

Prediction of static properties of LPBF AlSi10Mg samples post-treated by Friction Stir Processing or thermal treatments

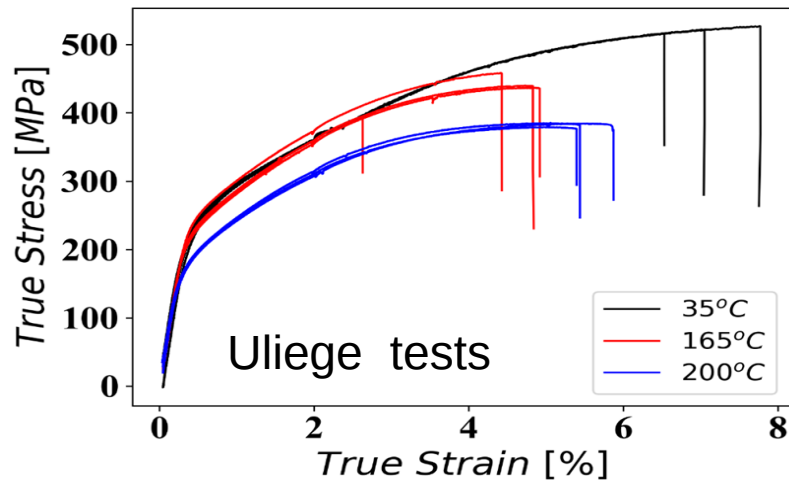
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¹ Materials and Solid Mechanics, University of Liège, Liège,
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Belgium

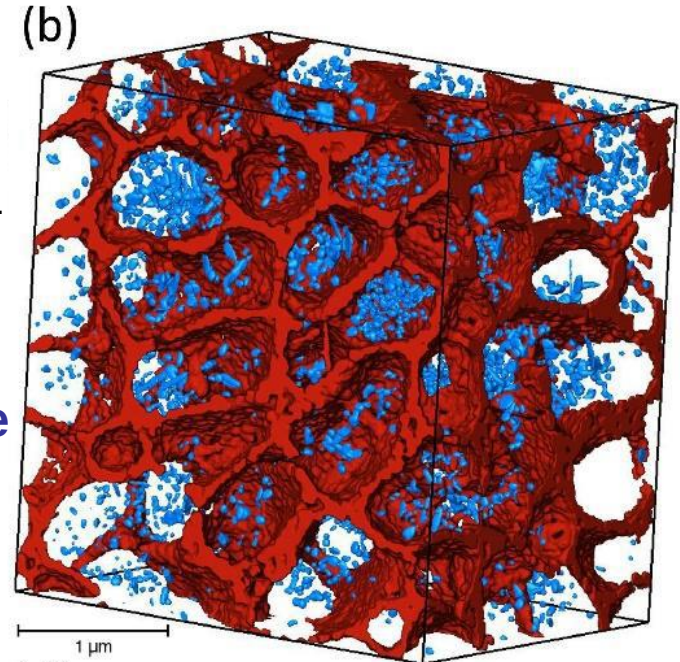
Experimental context

Tensile test AlSi10Mg SLM as – built versus build platform temperature

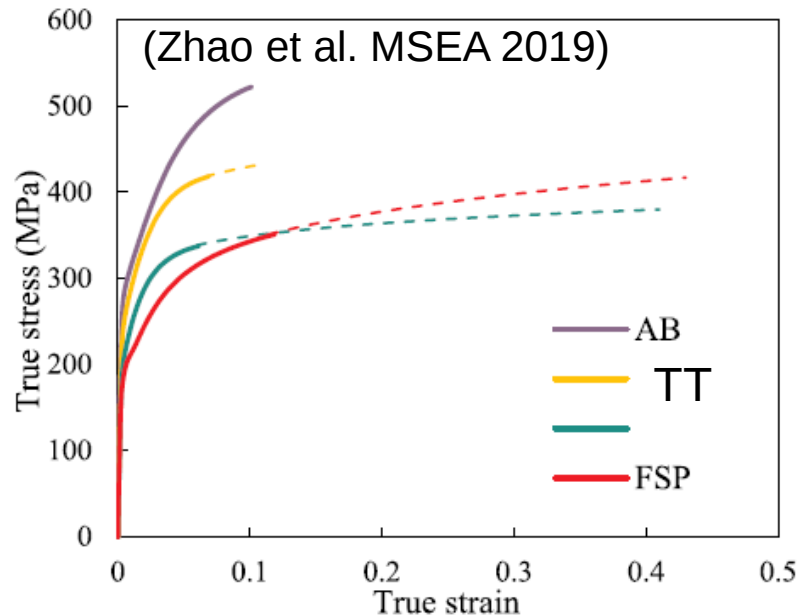


J.G. Santos
Macías Acta
Materialia 201
(2020)

**As built
microstructure
AB**



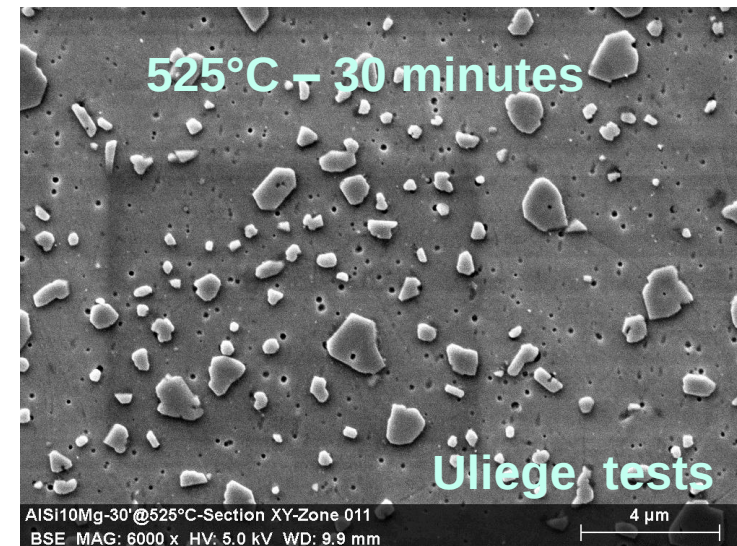
Post treatment effects (thermal treatment **TT** or Friction Stir Processing **FSP**)



+ DSC, SEM, DRX
→ Microstructure
Evolution AB

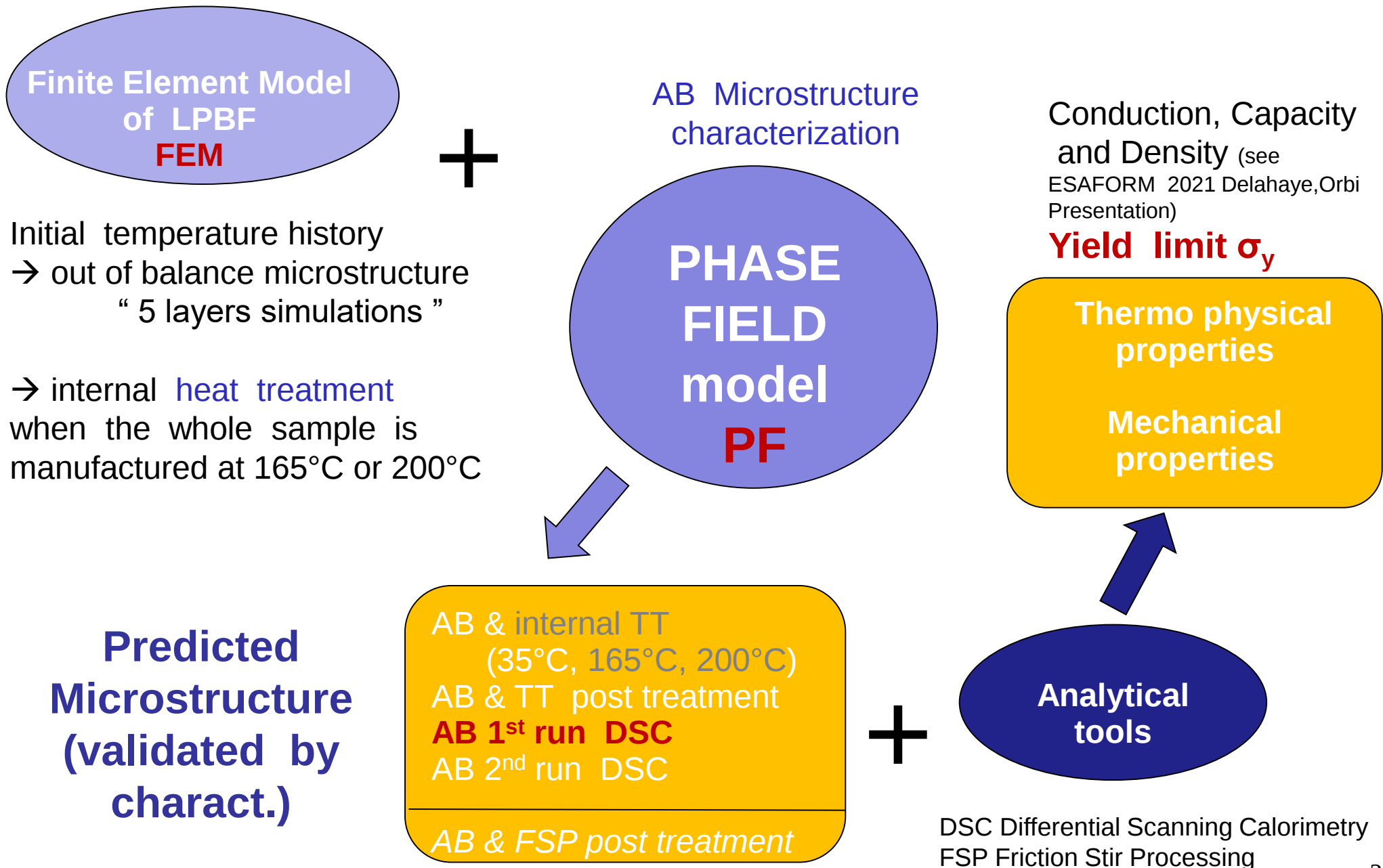
Nano indentation
→ **Local
Mechanical
properties**

Microstructure AB +TT



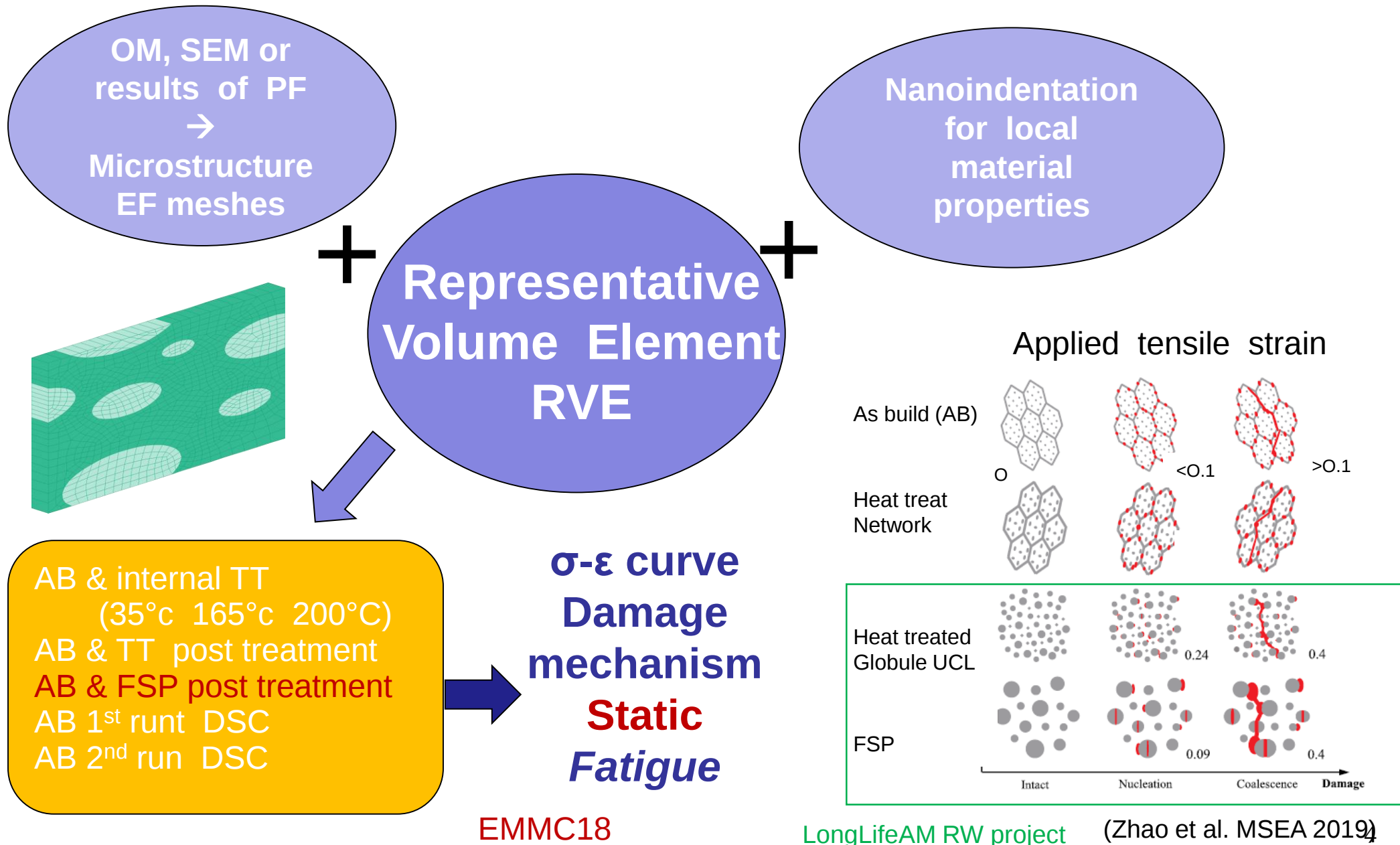
Toward Numerical Material Design

1. Microstructure Prediction & Properties



Toward Numerical Material Design

2. Microstructure Design through RVE



Is Phase Field

+ analytical tool able to provide

- the microstructure
- the thermophysical properties
- the mechanical properties σ_y

?

→ To be confident in Phase Field results:

**First predictions should be validated
by experiments**

Phase-Field model

AlSi10Mg simplified : Al-Si α -Al matrix + Si-diamond

Delahaye
et al.
Rice
2021

Novelties

Enhanced
diffusion

Elastic free
energy

Efficient
implementation

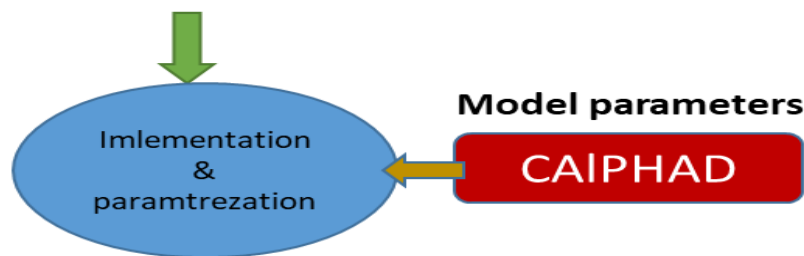
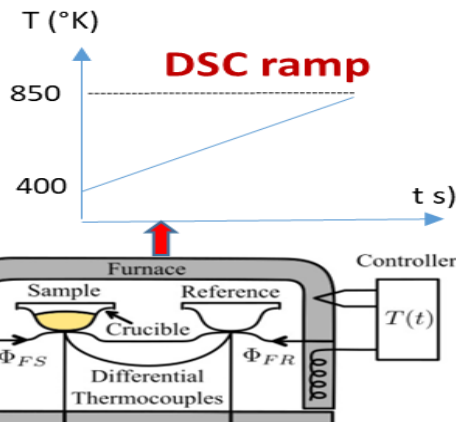
Anisotherm
al loading

KKS
definition

Adaptive
time
stepping

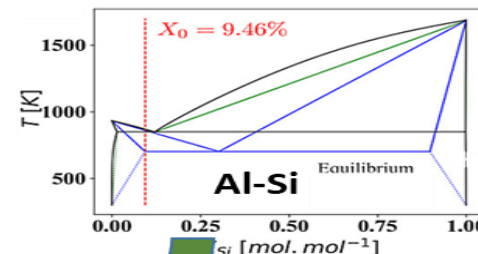
Uliege enhanced
Kim Kim Suzuki
"KKS" model

Fetni et al.
Complas
2021



Outputs

Microstructural changes, Si-content evolution, thermo-physical properties (e.g. Conductivity, heat capacity ...)



Analysis

See

- S.G. Kim Physical Review E 60 (6) (1999) 12
- J.Z. Zhu, Acta Materialia 52 (2004)

Phase-Field model validation

2D simulation of a AB AlSi10Mg heated at a rate 20 K/min for DSC modelling

Governing equations:

Cahn Hilliard

$$\frac{\partial X_{Si}}{\partial t^*} = D^* \nabla^* \cdot \left[\frac{f_{0X_{Si}\eta}}{f_{0X_{Si}X_{Si}}} \nabla^* \eta + \nabla^* X_{Si} \right]$$

Allen Cahn

$$\frac{\partial \eta}{\partial t^*} = -L^* \left(f_{0\eta}^* - \kappa^{*2} \nabla^{*2} \eta + e_{el\eta}^* \right)$$

η 1 → diamond Si phase
 0 → FCC Al phase
 X_{Si} molar fraction of Si
 F_0 homogeneous free energy density
 e_{el} elastic strain energy
 K interface contribution
 L interface kinetic coefficient
 D diffusion coefficient

* Modified due to excess of vacancies

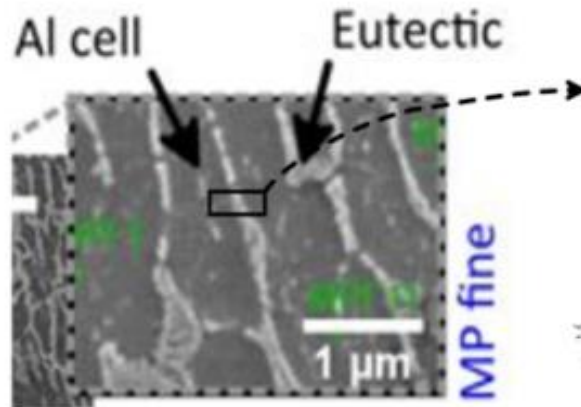
=> Fourier spectral method (FFT) with a semi-implicit form

$$\frac{\{X_{Si}\}_k^{n+1} - \{X_{Si}\}_k^n}{\Delta t} = D^* i\mathbf{k} \cdot \left\{ \frac{f_{0X_{Si}\eta}}{f_{0X_{Si}X_{Si}}} [i\mathbf{k}' \{\eta\}]_{k'}^n \right\}_k^n - D^* k^2 \{X_{Si}\}_k^{n+1}$$

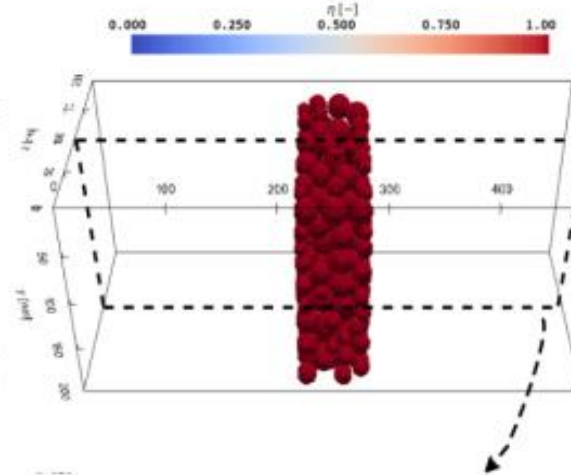
$$\frac{\{\eta\}_k^{n+1} - \{\eta\}_k^n}{\Delta t} = -L^* \left(\{f_{0\eta}^*\}_k^n + \kappa^{*2} k^2 \{\eta\}_k^{n+1} + \{e_{el\eta}\}_k^n \right)$$

Phase-Field enhanced KKS model

2D simulation of a Si precipitate “wall”
representative of AB microstructure

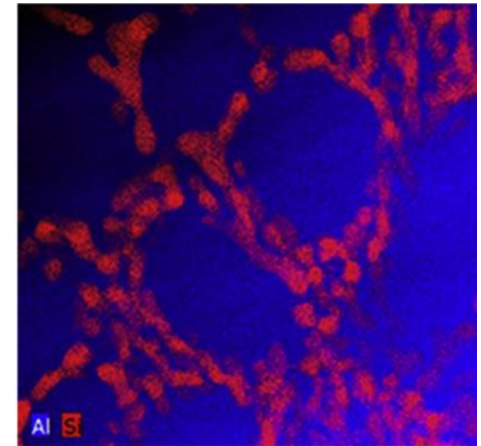


(a)



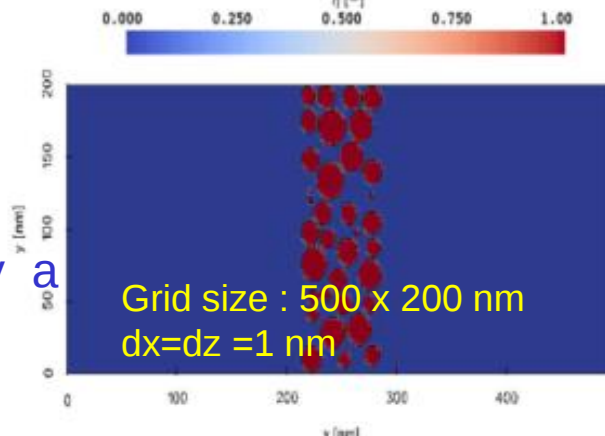
(b)

Loading:
heating rate 20
K/min



X.P. Li et al., Acta Mater. 95 (2015), 74-82

1st case L
(interface
mobility
coefficient)
bounded by a
fct of T_p°)

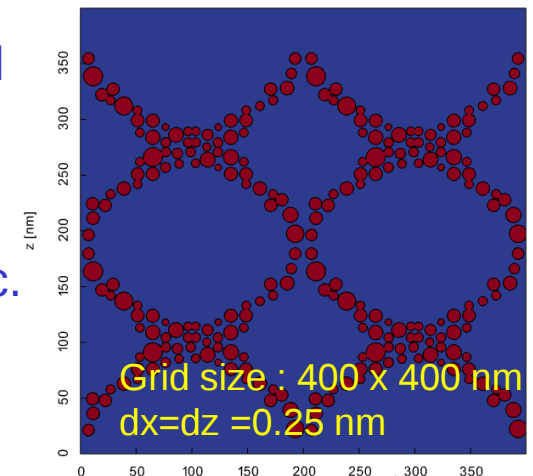


2nd case L not bounded

$L \downarrow$: microstr. evolution
interface controlled,
low transformation kinetic.

$L \uparrow$: diffusion-controlled,
high kinetic for $T_p^\circ \uparrow$

Eutectic network



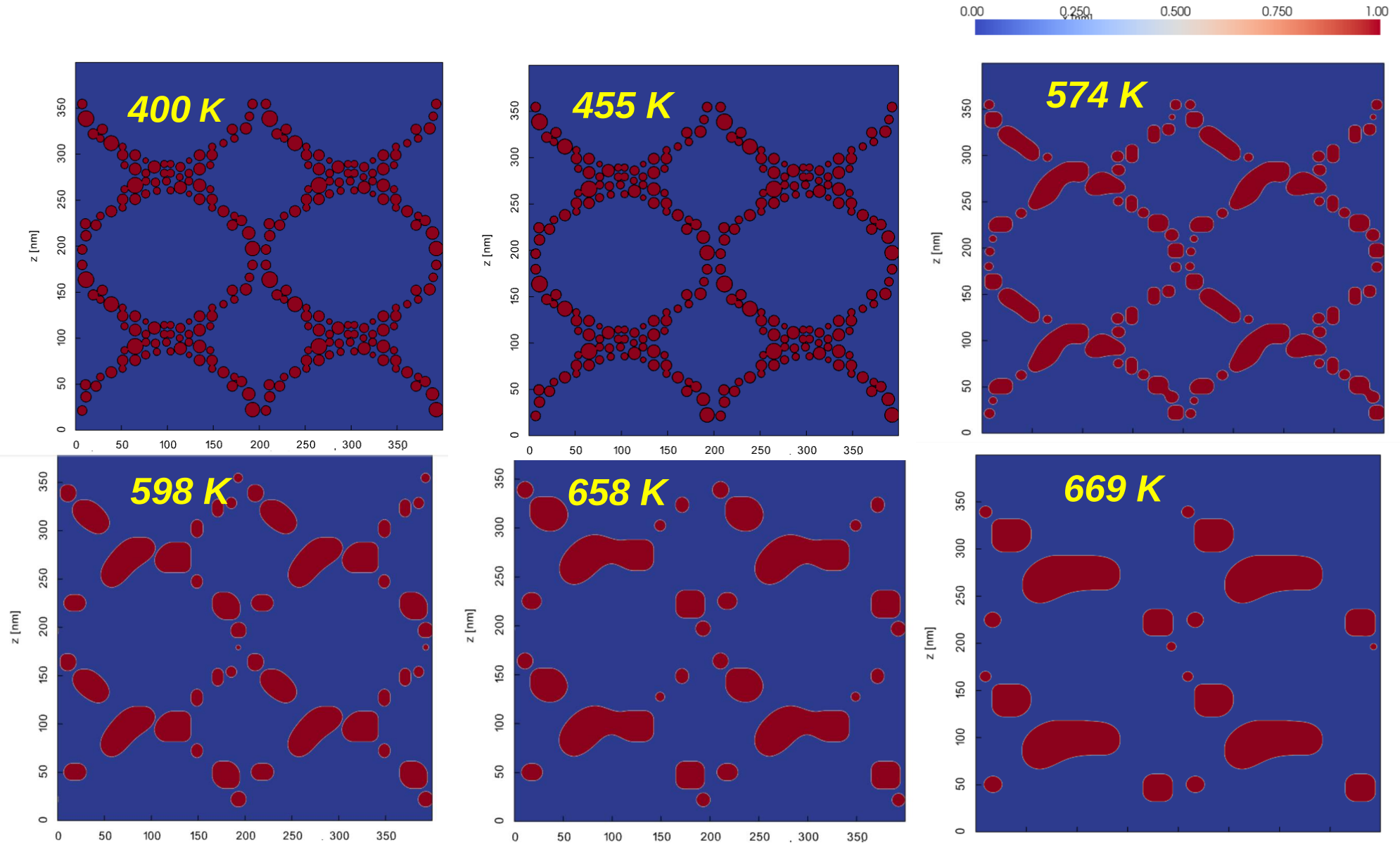
See Delahaye et. al ICAA2020 conf and
ESAFORM 2021 (Orbi pdf)

Initial Si particle : $\phi=20$ nm

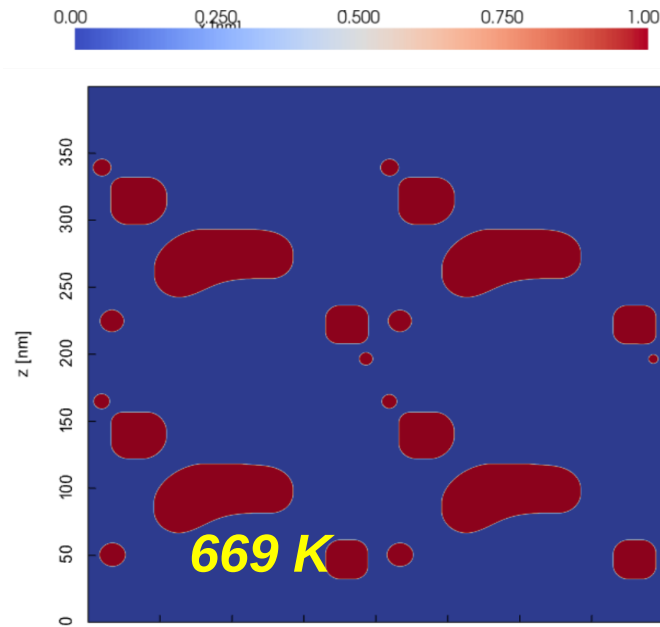
EMMC18 Representative network of
eutectic rich Si “walls” of AB

Phase-Field simulations

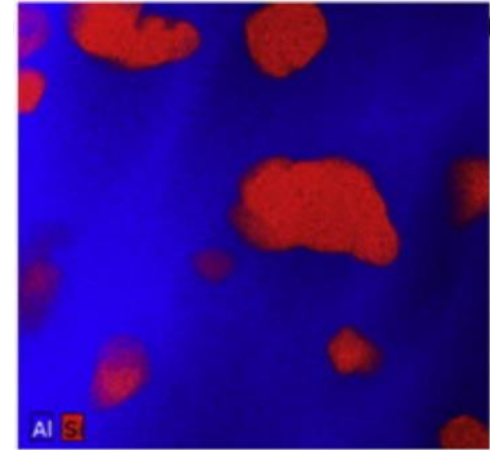
2D simulation of a Si precipitate wall heating rate 20 K/min // DSC 1st run



Phase-Field result versus experiment



- ⇒ Evidence of the coalescence and growth phenomena
- ⇒ rich-Si eutectic network disappears



STEM-EDX maps of the Al and Si distribution in the Al–12Si alloy, isothermal Loading at 500 °C for 4h

X.P. Li et al., Acta Mater. **95** (2015), 74-82

Delahaye et al.
Rice 2021 (Orbi Uliege)

Link with DSC capacity and conductivity curves ongoing

*Delahaye et al article,
submitted ActaMat*

Analytical tools based on microstructure

→ Prediction of mechanical properties

For α -Al matrix, Si particles

Analytical tools to compute macroscopic yield strength : σ_y

$$\sigma_y = \boxed{\sigma_i} + \boxed{\sigma_{ss}} + \boxed{\sigma_p} + \sigma_d \quad \nearrow \text{Dislocation hardening}$$

σ_i : Intrinsic yield strength: pure aluminium

σ_{ss} : Solid solution strengthening

σ_p : Precipitation strengthening contribution

In AB effect of
Build platform
Tp° 35°, 165°, 200°C
Eutectic walls and cells

In AB + FSP
Si particles, *ongoing*

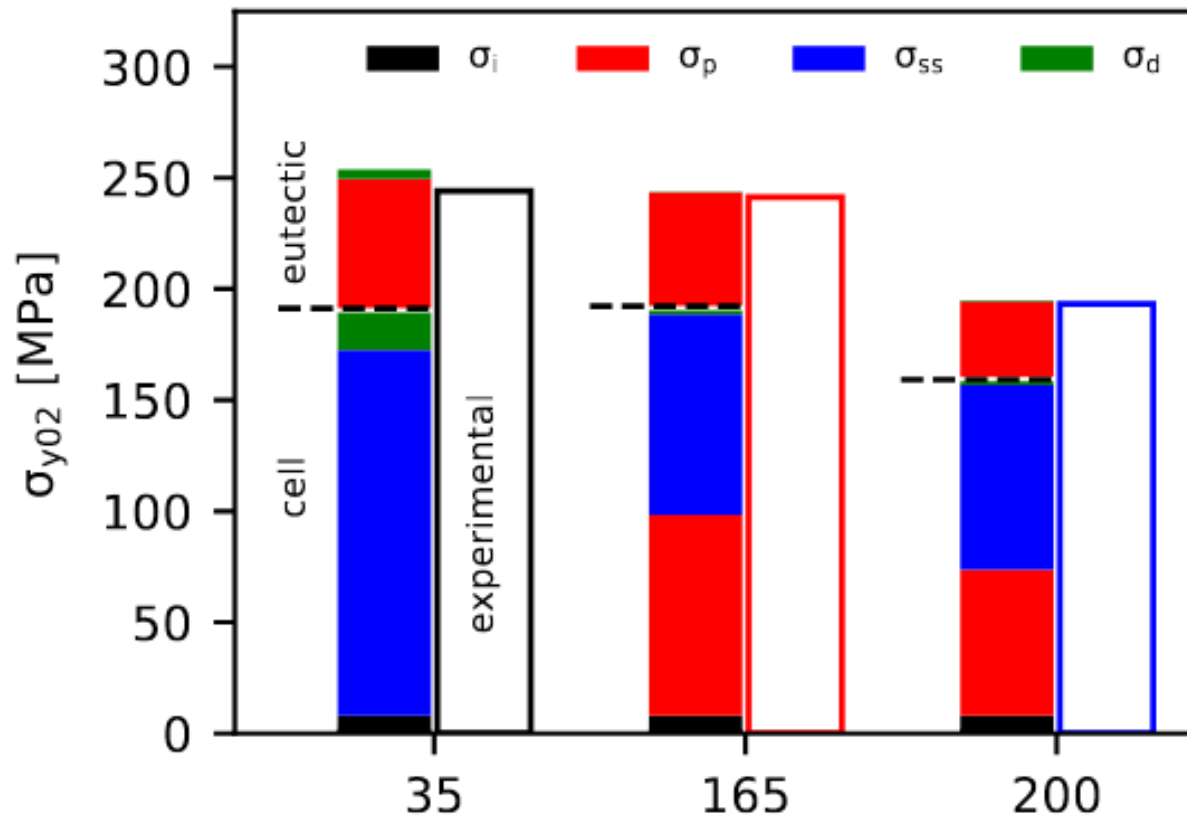
O. Bouaziz and P. Buessler. Mechanical behaviour of multiphase materials : an intermediate mixture law without fitting parameter Rev. Met. Paris 99.1 (Jan. 2002)

O. R. Myhr, Grong, and S. J. Andersen. Modelling of the age hardening behaviour of AlMgSi alloys". Acta Materialia 49.1 (2001)

Analytical tools based on microstructure

→ Prediction of mechanical properties

For As Built 35°C, 165°C, 200°C



σ_i Al yield strength

σ_{ss} Solid Solution

σ_d Si particles

σ_p particles strengthening
in eutectic or cell

+ isomechanical work between
the cells and the eutectic

→ the important effect
of the solid solution in the cells.

→ If temperature ↑:

Precipitation & coarsening
Eutectic ↓

Image and XRD analysis = input of analytical tools ;

Experimental yield stress from tensile tests

Is RVE model able to provide

- Macroscopic σ - ϵ AlSi10Mg for different microstructures
- Local strain and stress fields
- Damage mechanism

?

To be confident RVE results :

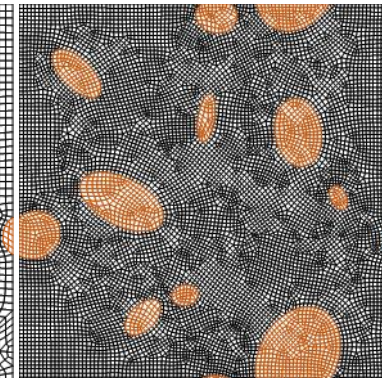
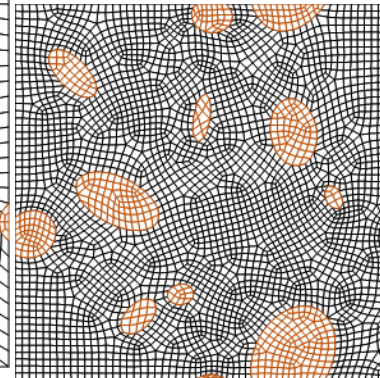
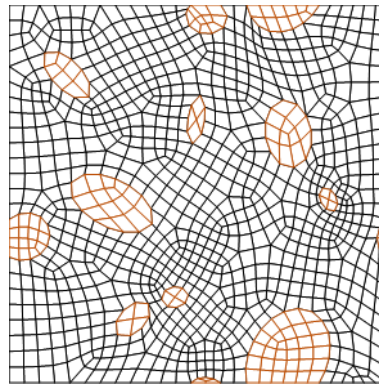
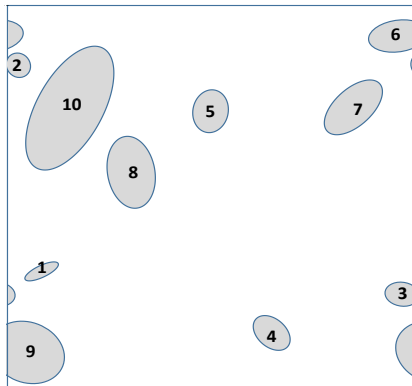
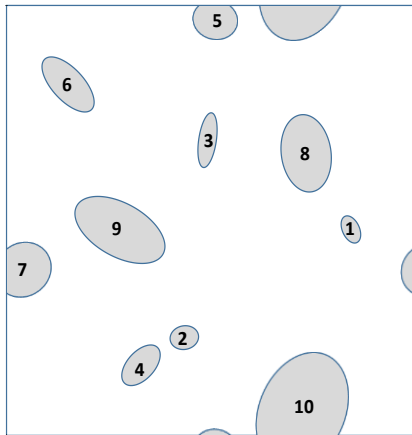
First prediction validated by experiment

AB + FSP → Matrix + Particles → RVE

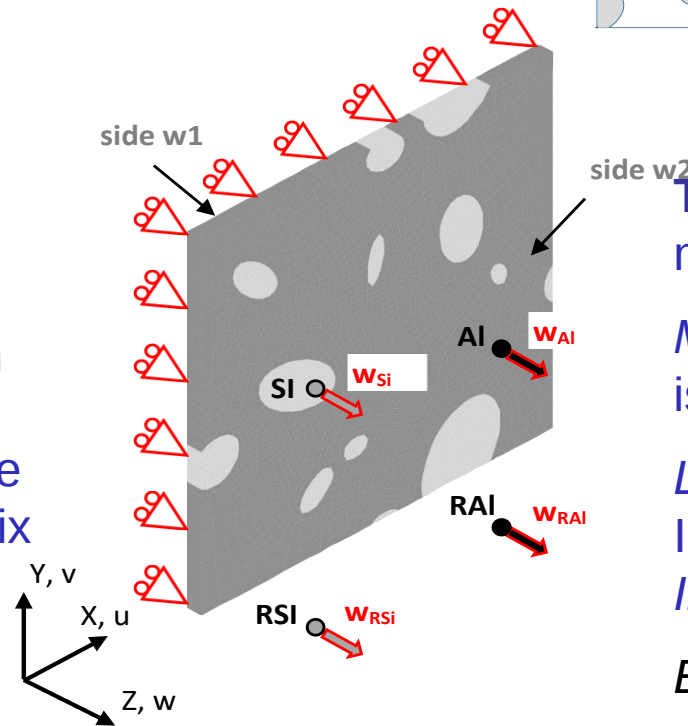
2D or 3D → 2.5D

Representative Size → 10 particles

Mesh density → medium



Strong
strength
ratio
Si particle
 α -Al matrix



Target: representativity of a
macro tensile test in Y dir.

Macro level : $\epsilon_x \approx \epsilon_z$
isotropic material

Local level: strength in z dir
Identical for all particles

Interface: Cohesive elements

Bouffieux et al. 2022

**σ - ϵ curve of
each
components?**

σ - ϵ curves of α -Al matrix, Si particles

AlSi10Mg AB + FSP = α -Al matrix + Si particles

Si : literature + nanoindentation of big particles (young modulus)

α -Al matrix: nano-indentation of α -Al matrix

and interactions with PF + analytical formulas

→ Possibility to validate our approach

→ Possibility to go toward virtual material state

*Tran Song Hoang
et. al submitted to
Int.Journal of
Mec.Sciences 2022*

+ Dedry et al.
Proc. ESAFORM
2021 (PoPuPs)

α -Al matrix characterisation by nanoindentations

1 point $(\epsilon_{r,\theta}, \sigma_{r,\theta})$ for each indenter characterized by its angle α

- Nanoindentation curves**

→ $F = C \cdot h^2$ with F: normal force, h: penetration depth, C: constant

→ $\frac{1}{E^*} = \frac{1 - \nu^2}{E} + \frac{1 - \nu_i^2}{E_i}$ with E^* : reduced modulus of the curve

- K.L. Johnson (J. Mech. Phys. Solids, 1970) → $\epsilon_{r,\theta} = K \cdot \cotan(\theta)$**

the characteristic strain $\epsilon_{r,\theta}$

θ : angle of the equivalent cone, $K = 0,105$ (Bucaille, Acta Mat. 51, 2003)

→ $\theta = \arctan\left(\sqrt{\frac{3 \cdot \sqrt{3}}{\pi}} \cdot \tan(\alpha)\right)$ with α : angle of indenter

- Dao's method (Acta Mat. 49, 2001) + Bucaille method (Acta Mat. 51, 2003)**

$$\Pi_{1\theta} = \frac{C_\theta}{\sigma_{r,\theta}} = \tan^2(\theta) \cdot \left\{ P1 \cdot \left[\ln\left(\frac{E^*}{\sigma_{r,\theta}}\right) \right]^3 + P2 \cdot \left[\ln\left(\frac{E^*}{\sigma_{r,\theta}}\right) \right]^2 + P3 \cdot \left[\ln\left(\frac{E^*}{\sigma_{r,\theta}}\right) \right] + P4 \right\}$$

the characteristic stress $\sigma_{r,\theta}$

P1	P2	P3	P4
0.02552	- 0.72526	6.34493	- 6.47458

α -Al matrix characterisation by nanoindentations

Indentations on grids with 3 different indenters $\rightarrow$ lowest curves for matrix

$\rightarrow$ Swift or Voce hardening law fitting

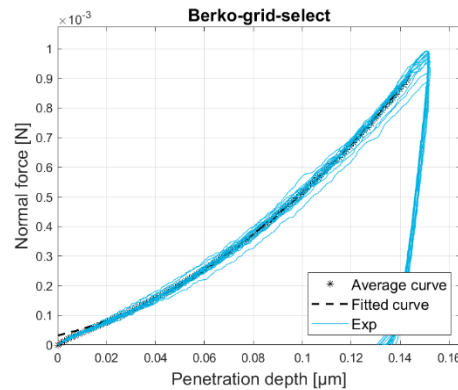
infinite solution if σ_y not defined

$\rightarrow \sigma_y$ from macro tensile macro

$\rightarrow$ Ok high ratio Si/ α -Al strength & low fraction of Si particles (*Tran et. Al 2022*)

Berkovich

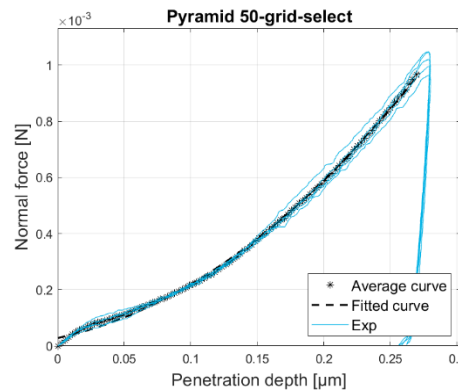
θ_1



V

50°

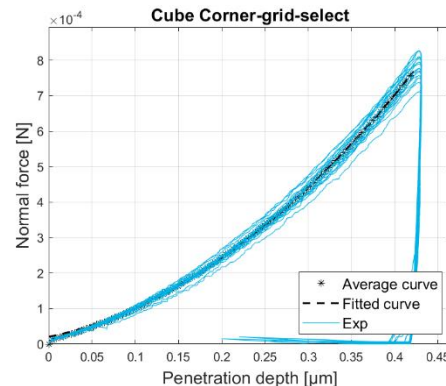
θ_2



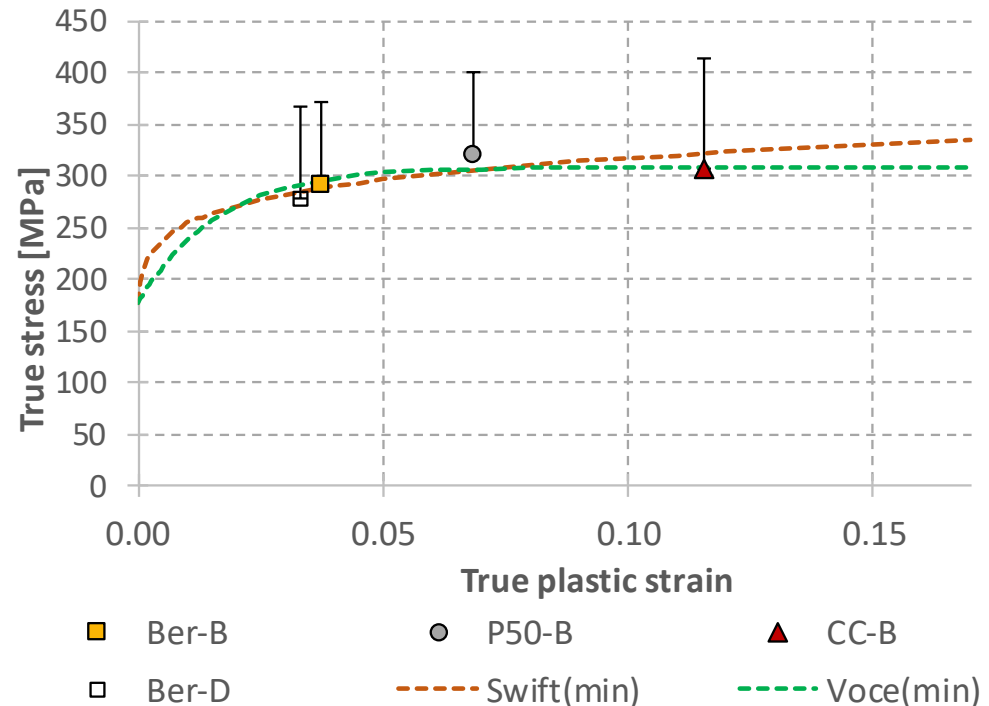
V

Cube corner

θ_3



FSP - matrix

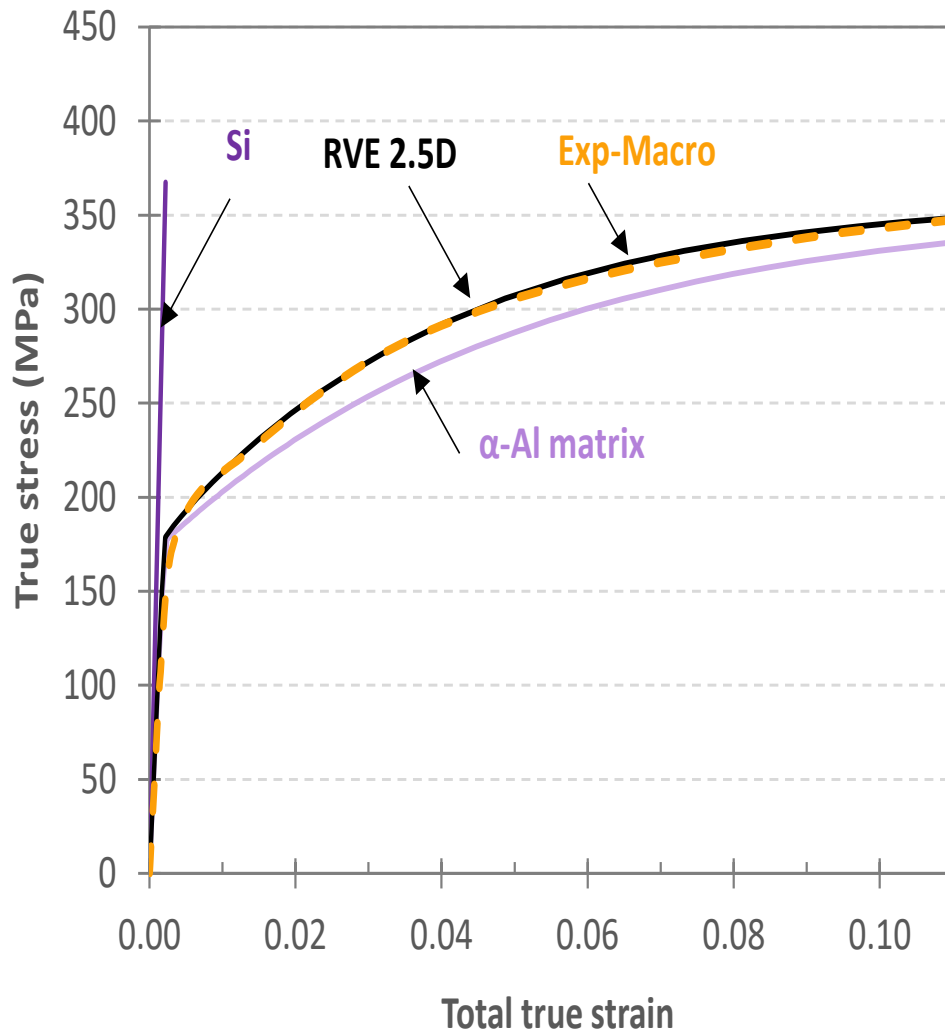


O. Dedry, C. Bouffieux, H;S.Tran, J. Macías, A.M. Habraken, A. Mertens, (2021) ESAFORM proceedings

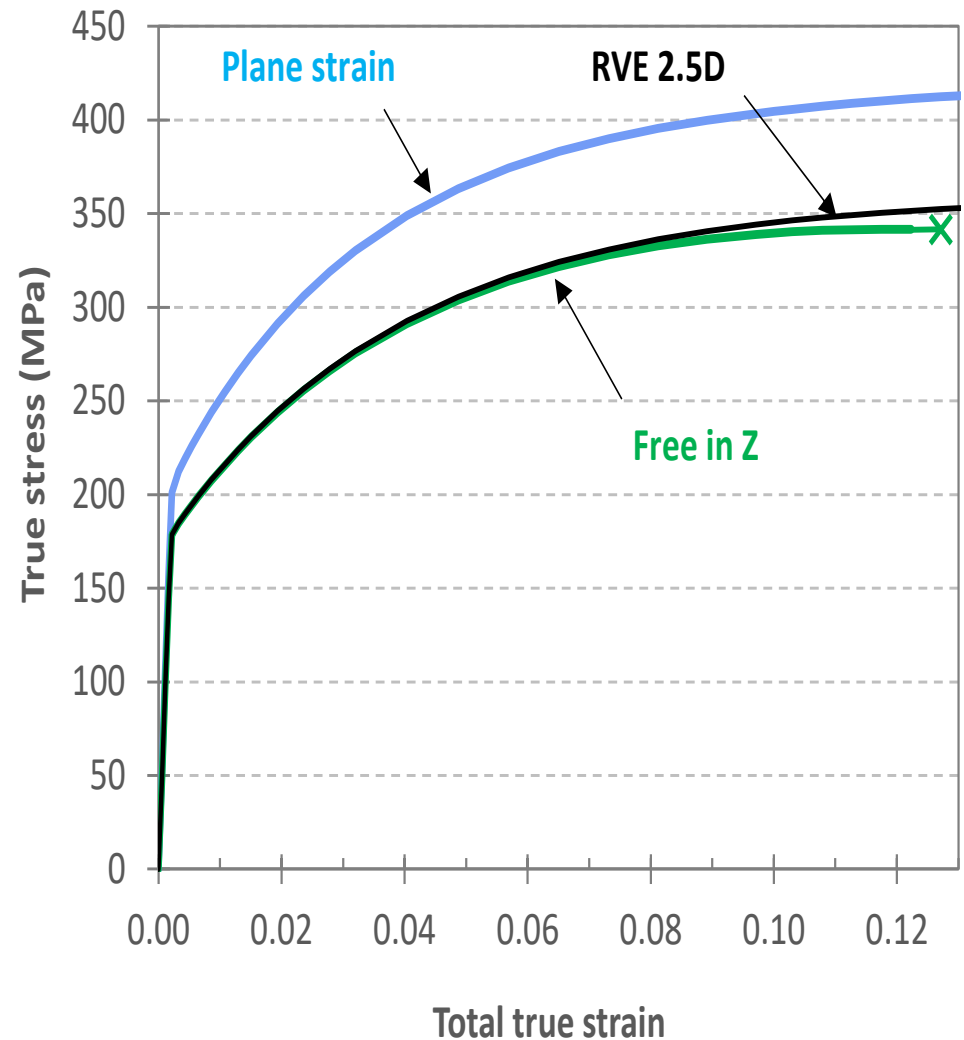
Macroscopic σ - ϵ computed from RVE

Tensile test in y direction

Experimental validation



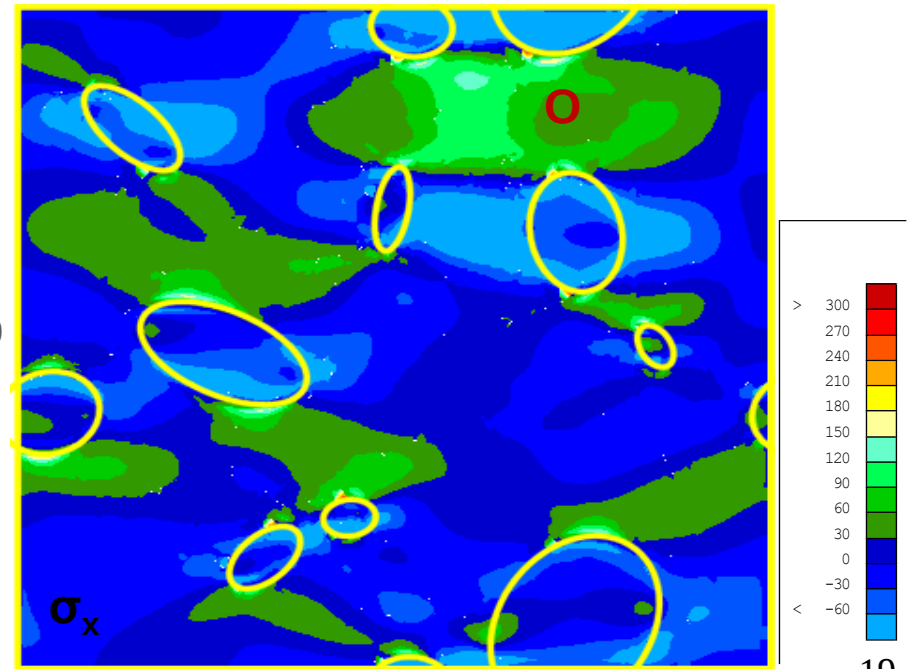
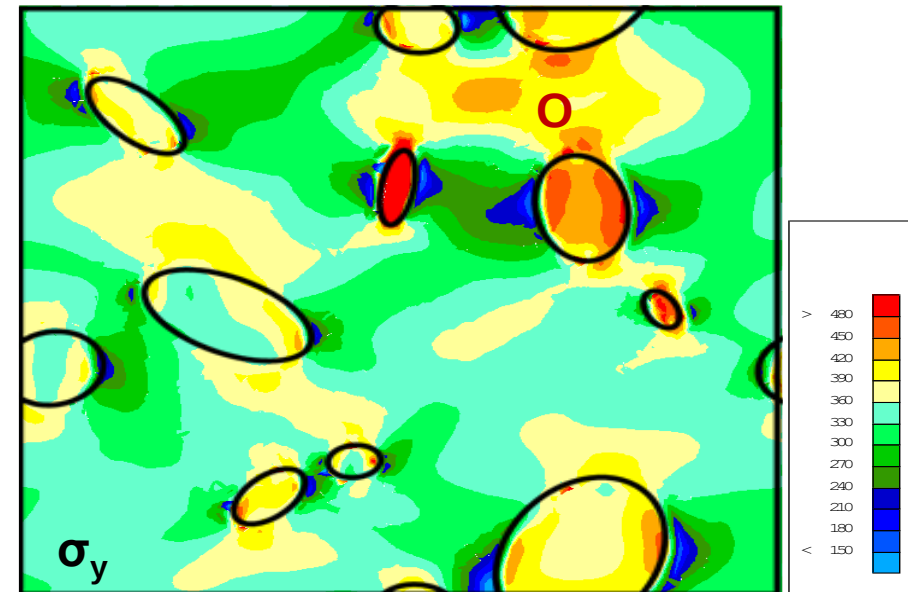
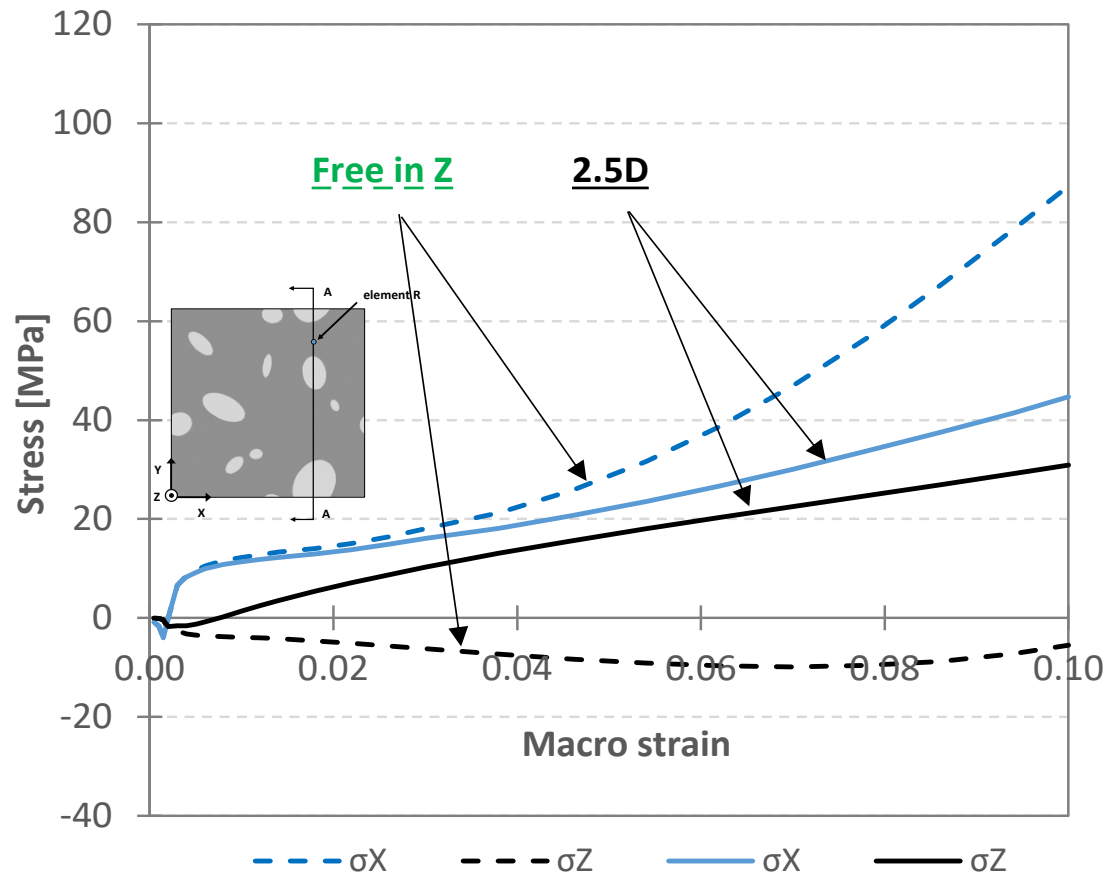
Effect of z boundary condition



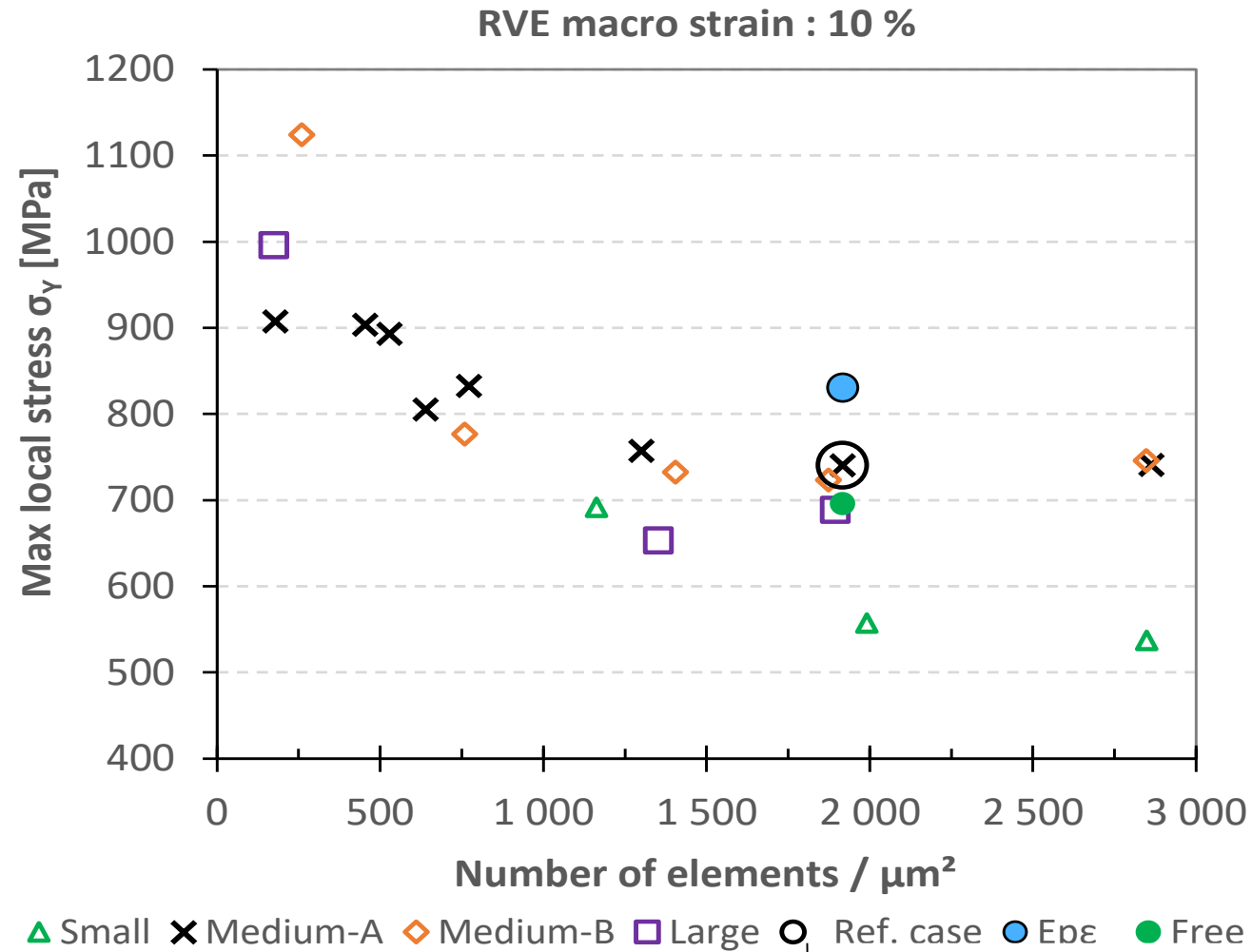
Local stress field

Periodic conditions in XY plane
Force applied in y

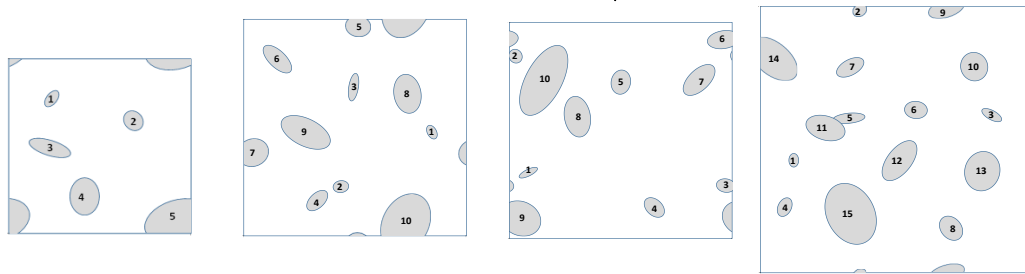
Effect of Boundary conditions in z direction



Sensitivity of local max σ_y to mesh & RVE size



For
Medium-A
RVE
Effect of
boundary
condition



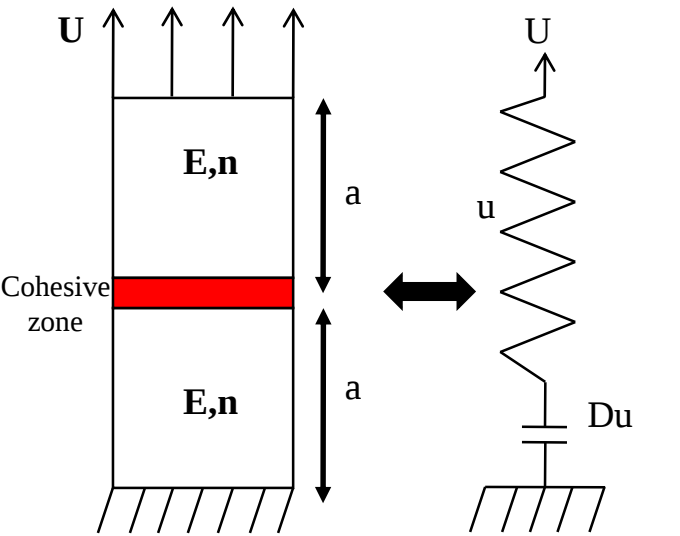
2.5D

Plane
strain

No macro stress
however effect of
strength heterogeneity
(3D law 1 element
layer mesh)

Damage mechanism in static loading

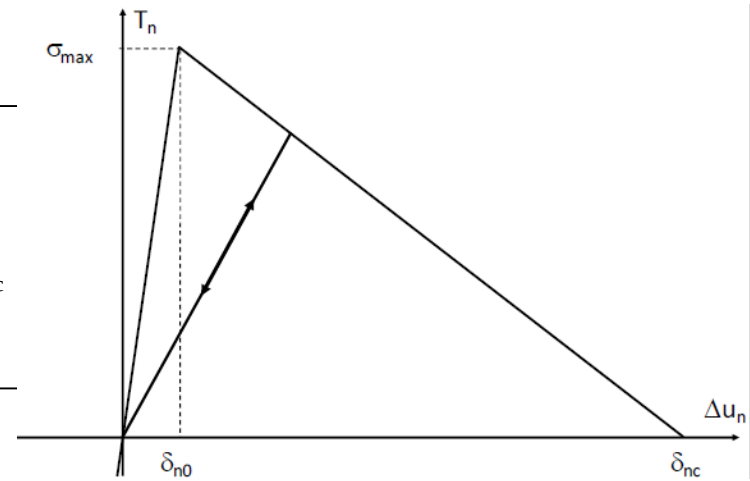
→ Cohesive interface elements



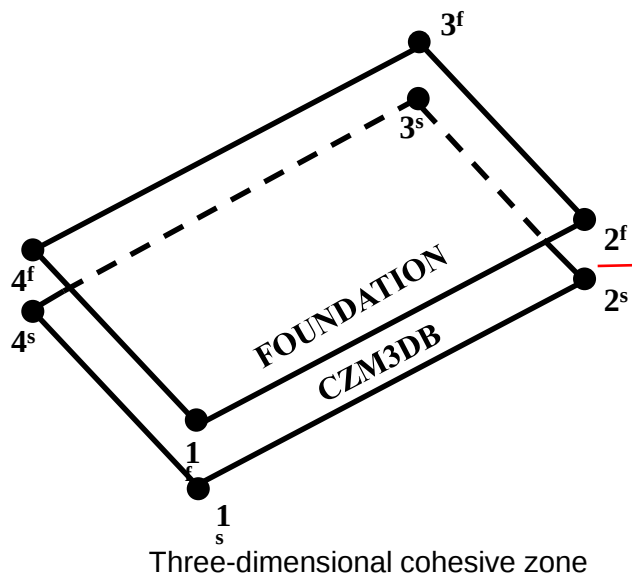
Uniaxial problem to illustrate the jump displacement

$$T = \begin{cases} \frac{\sigma_{\max}}{\delta_0} \Delta u & \text{if } \Delta u < \delta_0 \\ \sigma_{\max} \frac{\delta_c - \Delta u}{\delta_c - \delta_0} & \text{if } \delta_0 \leq \Delta u \leq \delta_c \\ 0 & \text{if } \Delta u > \delta_c \end{cases}$$

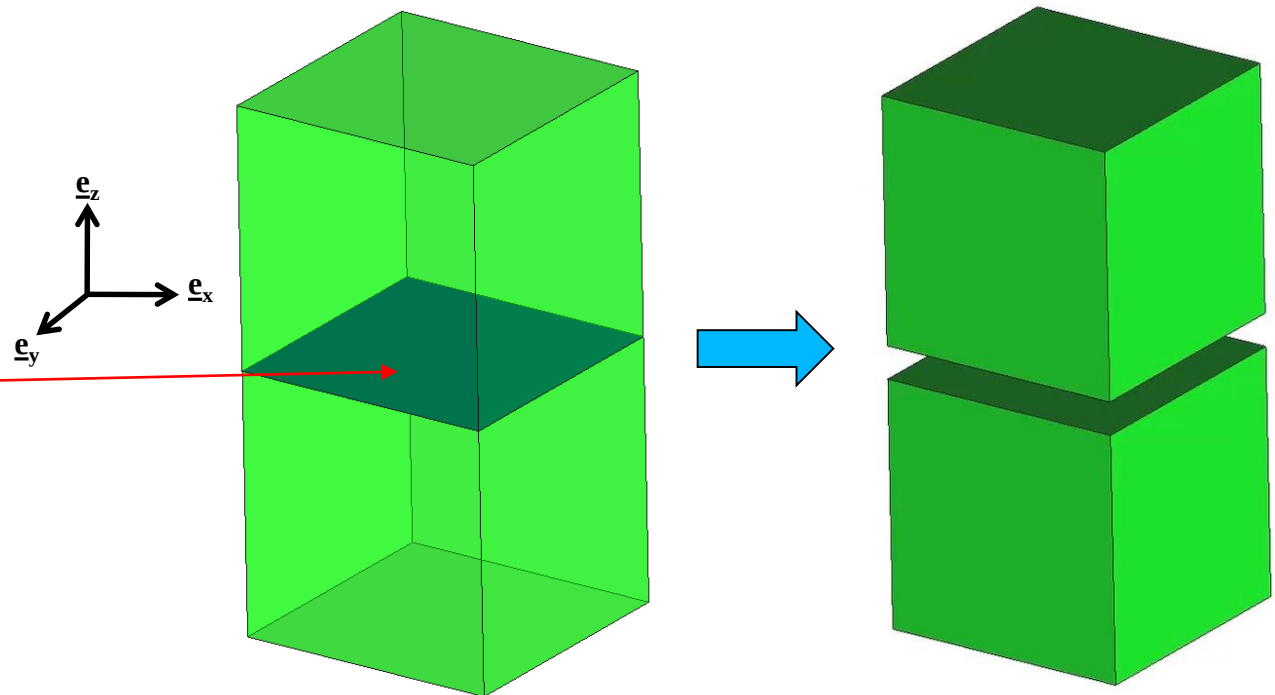
Bilinear law



Traction separation law

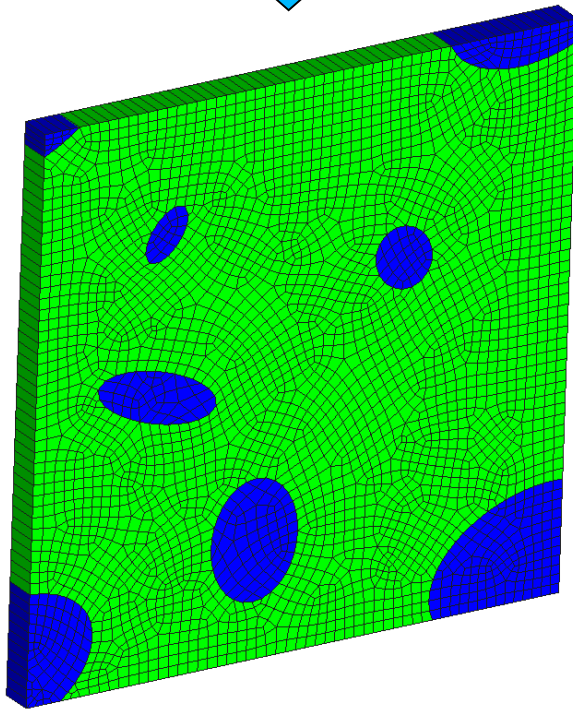
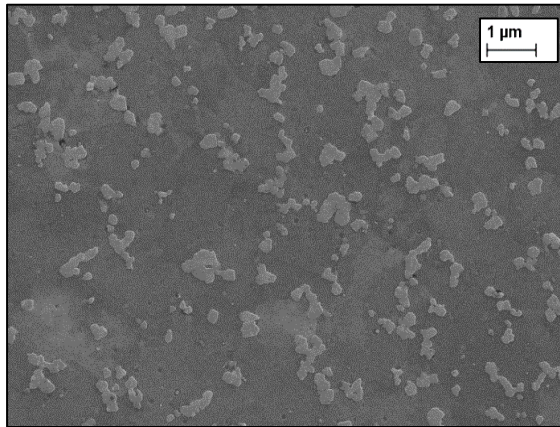


Three-dimensional cohesive zone



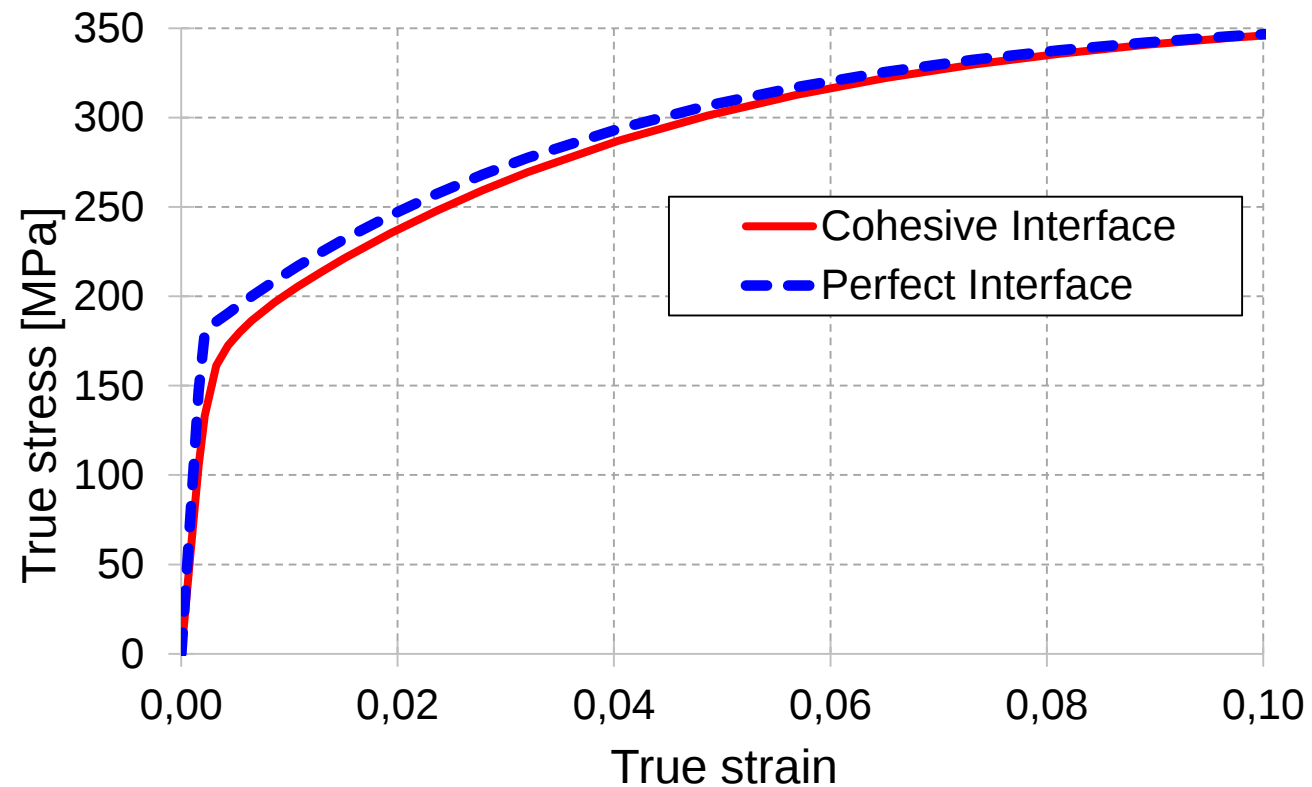
Cohesive zone modelling

Microstructure of AlSi10Mg after FSP



Finite element model of the Representative Volume Element (RVE)

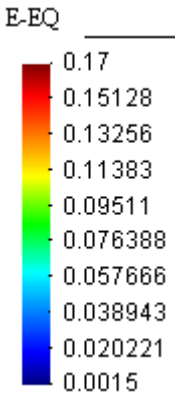
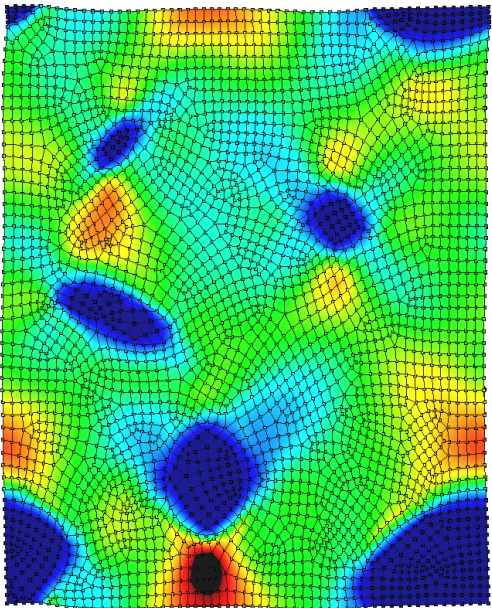
$\sigma_{\max}$	δ_{n0}	δ_{nc}	$\tau_{\max}$	δ_{t0}	δ_{tc}
550	5.5E-6	6E-6	550.	5.5E-6	6E-6



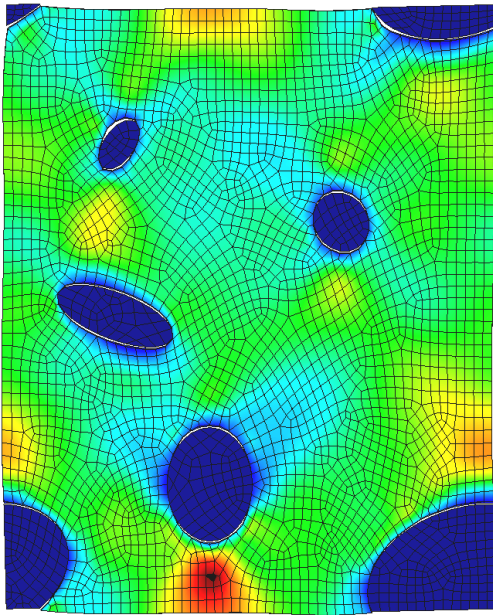
Sensitivity of local field assumption at macro strain 0.1

Equivalent Strain

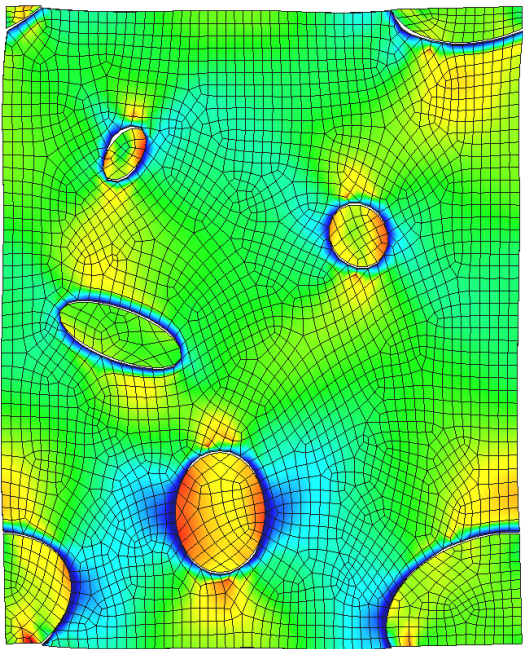
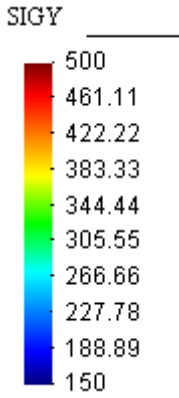
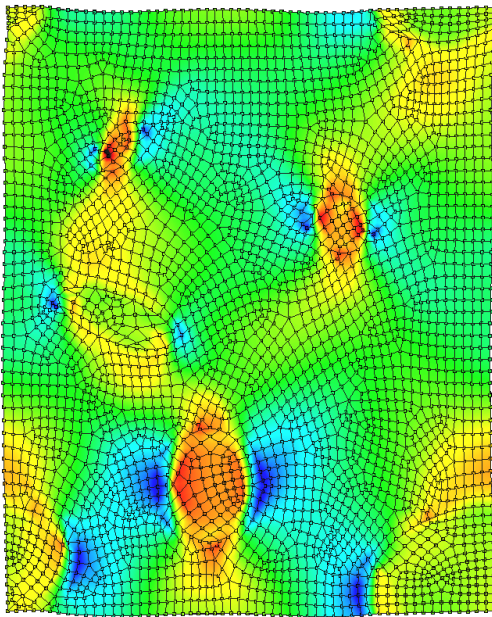
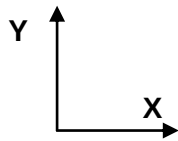
Perfect Interfaces



Cohesive Interfaces



Stress-YY



Toward numerically optimize post treatments of AB (TT, FSP) ?

2.5D RVE developed → validated macro stress strain tensile curve ✓
→ local stress and strain fields available ✓
→ damage mechanism in static loading *ongoing*
(Input data from experiments or Phase Field approach)

Phase field → microstructures predicted from T_p° history ✓
→ validated by 1st run DSC curve ✓
+ microstructure evolution (EMMC18)

Analytical tools → validated mechanical properties
on AB 35°C, 165°C, 200°C ✓
(Input data from experiments, from PF *ongoing*)
→ validated thermophysical properties on AB 35°C ✓
(Input data PF, Delahaye et al. Rice 2021, ESAFORM 2021)

Next steps:
fatigue
fatigue experimental campaign
RVE predictions via damage constitutive laws