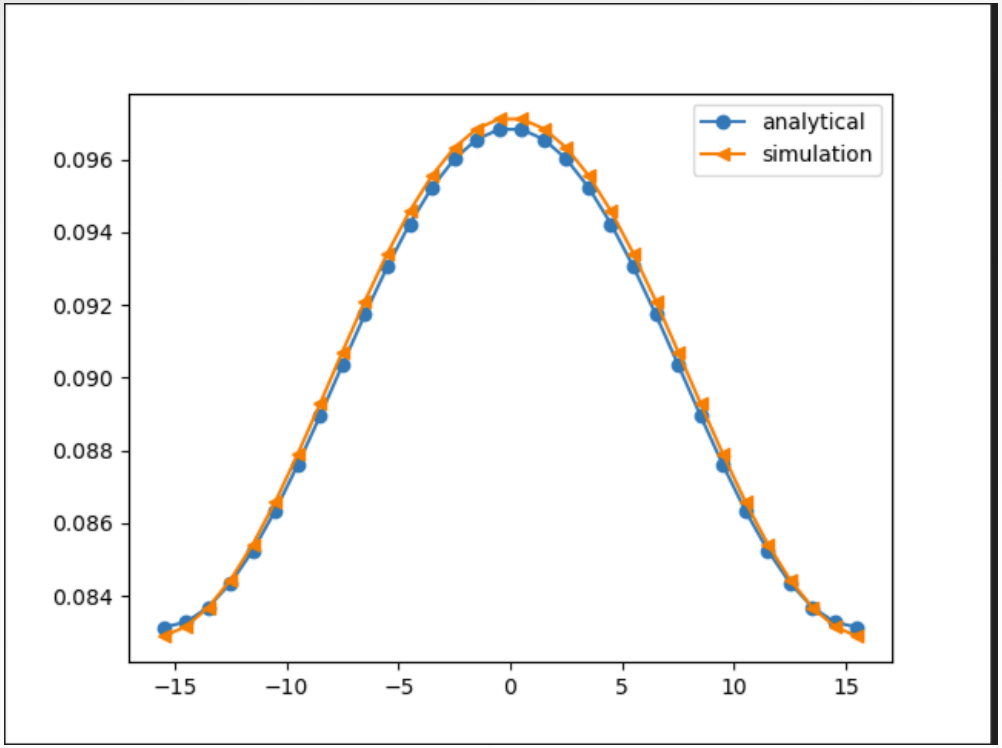
Assign new phase properties to the damaged region with lower equilibrium concentration

$$G = \phi^2 \tilde{\psi_E}^M + \left(1-\phi^2\right)\tilde{\psi_E}^A + \frac{G_c}{l_c}\left(1-\phi\right) + \frac{1}{2} l_c G_c |\nabla \phi|^2$$

- More complicated and numerically challenging
- Not sure if it is needed for what we want to study
- Needs sanity checks

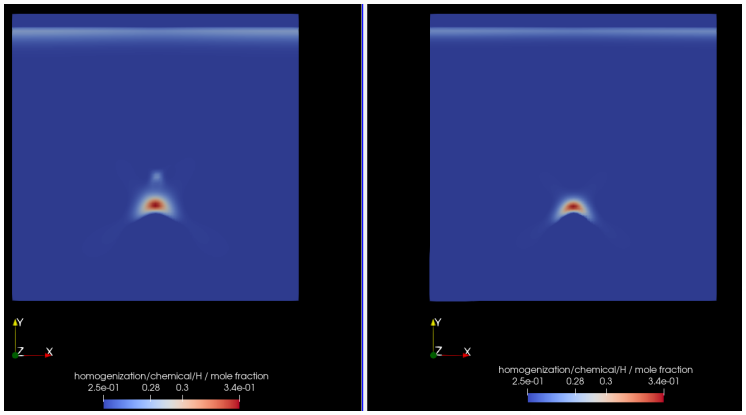


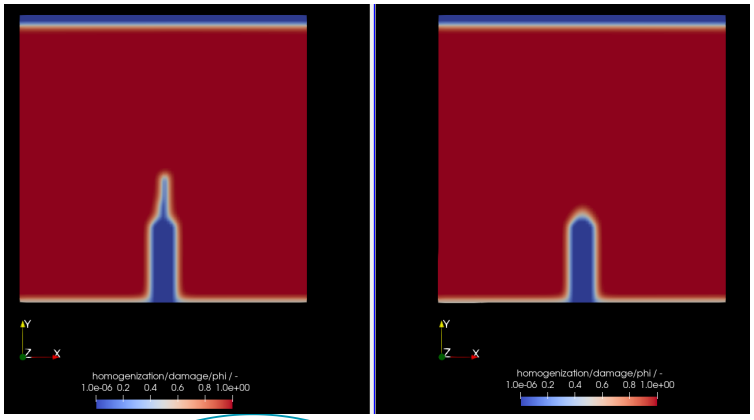
Validation of the solver

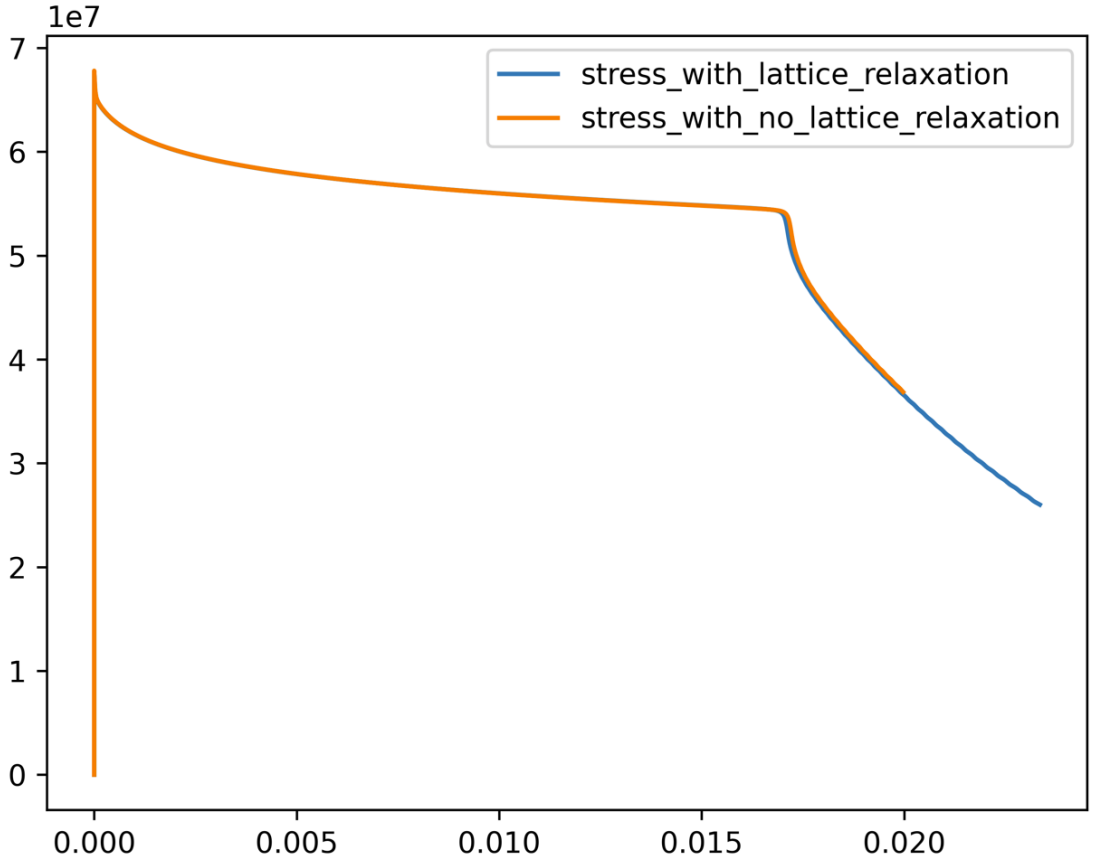


Problems with the diffusion-damage coupling

- Increased concentration at GBs:
  - Currently I artificially increase the concentration using a higher molar volume
  - Also tried using a higher slope for degradation for W_crit
  - Physically, the description of dislocations and GBs in the model should help circumvent this problem
- Solute trapped inside the damaged region:
  - Known problem with coupling Allen-Cahn and Cahn-Hilliard






1e7
7
6
5
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0.000
0.005
0.010
0.015
0.020
stress_with_lattice_relaxation
stress_with_no_lattice_relaxation