Full-field modeling of spheroidization phenomenon in α/β titanium alloys during hot-deformation and subsequent annealing at a given temperature.

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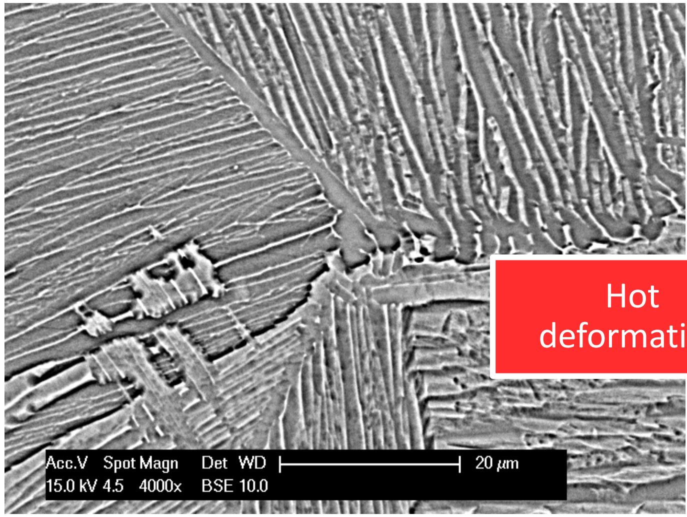
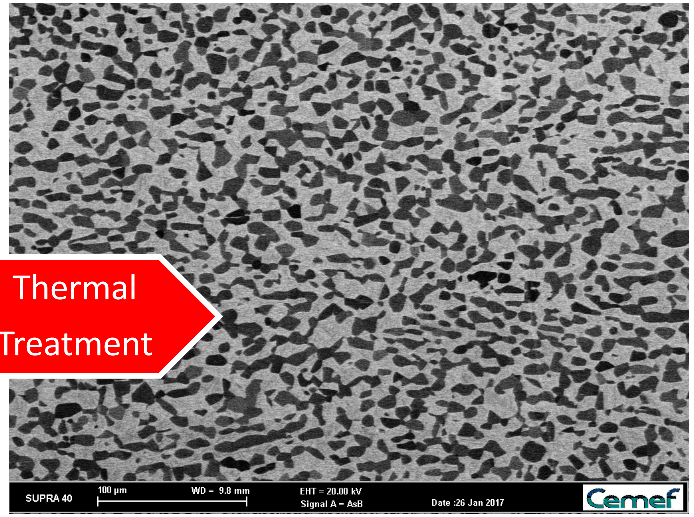
Overview

What is spheroidization in α/β titanium alloys ?



Hot deformation + Thermal Treatment



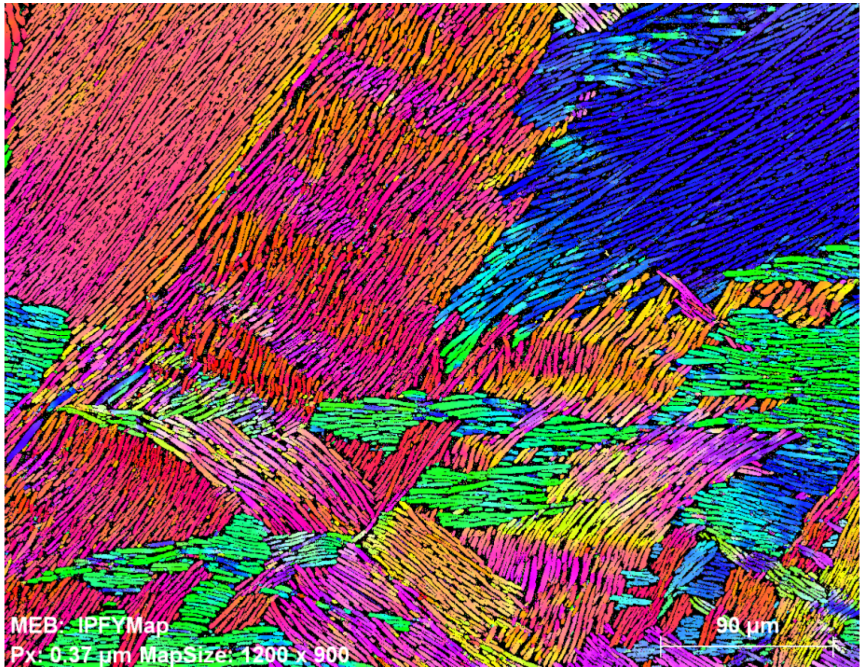
Why?

- **α/β titanium alloys show attractive mechanical properties for industrial use.**
- **Spheroidization is a very important phenomenon for the microstructural control**
- **Speroidized microstructure shows enhanced strength and ductility**

Goals

To develop a global experimental and numerical framework in order to understand and simulate the phenomenon of spheroidization

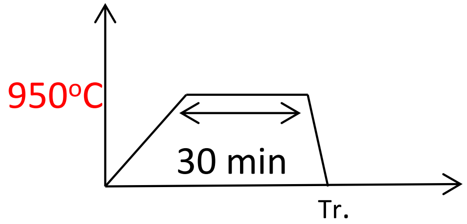
Which are the main governing mechanisms?



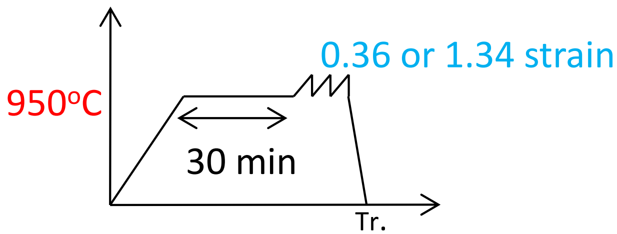
Titanium
α phase

- β Grains Size ≈ 0.25 – 0.7mm
  - Laths thickness ≈ 1-2 µm

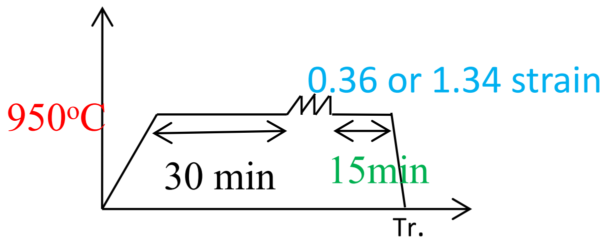
Initial state



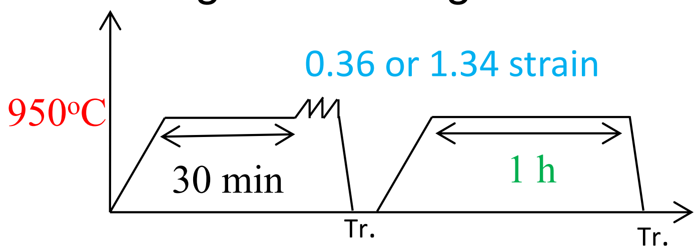
Deformed state



Short annealing state

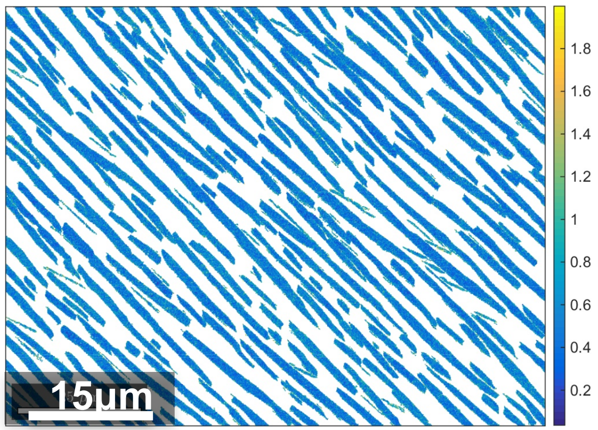


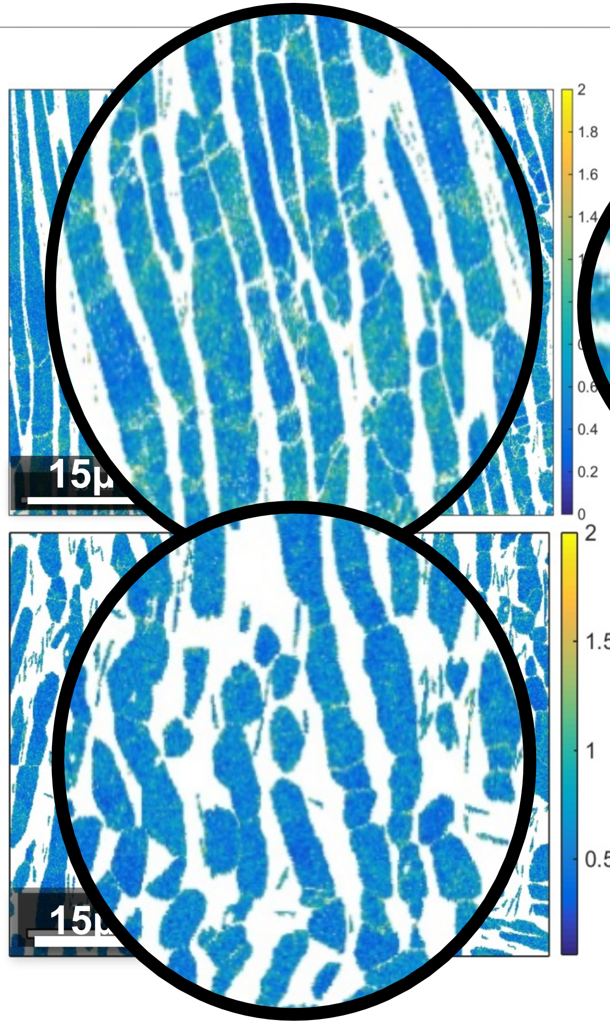
Longer annealing state



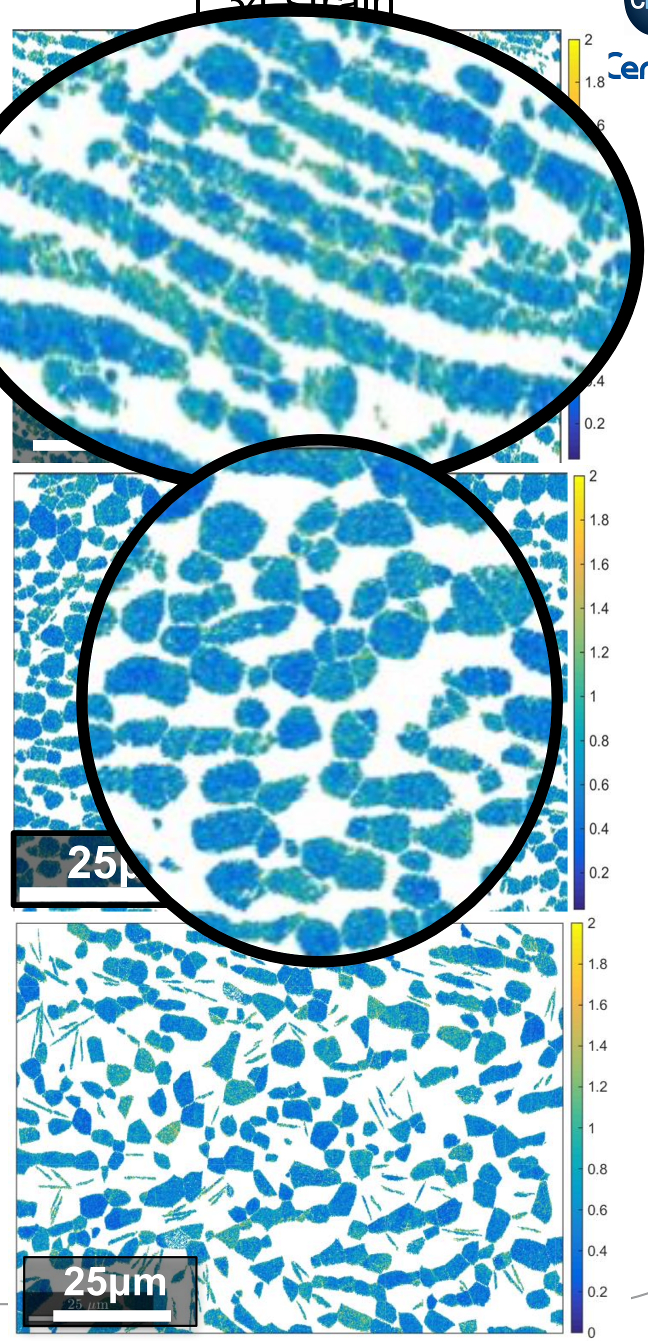
Microstructural evolution

Before deformation





1.34 strain



+ 15min annealing

Conclusions

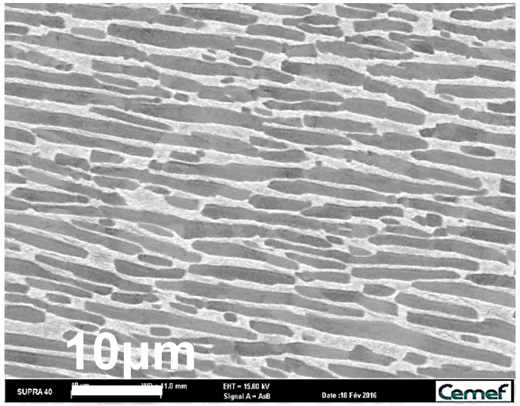
The higher the strain the quicker is the evolution during annealing

+ 1h annealing

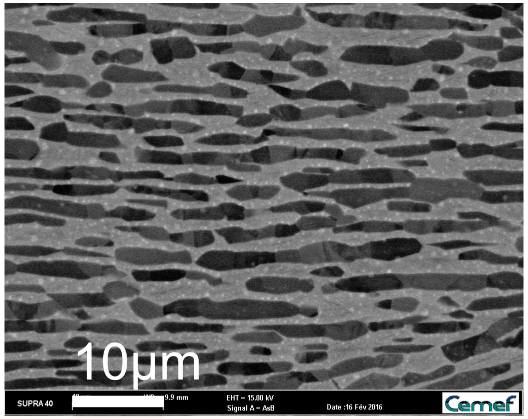
Quantification of microstructural evolution

0.36 strain

350 laths measured



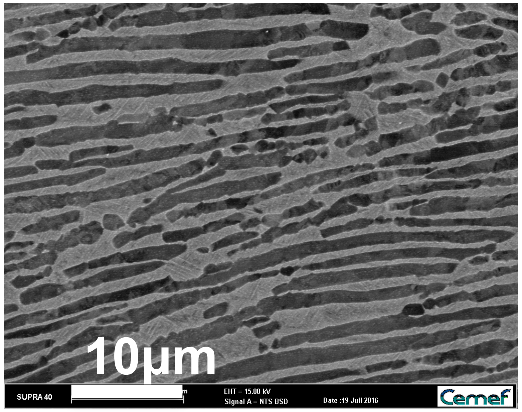
Deformed



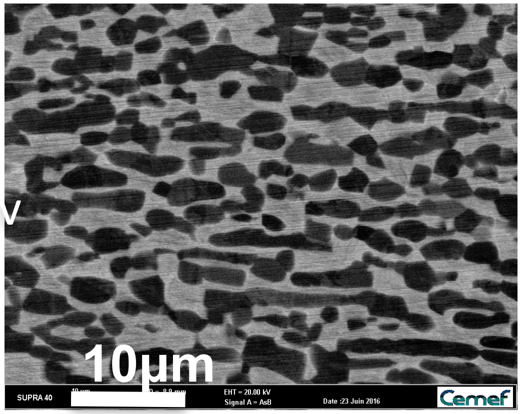
Deformed +15 min annealed

1.34 strain

450 laths measured

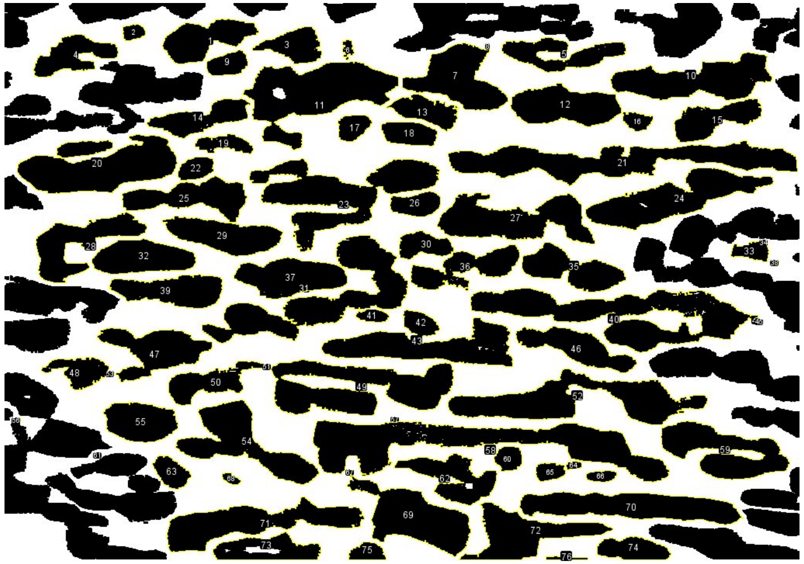


Deformed



Deformed +15 min annealed

Binarization with ImageJ

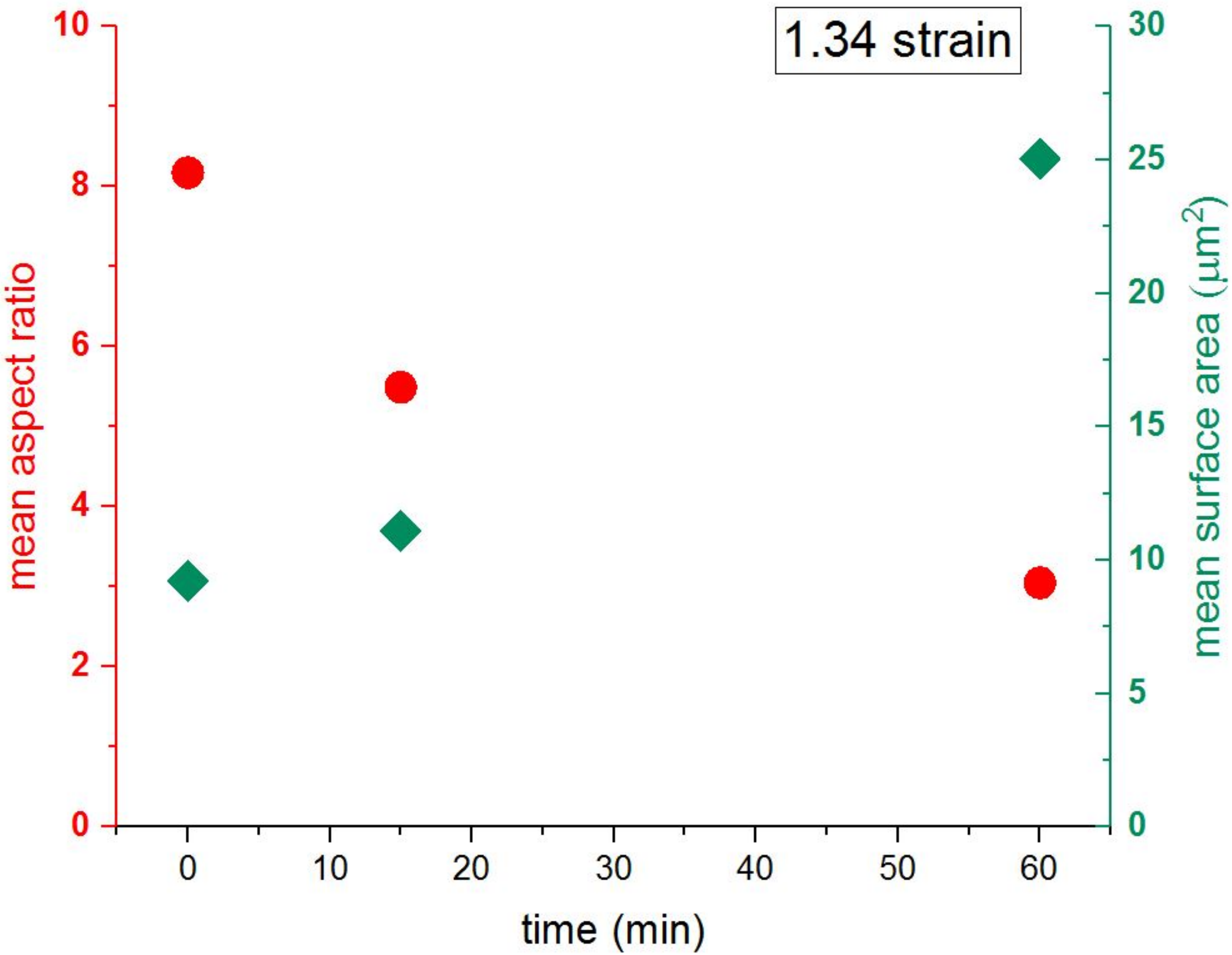


We want to measure

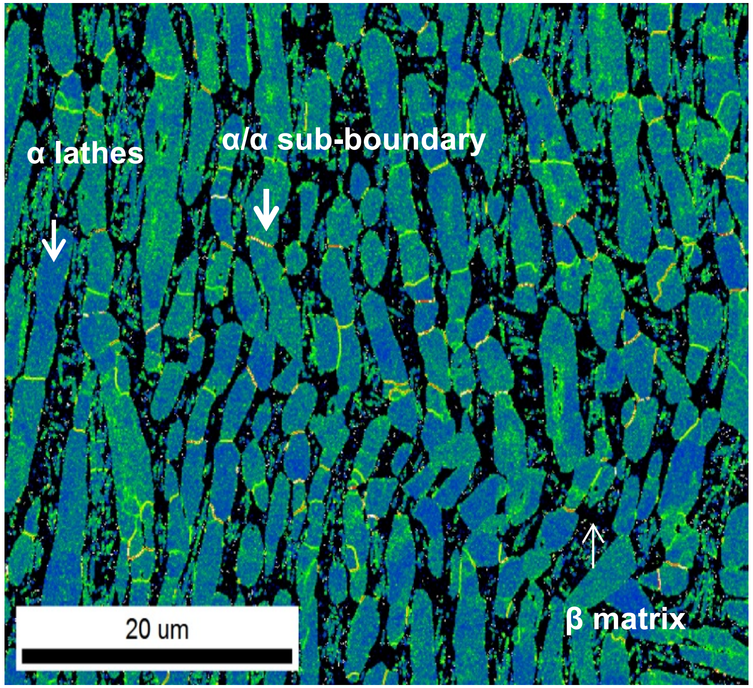
- Aspect ratio
- Particle area

$$Aspect\ ratio = \frac{major\ radius}{minor\ radius}$$

Quantification of microstructural evolution



Overview of the physical mechanisms



KAM map of
lamellar microstructure after
deformation and annealing

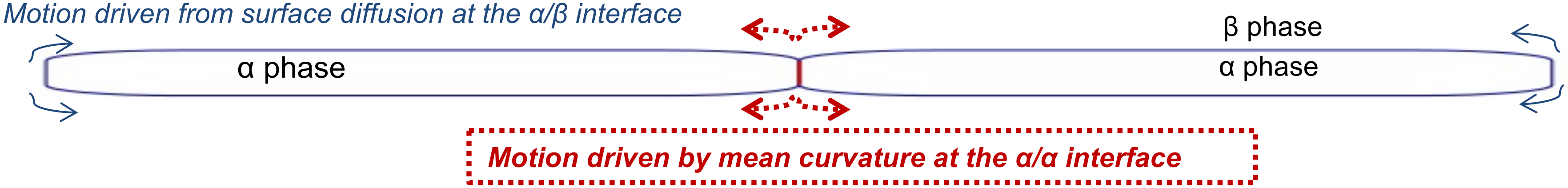
observations

Applying hot deformation
↓
Local misorientations developed in α lamellaes
↓
Formation of α/α subboundaries

Governing Mechanisms

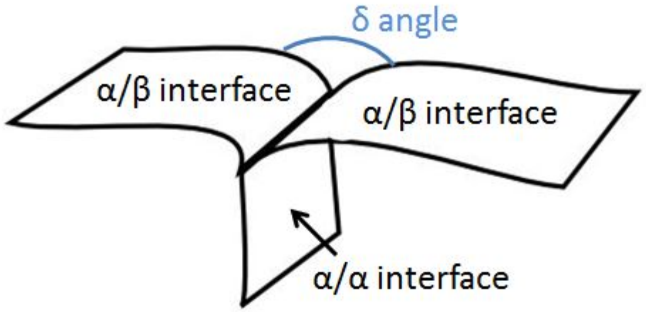
- Crystal plasticity
- Surface diffusion in α/β interfaces
- Motion by mean curvature in α/α interfaces
- Coarsening

Splitting of lamellae



FE/ Level-Set Method

Simulating Grooving



Distance function

$$\varphi(x,t) = \pm d(x,\Gamma(t))$$

Outside normal

$$\vec{n} = -\frac{\nabla\varphi}{\|\nabla\varphi\|}$$

Mean curvature

$$\kappa = -\boldsymbol{\nabla}\frac{\nabla\varphi}{\|\nabla\varphi\|}$$

Mathematical formulation
coupling of two different motion velocities

$$\overrightarrow{v_n} = (-(C_o\ \Delta_s\kappa) + A\kappa)\overrightarrow{n}$$

$$C_0 = \begin{cases} \dfrac{-\gamma_{\alpha\beta} v \Omega^2 D_{\alpha\beta}}{kT} & \text{at the } \alpha/\beta \text{ interface} \\ 0 & \text{everywhere else} \end{cases}$$

$$A = \begin{cases} \dfrac{\gamma_{\alpha a} b f \Omega}{kT}\ e^{-\frac{Q}{RT}} & \text{at the } \alpha/\alpha \text{ interface} \\ 0 & \text{everywhere else} \end{cases}$$

FE/ Level-Set Method

$\phi(x)$

Calculation of curvature κ and velocity v_n
*(use of the surface diffusion estimation solver developed by Bruchon, Pino Muñoz et al. *)*

Enhanced Lagrangian framework

$$\overrightarrow{\boldsymbol{v_n}} = [-C_0(\Delta_s \kappa) + A\kappa]\overrightarrow{\boldsymbol{n}}$$

Analytical exact reinitialization**

$$\|\widetilde{\varphi(x)} = 1\|$$

$\widetilde{\varphi(x)}$

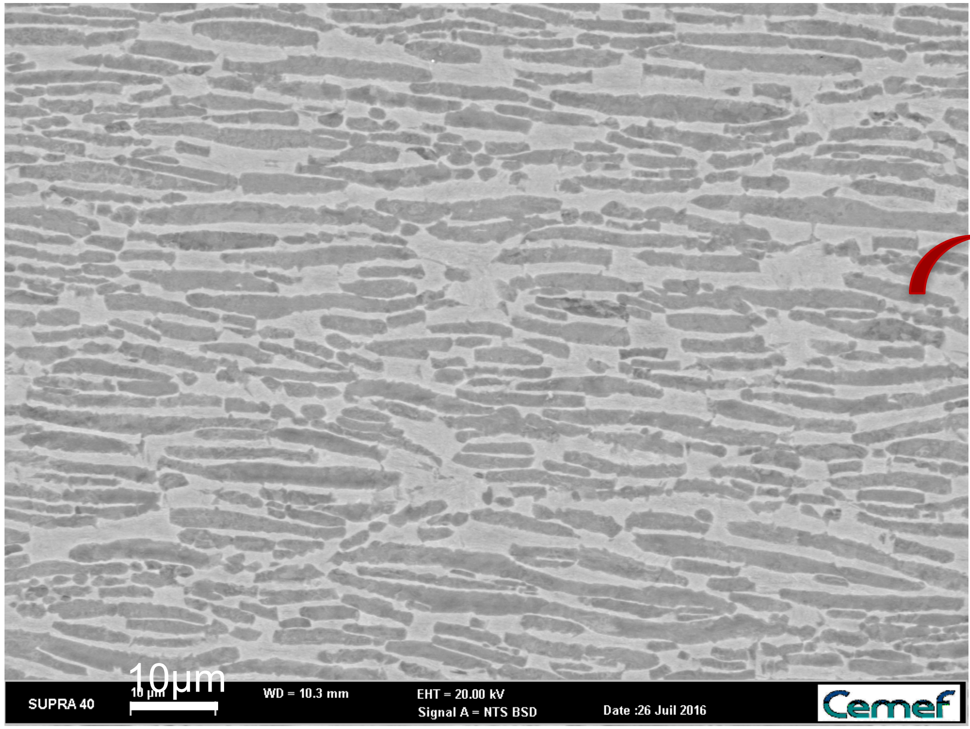
- No validation/calibration of unphysical parameters necessary to reinitialize
- It enables the exact description of $\boldsymbol{n}$ (no P1 interpolation of LS)

*D. Pino Muñoz, J. Bruchon, F. Valdivieso, S. Drapier, Solid-state sintering simulation: surface, volume and grain boundary diffusions, Conference: ECCOMAS 2012 - European Congress on Computational Methods in Applied Sciences and Engineering, 2012

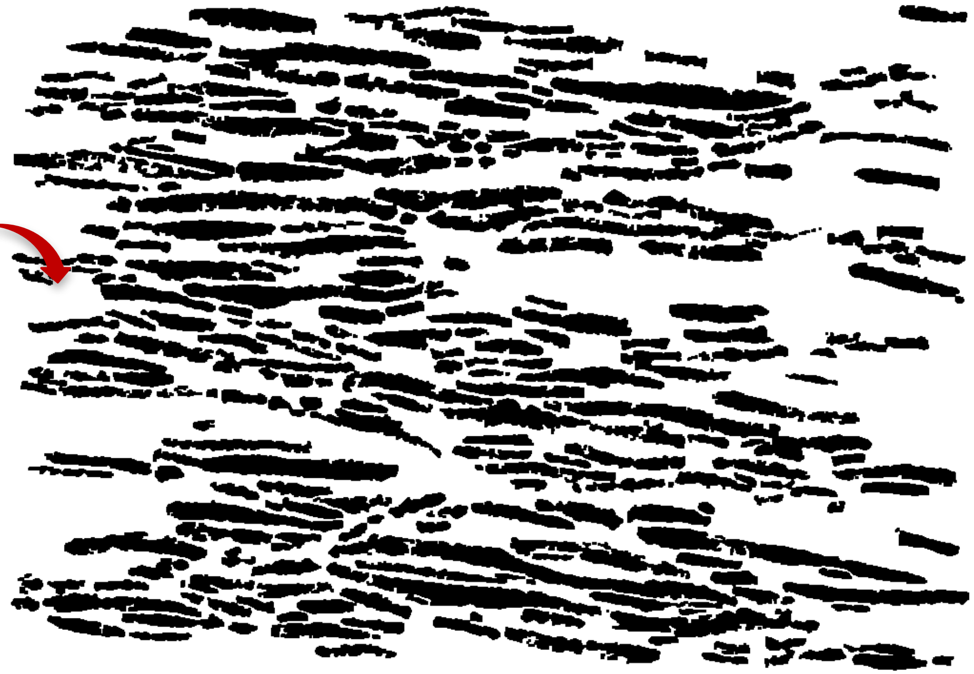
**M. Shakoor, B. Scholtes, P.-O. Bouchard, and M. Bernacki. An efficient and parallel level set reinitialization method - application to micromechanics and microstructural evolutions. Applied Mathematical Modelling, 2015.

Immersion of microstructure

Extraction of real α colonies from experimental images and application of surface diffusion



Experimental picture of LNx4 deformed



- Binarization and image treatment with “Image J”
- Extract of the distance function with “Image J”

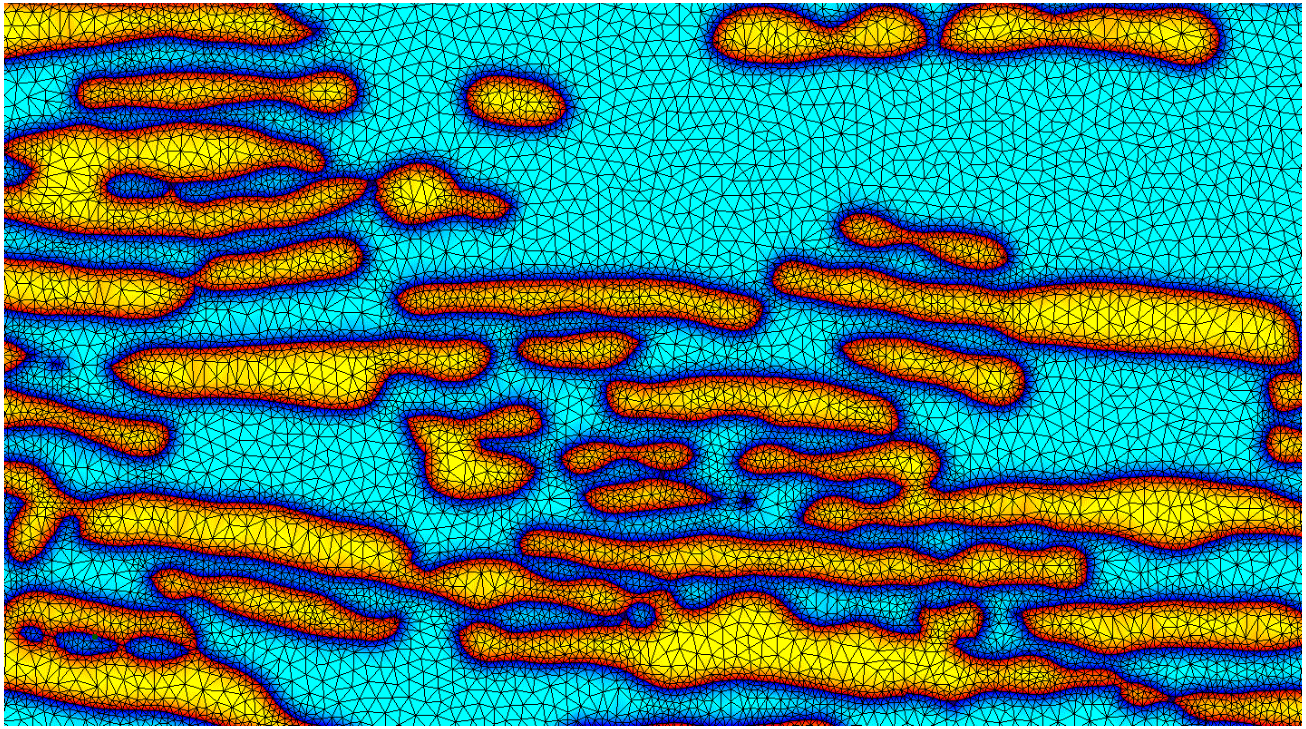
Enhanced Lagrangian framework

New topological mesher (Fitz)

- Body fitted meshing and remeshing is possible with this technic

Necessary use of adaptive mesh

- **Efficient representation of the α laths**
- **Following the shape evolution of the interfaces**
- **More efficient regarding volume loss**



Mesh quality

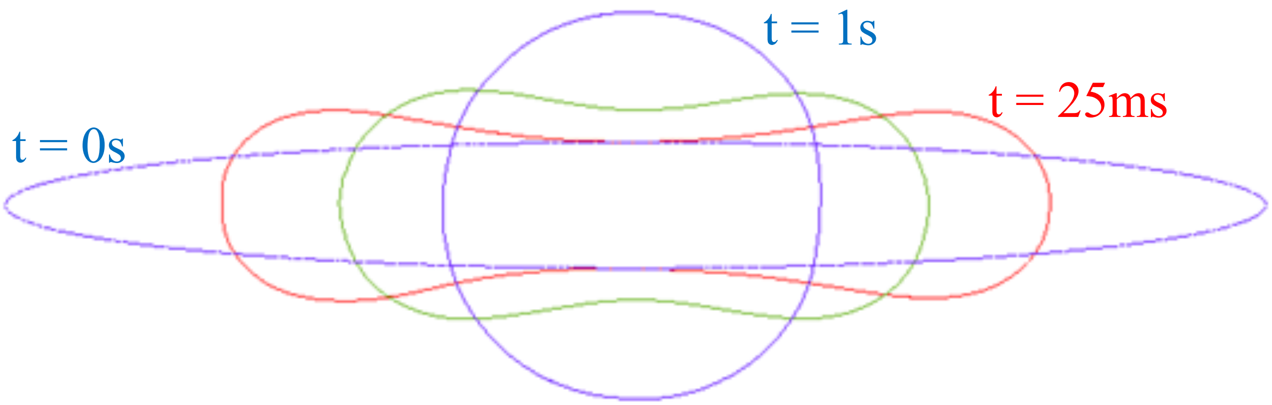
Extraction of real α colonies from experimental images and application of surface diffusion

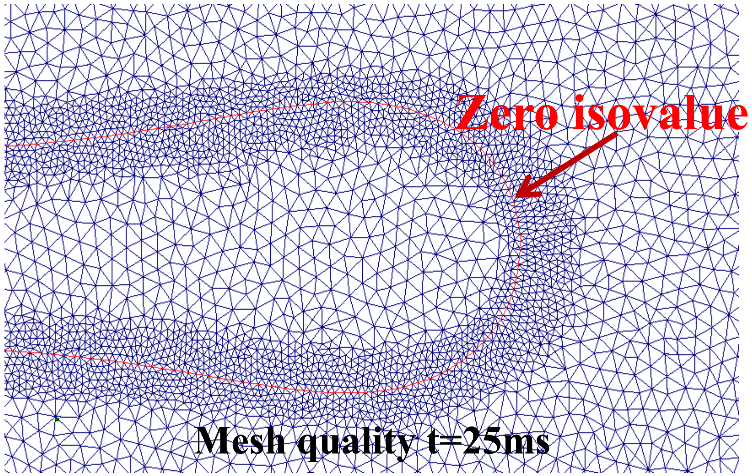
M. Shakoor, P.-O. Bouchard, and M. Bernacki. An adaptive level-set method with enhanced volume conservation for simulations in multiphase domains. International Journal for Numerical Methods in Engineering, 2016.

Motion by surface diffusion

$$\overrightarrow{v_n} = (C_o \, \Delta_s \kappa)\overrightarrow{n}$$

Zero iso-surface evolution

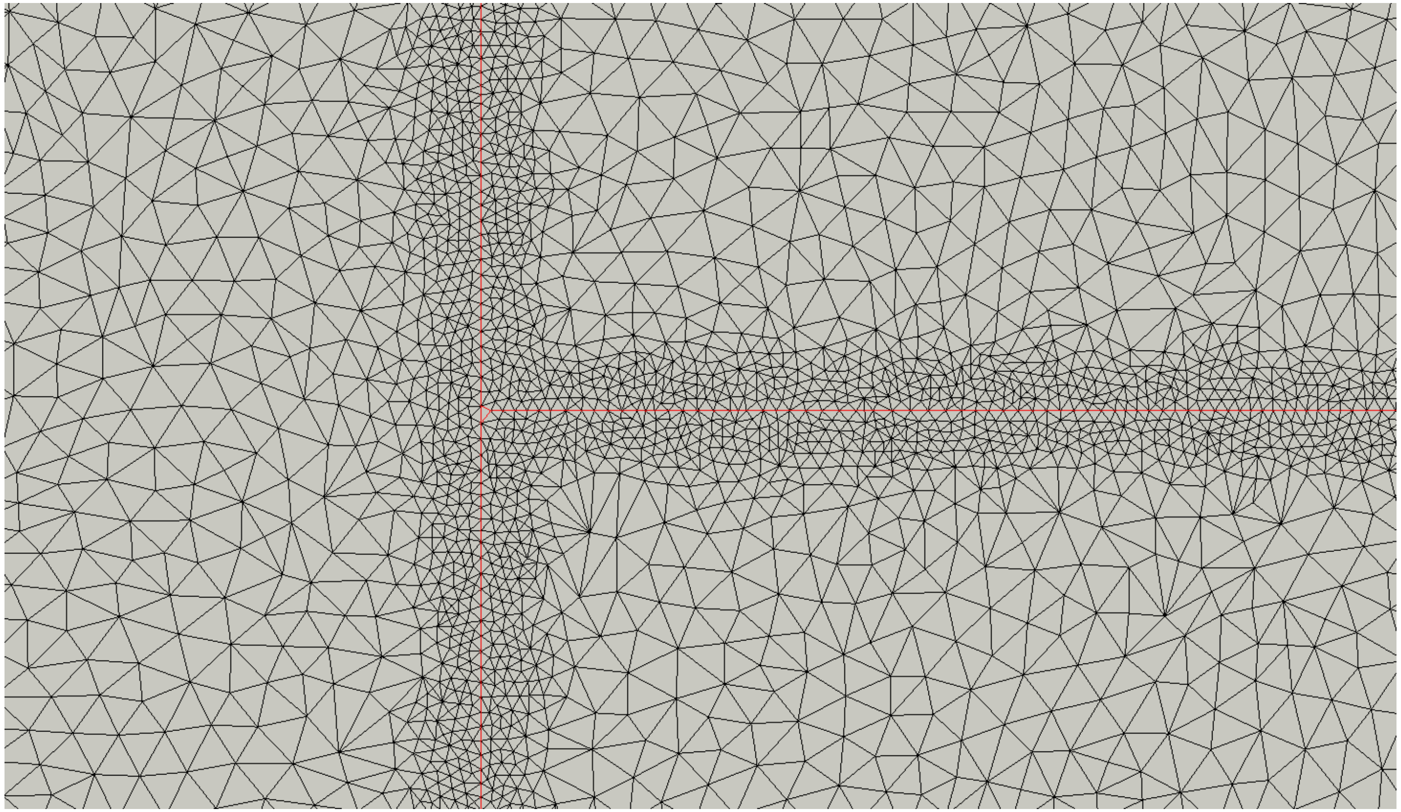




Mesh adaptation technique	Method 2
Time step (ms)	10
Time (s)	1
h_{el} close to surface (µm)	1
time calculation (12CPUs)	2min
Volume loss	**1.5%**

Motion by mean curvature

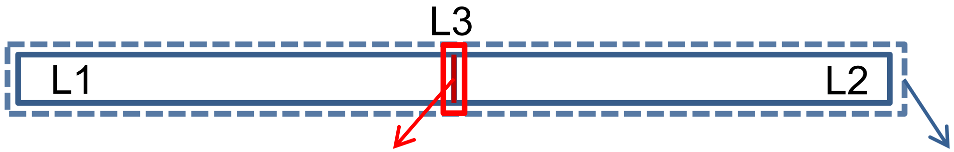
$$\overrightarrow{v_{curv}} = (A\kappa)\overrightarrow{n}$$



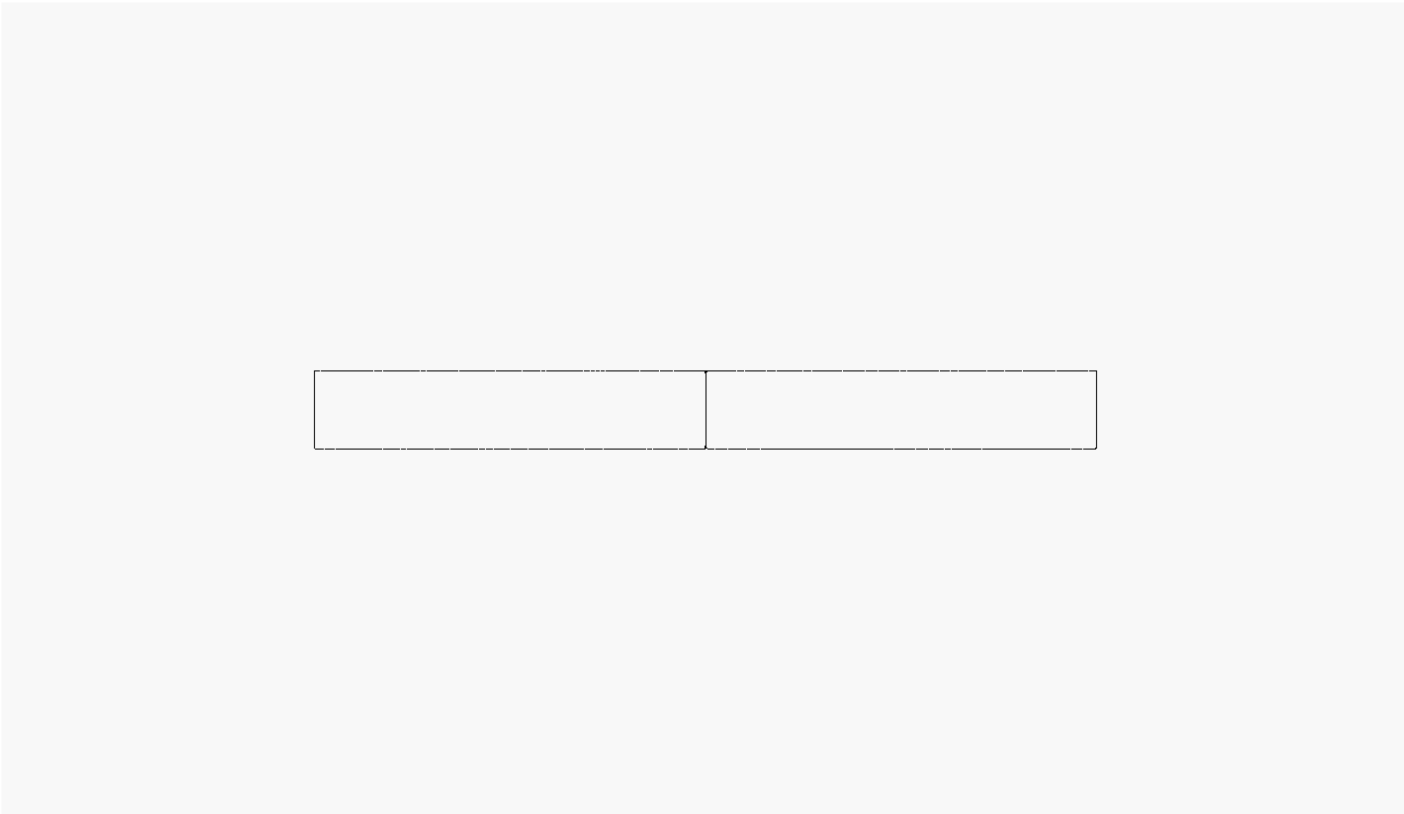
simple case of triple junction in a Lagragian Framework

Calculation time: 8 min

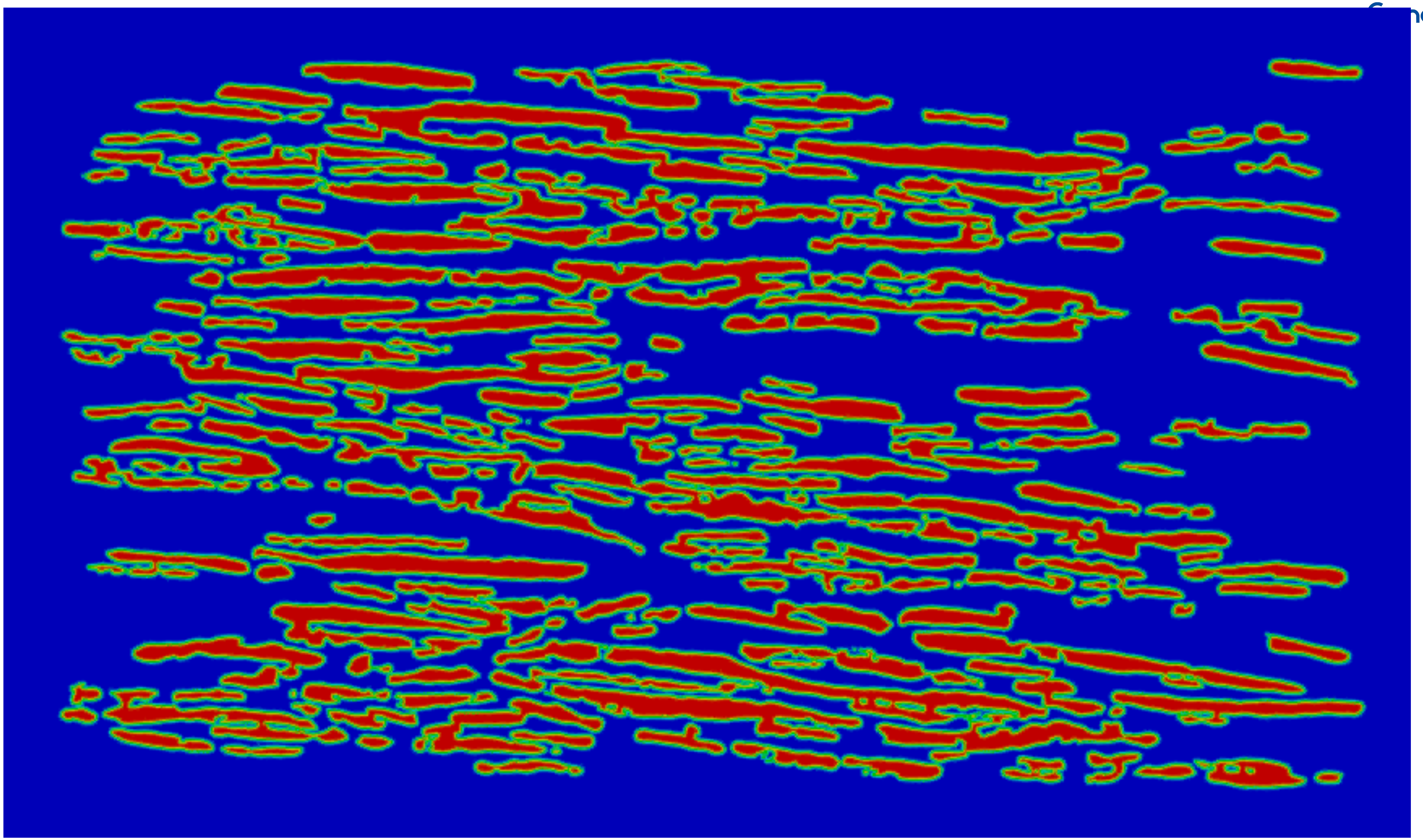
Coupling of surface diffusion and motion by mean curvature



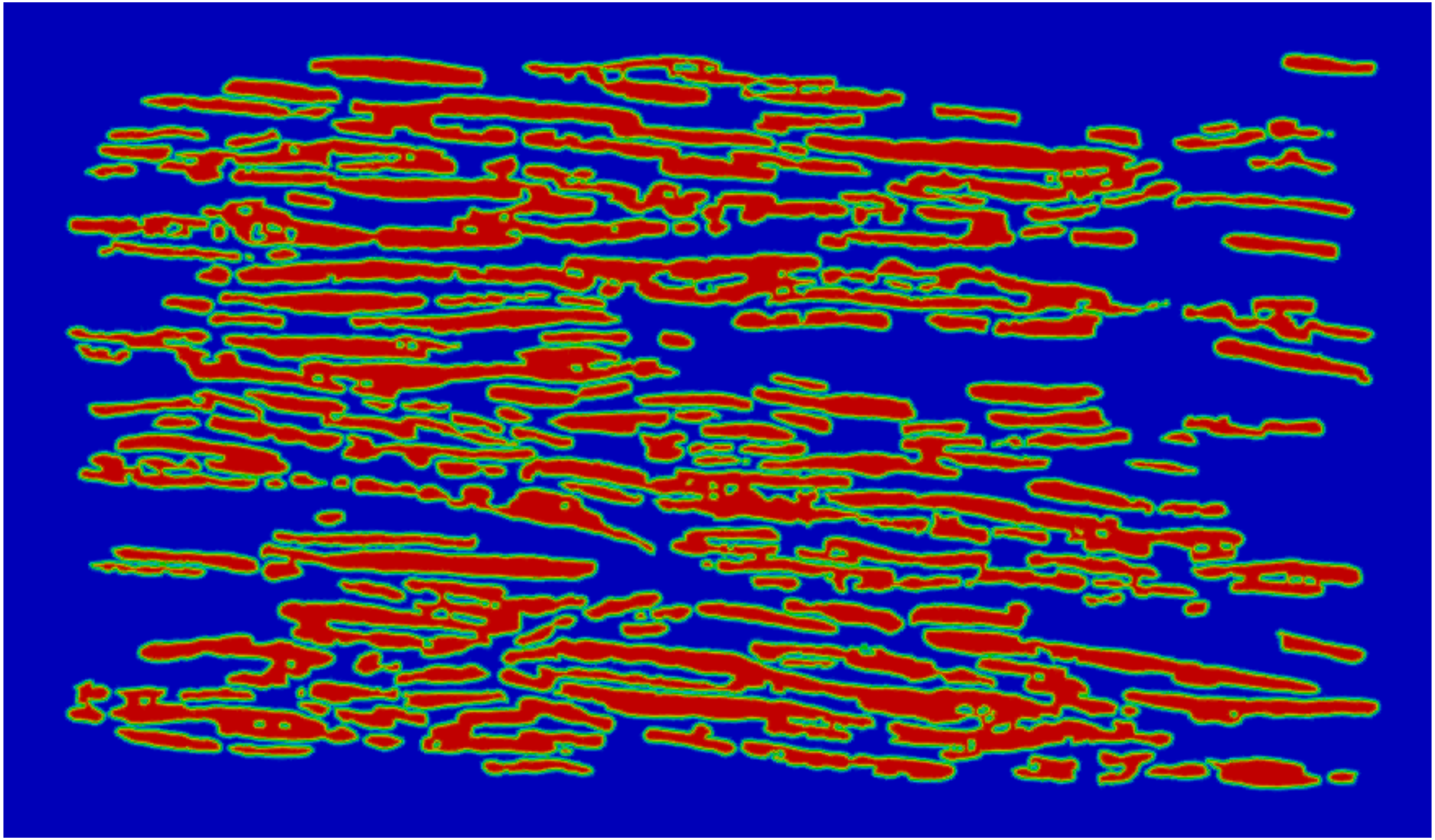
$$\overrightarrow{v_{curv}} = (A\kappa)\vec{n} \qquad \overrightarrow{\boldsymbol{v_{surf}}} = C_0(\Delta_s\kappa)\vec{\boldsymbol{n}}$$



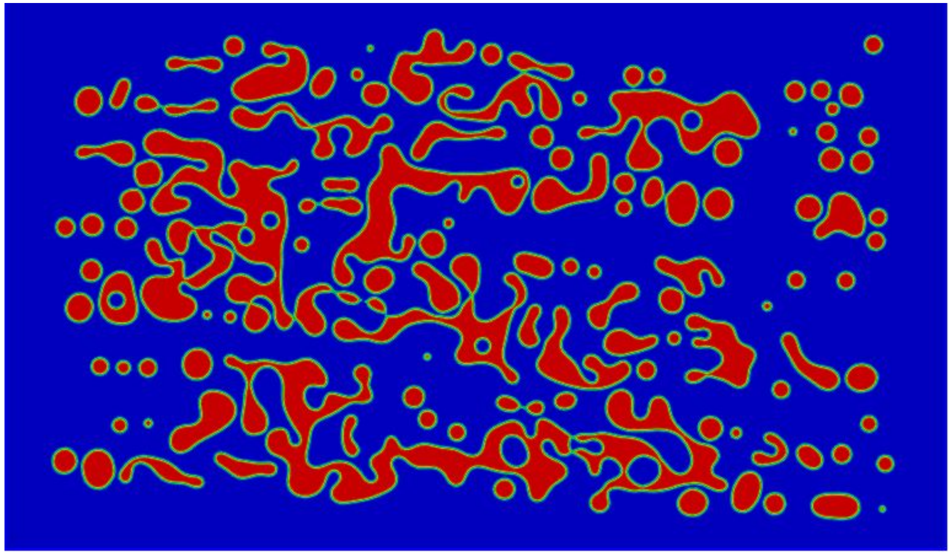
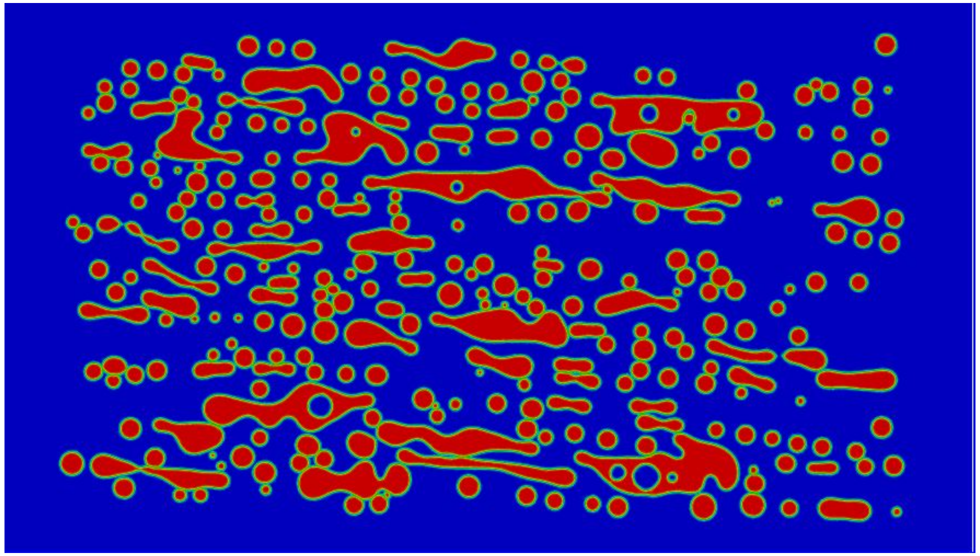
Surface diffusion in real microstructure



Motion by surface diffusion coupled with motion by mean curvature



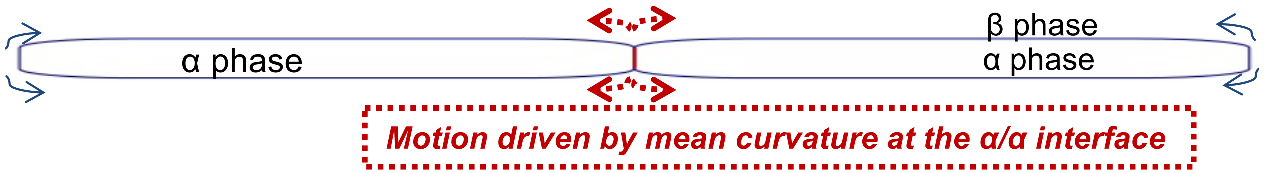
Comparison

Surface diffusion	Surface diffusion + motion by mean curvature
	
Volume loss approximation: 2.8%	No unphysical coalescence Volume loss approximation: 0,1%

Conclusions

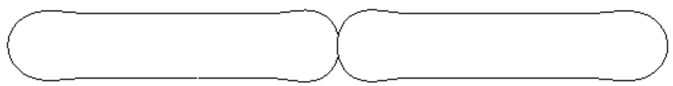
1. Governing mechanisms for the first stages of annealing

Motion driven from surface diffusion at the α/β interface

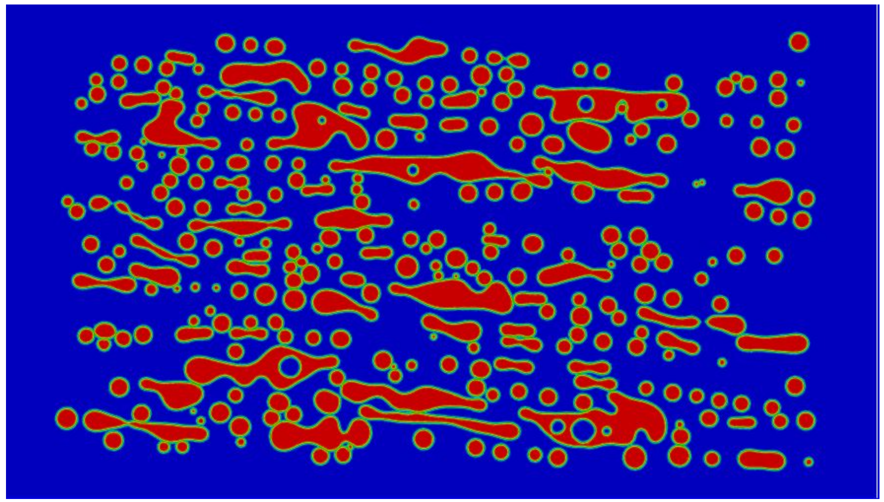


2. Efficiently simulated the splitting of the lamellae

$$\overrightarrow{v_n} = (-(C_o\ \Delta_s \kappa) + A\kappa)\overrightarrow{n}$$



3. Simulated the coupling of the mechanisms on real microstructure



Perspectives

- Estimation of the right values for coefficients Co and A $\overrightarrow{v_n} = (-(C_o\ \Delta_s \kappa) + A\kappa)\overrightarrow{n}$
- Simulating coarsening
- Simulating crystal plasticity during deformation for the formation of sub-boundaries

Thank you for your attention!