10/07/20

4D experimental testing and simulations for statistical analysis of crystal plasticity in structural materials

BIGMECA COPIL

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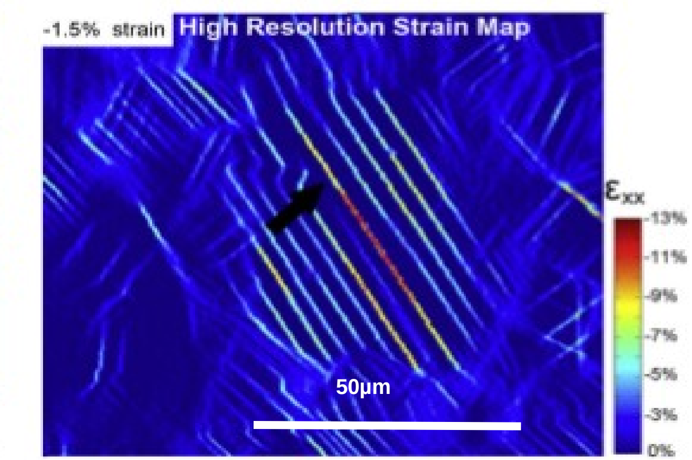
Agenda

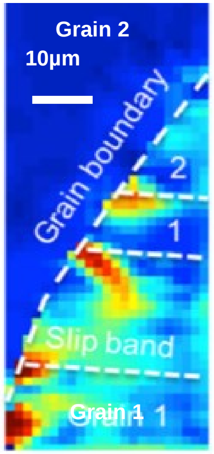
- Overview
- Multimodal experimental data
  - Digital twins reconstruction
  - Lab tensile tests
  - SEM in-situ campaigns
  - 3D LabDCT scans
- Simulation data
  - Behavior law model
  - Parameters identification
  - Meshing
  - Simulations (FEA,FFT)
- Achievement & Outlook

Overview - Background

- **Motivation** : Establish Process-**Structure-Properties** relationships.
- **Mechanisms investigated** :
  - Intra-granular slip systems activation
  - Inter-granular plasticity propagation
  - Influence and evolution of dislocations
  - Lattice curvature evolution



Slip bands - SEM in-situ microscopy (Stinville et al., 2016)

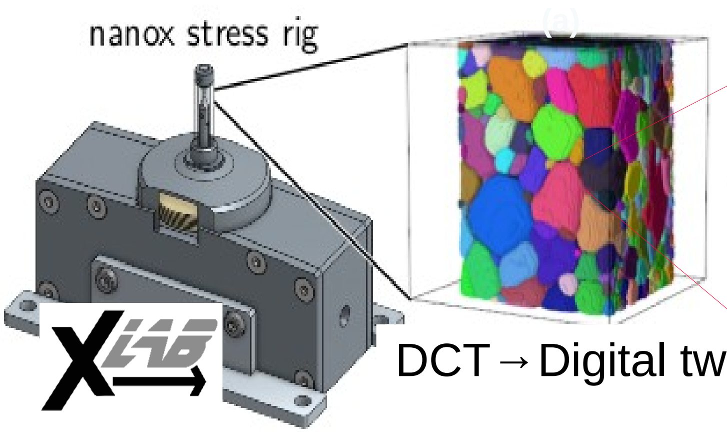


Dislocations concentration DAXM microscopy (Guo et al., 2020)

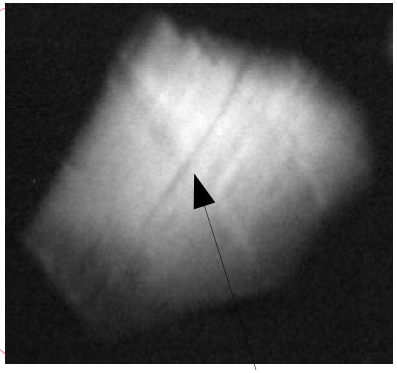
DAXM: Differential Aperture Xray Microscopy
SEM : Scanning Electron Microscopy

Overview - DCT opportunity

- DCT at ESRF (Ludwig et al., 2009) (Reischig et al., 2013)
- DCT compatible in-situ stress rigs (Xlab) (Gueninchault, 2016)
- First signs of plasticity in volume : Slip bands, lattice curvature (Proudhon, 2018)
- New laboratory sources : LabDCT - ZEISS



DCT→Digital twin



Slip band

Zeiss Xradia Versa X-ray Microscope with LabDCT

3DXRD : 3D X-ray Diffraction
DCT : Diffraction Contrast Tomography

ESRF : European synchrotron (Grenoble)
In-situ = 4D = Measure of deformations during the test = adding temporal dimension

Overview - Problem

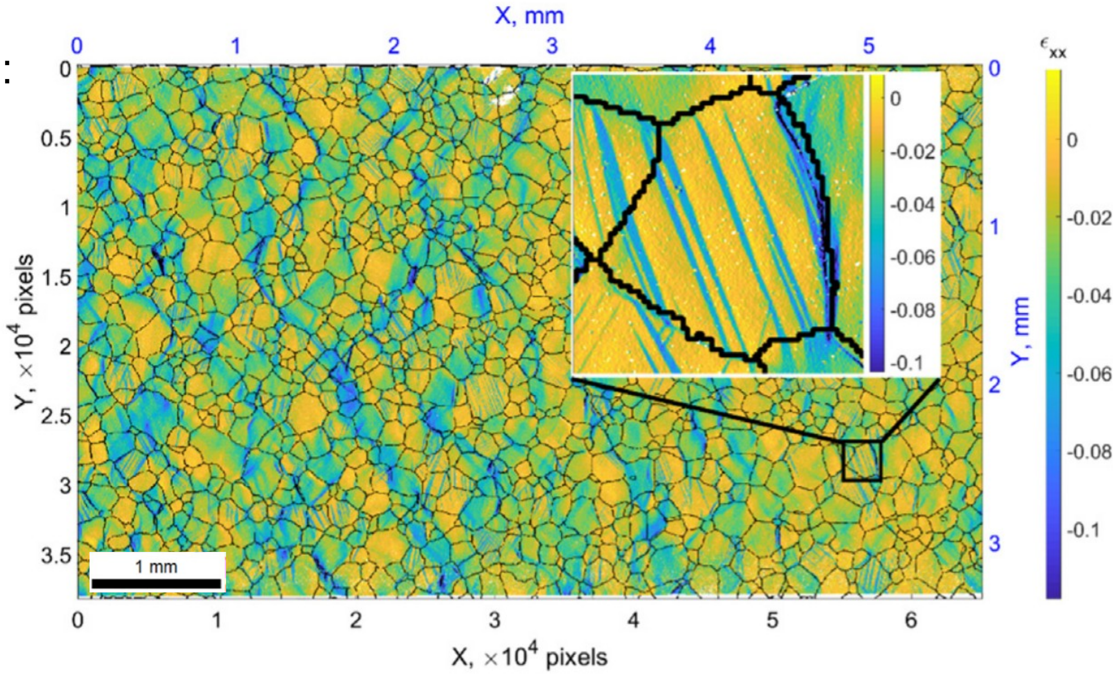
Complexity of mechanical mechanisms at mesoscopic scale (~10^3 grains)
(**plasticity**, damage and fracture, crack propagation, twinning)

⇩

Current approaches limited to
extract physical data, derive behavior models in realistic time frame

Case study (Chen et Daly, 2018):

- Twinning in Magnesium
  Large FOV (1,400 grains)
- SEM-DIC : 10^8 data points
- How to extract single grain twinning information ?



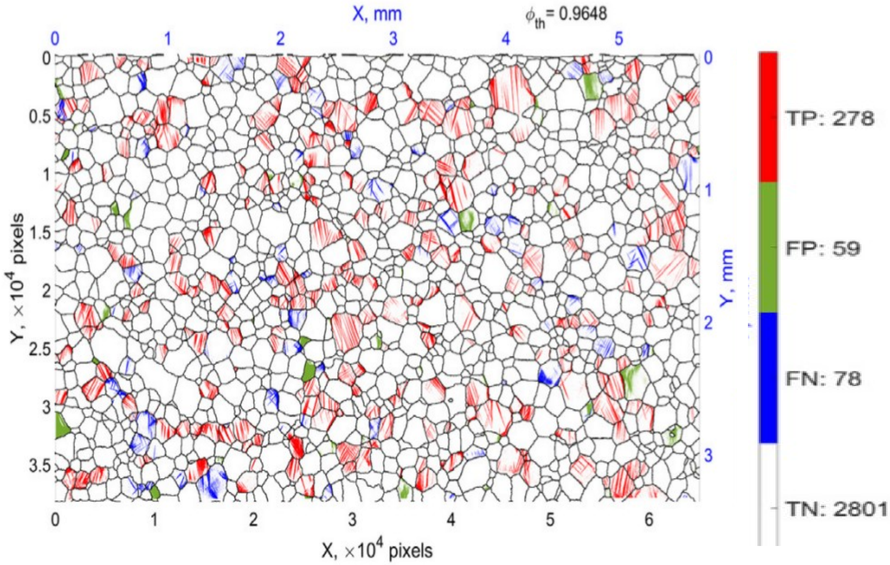
DIC : Digital Image Correlation
FOV: Field of view
SEM: Scanning Electron Microscope

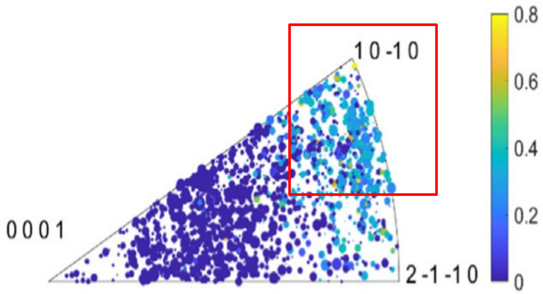
Overview - Machine Learning opportunity

- **Statistical learning** applied to mechanics
  allows to extract physics based data from large datasets

- **Combined** with :
  - CDM expertise: characterization, simulation
  - DCT technique : 4D - Deployment at SOLEIL, 3D - LabDCT

Potential to unlock statistically plasticity mechanims at mesoscopic scale



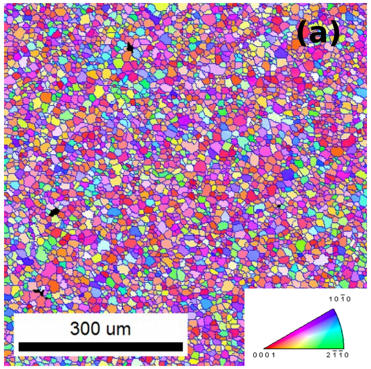


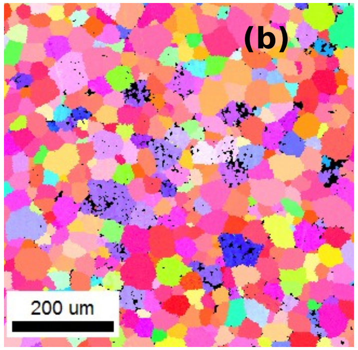
Ratio of plasticity
by twinning/total plasticity
per grain (size, orientation)

CDM : Centre des Matériaux
DCT : Diffraction Contrast Tomography
SOLEIL : Synchrotron at Plateau de Saclay (Paris Area)

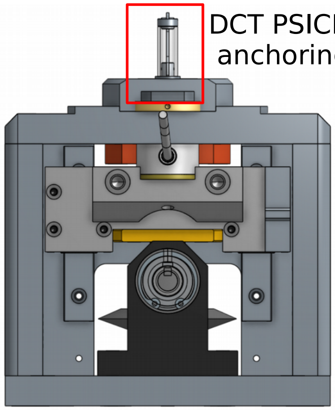
Previous status reminder (06/09/20)

- **Material**: Titanium (T40) Phase-α, HCP lattice





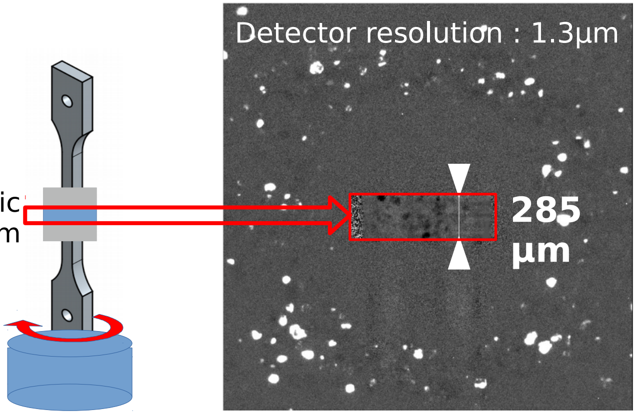
EBSD :
(a) Initial grain size ~ **15µm**,
(b) : After Heat treatment (855°C, 17h, 24h, Argon) : ~ **50µm**



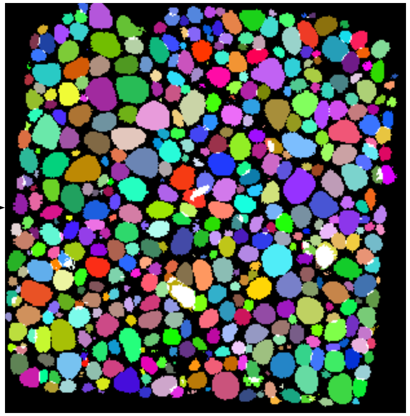
DCT PSICHE compatible anchoring block

BULKY

Monochromatic Xray beam



1 radiograph = 1 projection/3600 (2s)
1 scan = 3600 projections → 2100 grains
3 scans → ~ **5000 grains**



(Ludwig et al. 2009)
(Reishig et al. 2013)

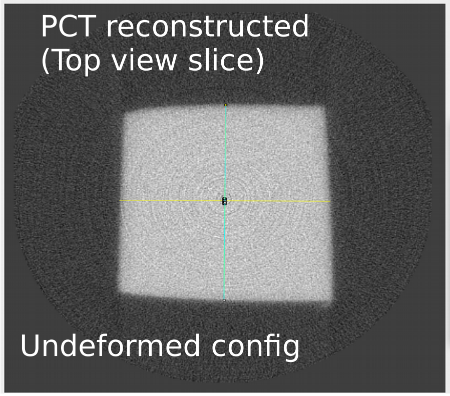
Digital twins : 6 single scans successfully reconstructed both for 3D and 4D resolutions

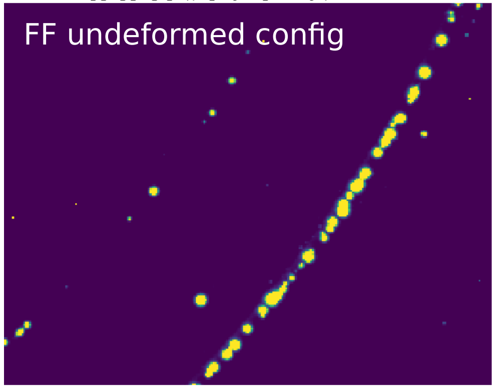
DCT = Diffraction Contrast Tomography
EDM = Electrical Discharge Machining
EBSD : Electron Back Scattered Diffraction

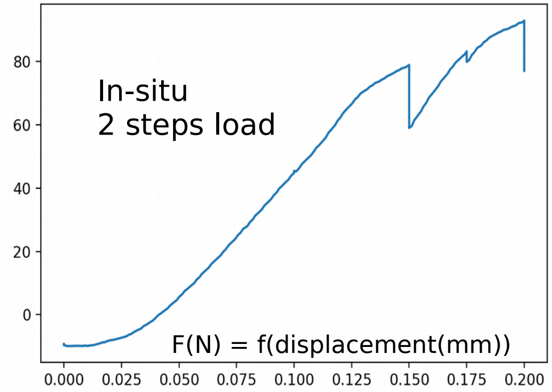
FF = Far Field
HCP = Hexagonal Closed Pack
PCT = Phase Contrast Tomography

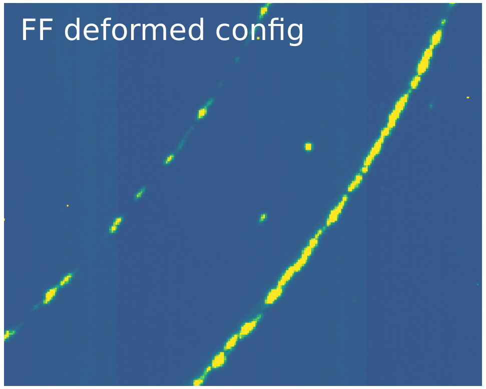
Experimental data – PSICHE data

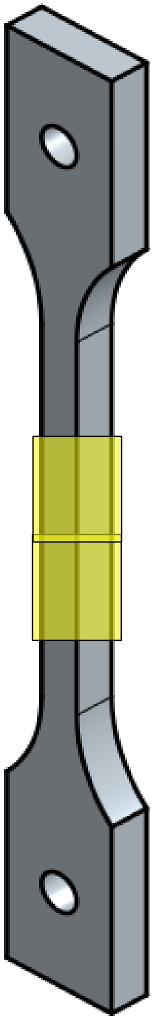
- PCT, FF and in-situ log data recovered from PSICHE
- PCT data cleaned and used to generate absorption masks







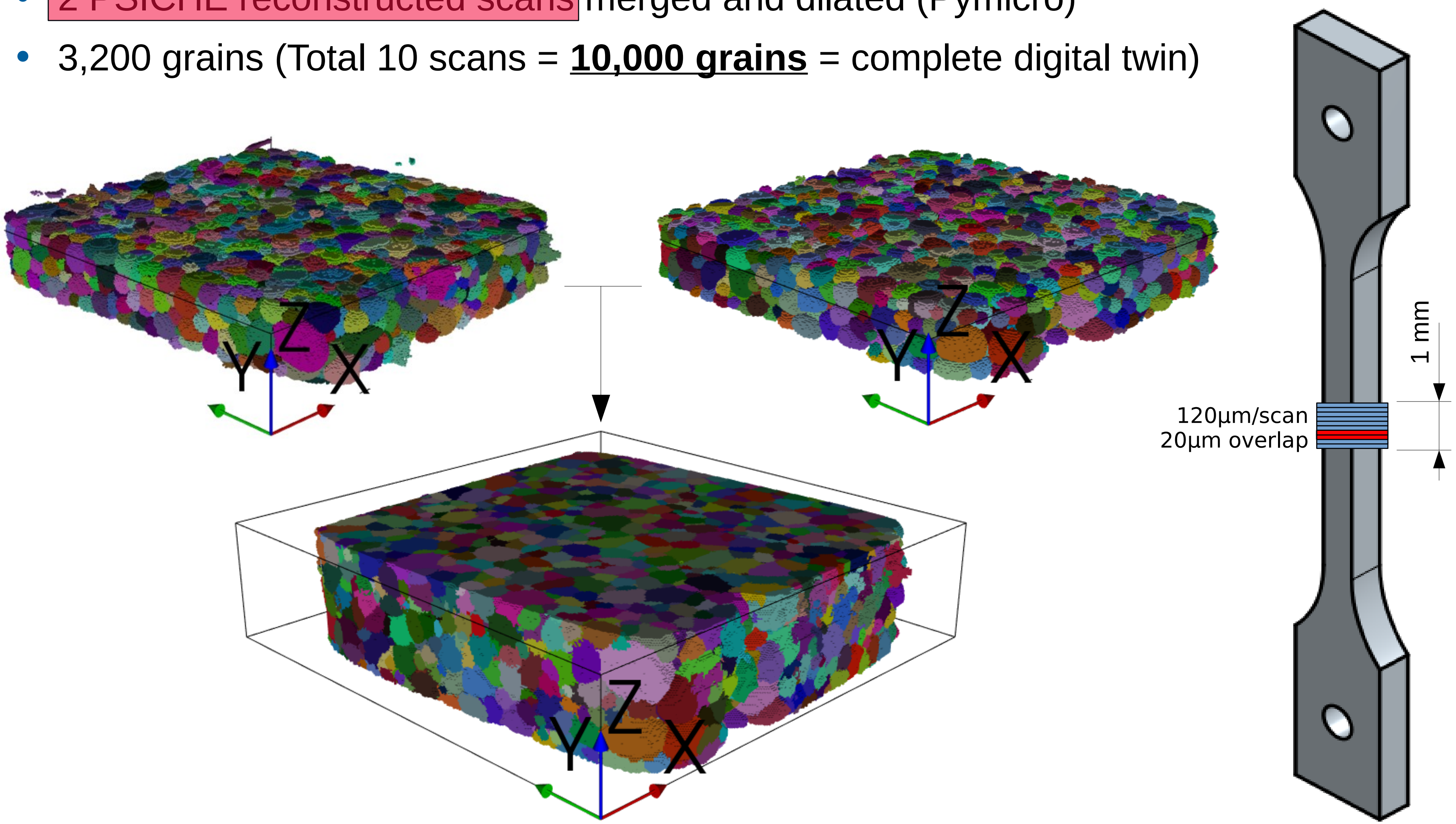




FF : Far Field
PCT: Phase Contrast Tomography

Experimental data – PSICHE Digital twins

- 2 PSICHE reconstructed scans merged and dilated (Pymicro)
- 3,200 grains (Total 10 scans = **<u>10,000 grains</u>** = complete digital twin)

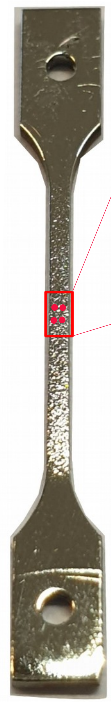


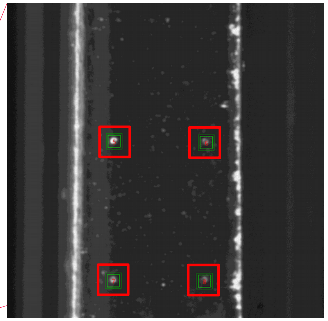
Pymicro: Pypi library: https://pypi.org/project/pymicro/

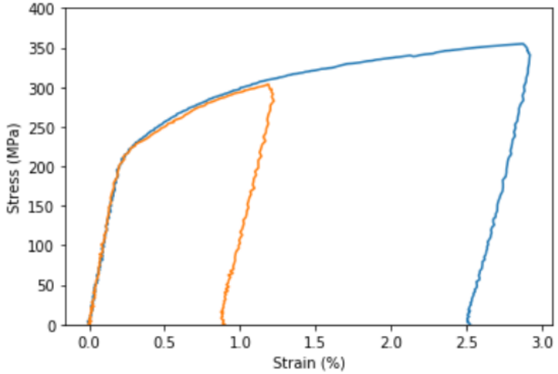
Experimental data – Lab tensile tests

- Monotonic tensile test with Bulky + post treatment with ARIANE routine

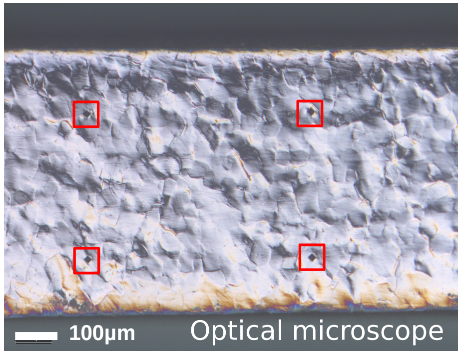
Samples (same batch)	ET9_3_	ET9_5
Initial section	0.63 mm²	0.67 mm²
Cross-head speed	2 µm/s	2 µm/s
L0 (µ-indents)	2,400 µm	2,400 µm
Force max	223 N	200
ε_{TOTAL}	2.88 %	1.2 %
ε_P	**2.5 %**	**0.8 %**
σMAX	354 MPa	299 MPa
E homogenized	105,000 MPa	

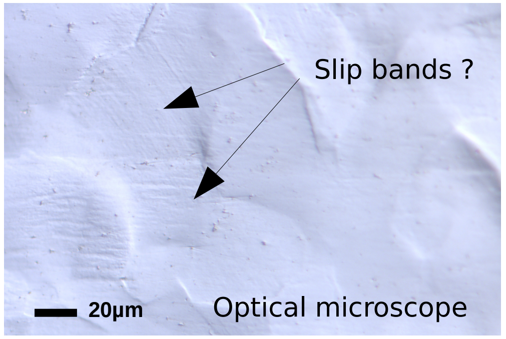






- **Micrography**:
  Optical : Out of plane plasticity
  SEM : No slip bands visible directly





- **Interpretation** :
  T40 too pure. Limited localization of dislocations accumulation for strains < 3 % = DCT limit

➡ Nano speckle needed for SEM-DIC

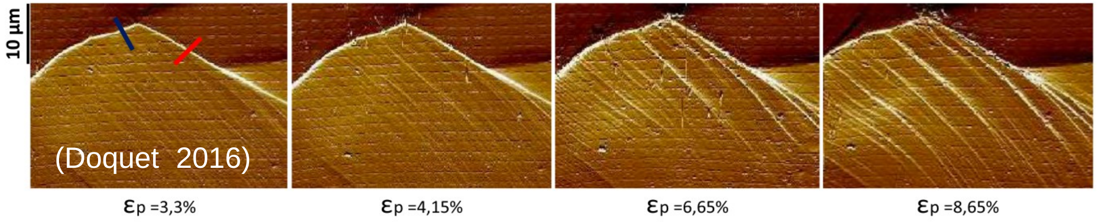


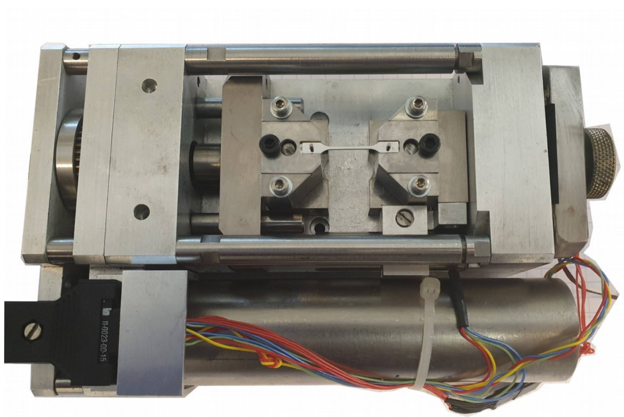
Fig. 8. Evolution of in-plane and out-of-plane sliding for two grain boundaries in Grade 2 Ti.

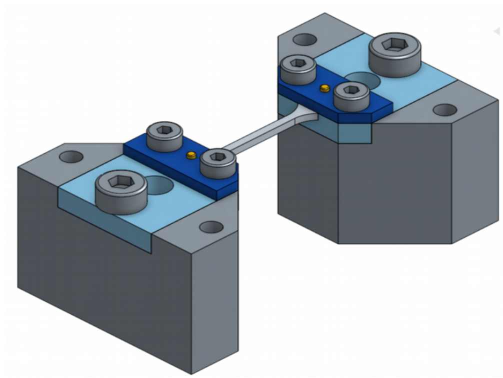
CDM : Centre des Matériaux
DCT: Diffraction Contrast Tomography
DIC = Digital Image Correlation

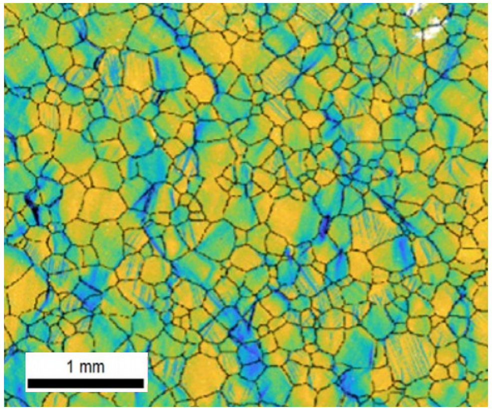
SEM: Scanning Electron Microscopy

Experimental data: SEM in-situ preparation

- **DCT 4D data :**
  - Reconstruction limited to $\varepsilon_P = 3\ \%$ → No access to slip bands for T40
  - Explore ability to access to **lattice curvature**
- **SEM surface data :**
  - In-situ machine available + new adapters
  - Currently, cannot take advantage of secondary electrons scanning
  - Ability to access to **lattice curvature** with EBSD
  - Need to test SEM capacity to tilt in-situ machine (otherwise: ex-situ)
  - Explore **SEM-DIC** technique: Potential to access to **slip bands traces**
  - DMS student support: Kenza ZOUGAGH







(Chen et Daly, 2018)

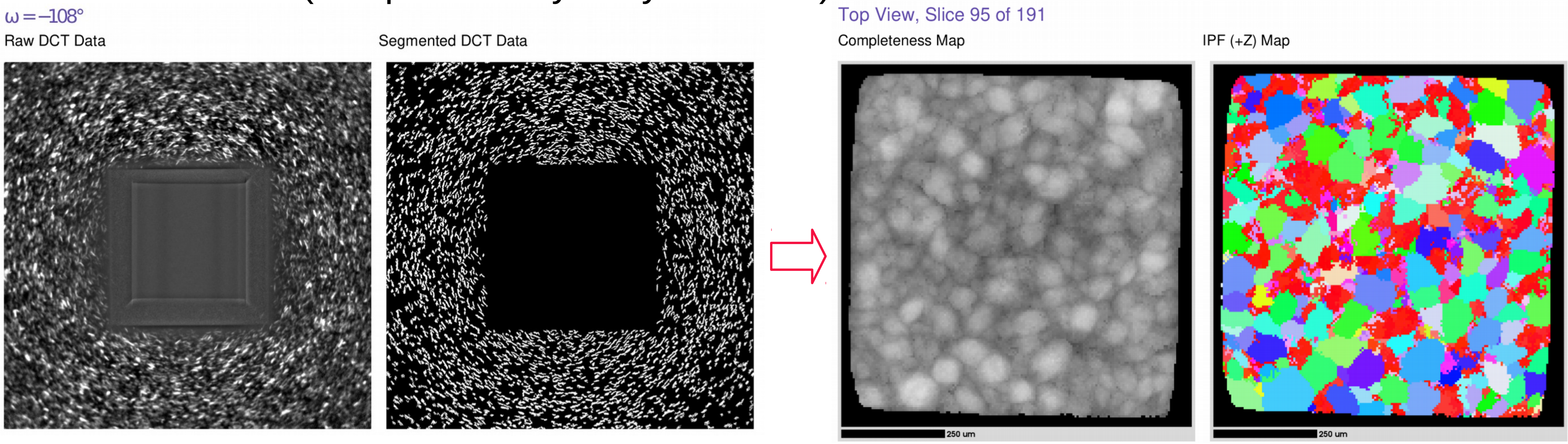
DCT: Diffraction Contrast Tomography
EBSD : Electron Back Scattered Diffraction
SEM: Scanning Electron Microscopy
DIC : Digital Image Correlation
UCSB: University of California Santa Barbara

Experimental data - 3D LabDCT

- **Lund University** owns a LabDCT
- 2 samples sent for scanning :
  - 800x800µm section
  - Reference EBSD + SEM Mapping
- **Results** :
  - Promising. Some artefacts
  - Need samples with smaller sections
  - → New batch : 21 samples 600x600µm section

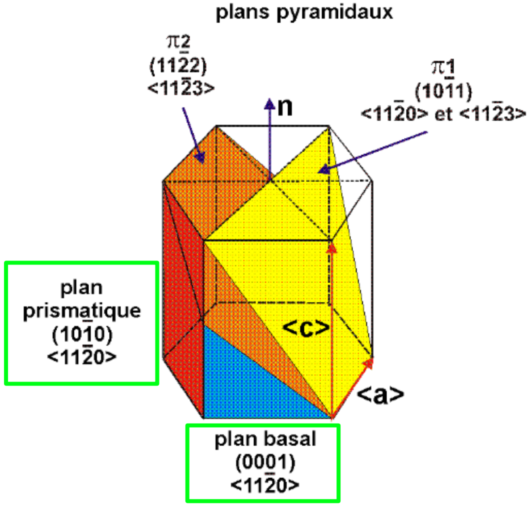
Zeiss Xradia Versa X-ray Microscope with LabDCT

- **Opportunity** : Combine Lab 3D DCT with SEM data on each sample (complementary to synchrotron)

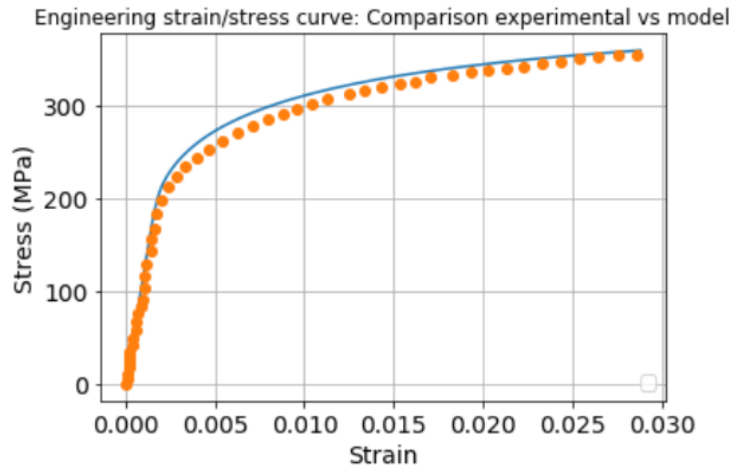


Simulated data – Behavior model

- **Material** : Titanium (T40) Phase-α, HCP lattice, c/a = 1.58
- **Model**: Crystal plasticity:
  - Elastic orthotropic (Simmons and Wang, 1971)
  - Active slip systems: prismatic, basal
  - Flow rule: Norton $$\dot{\gamma}^s = \mathrm{sign}(\tau^s)\left\langle \frac{|\tau^s| - \tau_c^s}{K} \right\rangle^n$$
  - Hardening: Isotropic non linear.
    Only self hardening $$R = \mathtt{R0} + \mathtt{Q}\left(1 - e^{-\mathtt{b}p}\right)$$

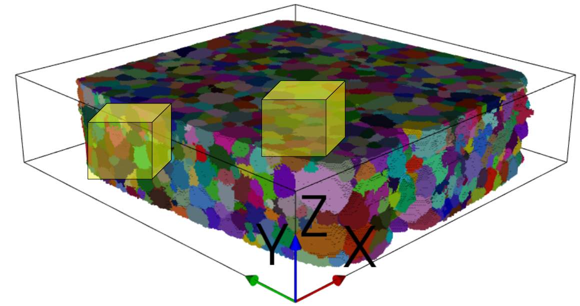


- **Parameters identification**: First fitting

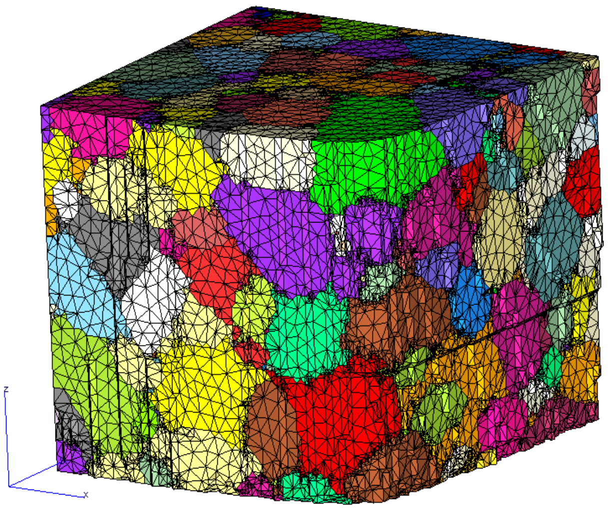


Simulated data – Meshing

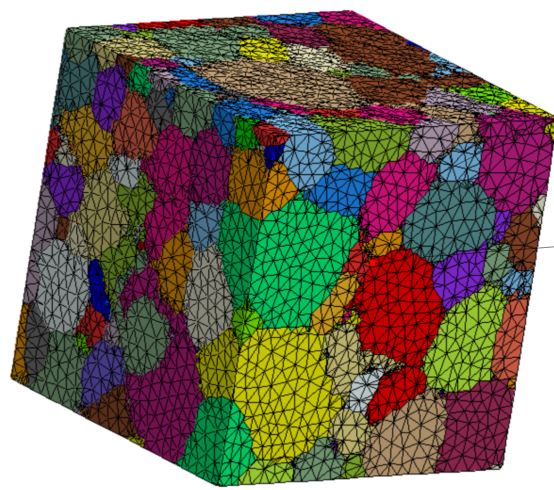
- 2 sub volumes extracted from PSICHE volume ~ 300 grains



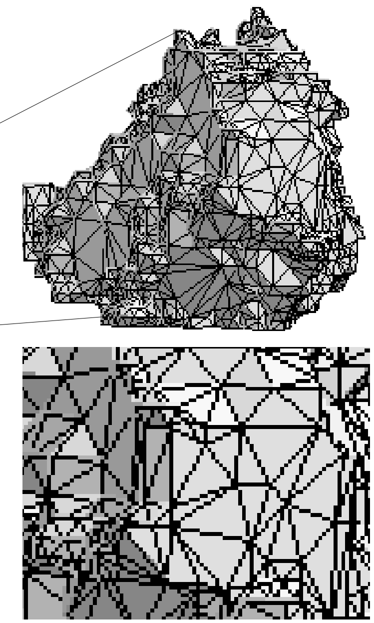
- Morphological meshing (F. N'GUYEN)
  Attempt 1 : Rough grains, distorted elements, artefacts ELSET



Volume corner : Free surface

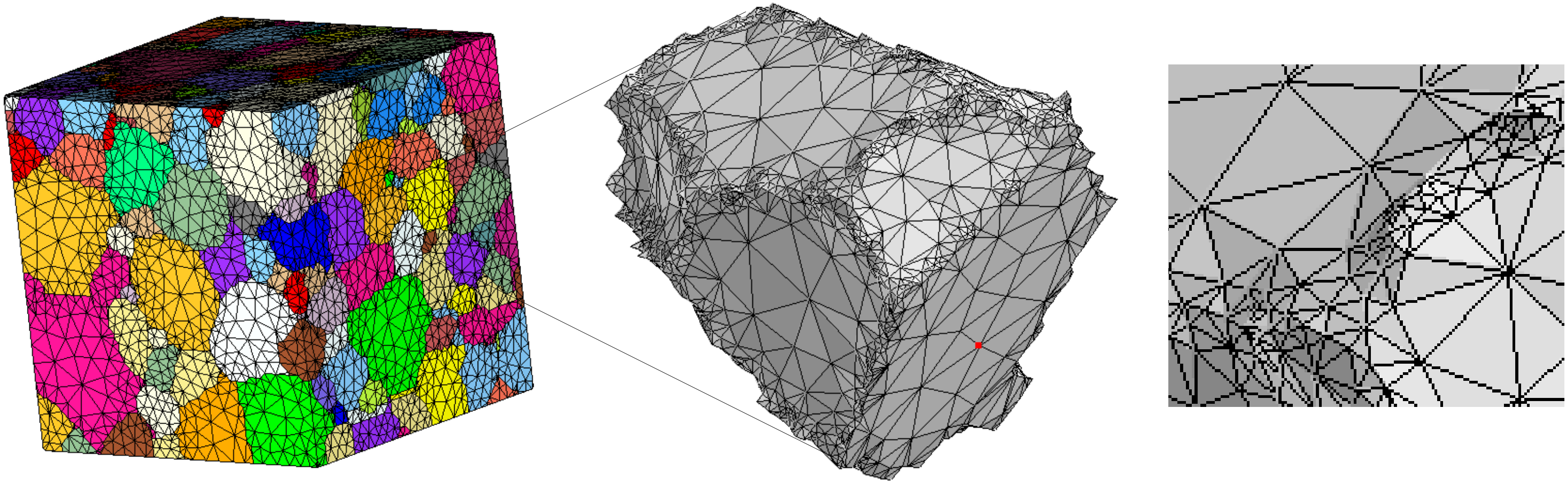


Volume middle
74x72x70 voxels : 316 grains



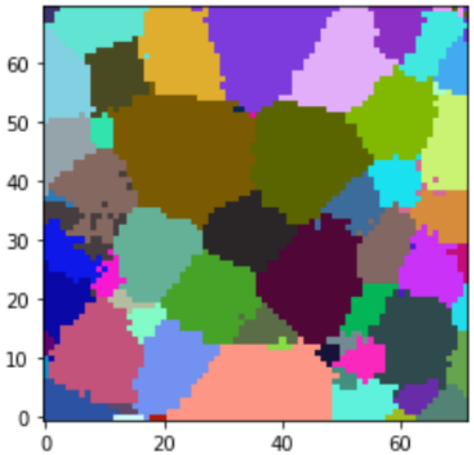
Simulated data – Meshing

- Ad hoc mesh strategy
- Mesh criteria : Undistorted elements, #elements, smooth surface on ELSET
- **1st** morphological post-treatment : obtain acceptable meshing aspect
  Convexify ELSET + adapt geodesic triangulation density to grains size

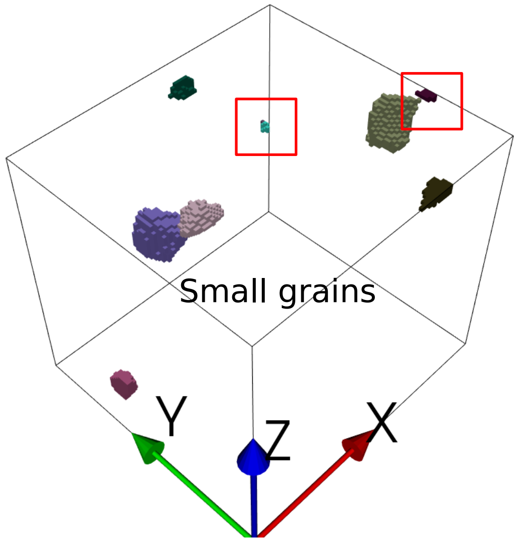


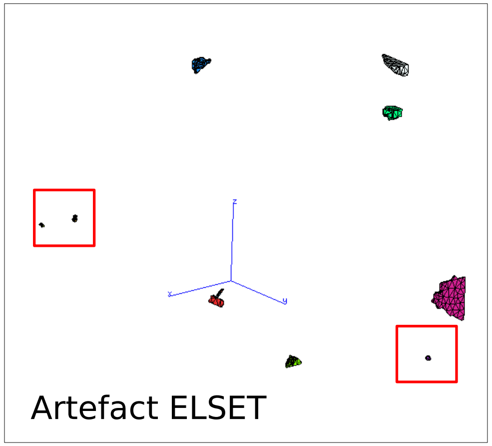
Simulated data – Meshing

- **2nd** morphological post-treatment : delete artefact ELSET
  - Original grain map : 316 grains - low connexity
  - 560 ELSET - high connexity
  - Treatment → **302 ELSET, 75,392 elements**
  - Small grains discarded
- **3rd** treatment : ELSET reindexation to match original grain map IDs



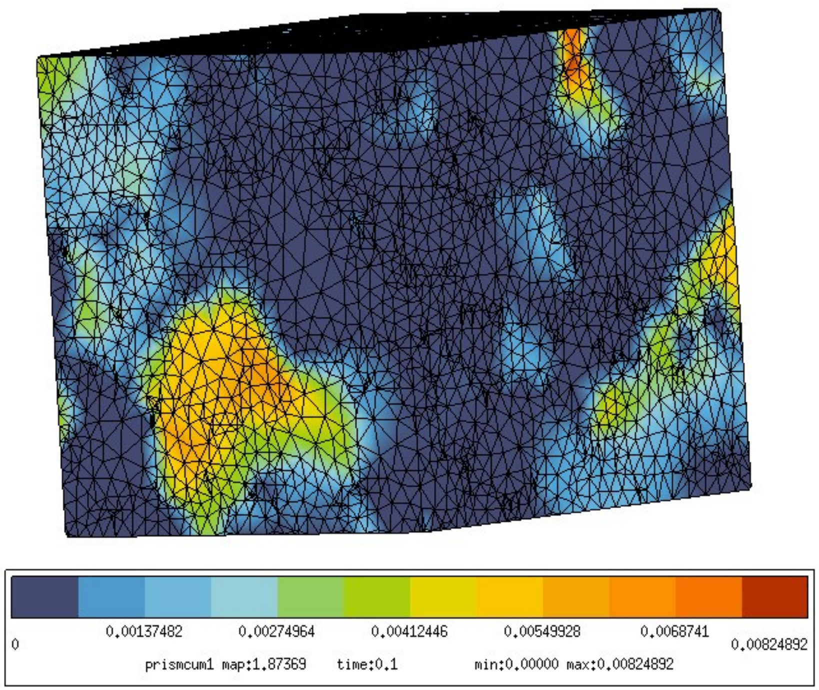
Grain map slice (top view)
Detector : 2.85µm resolution

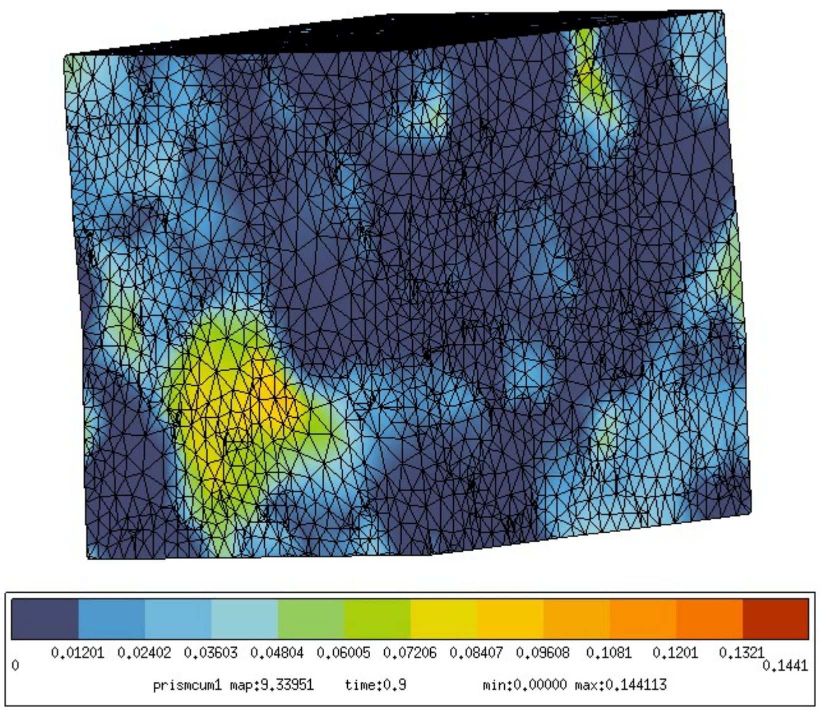




Simulated data – Zset FEA Simulation

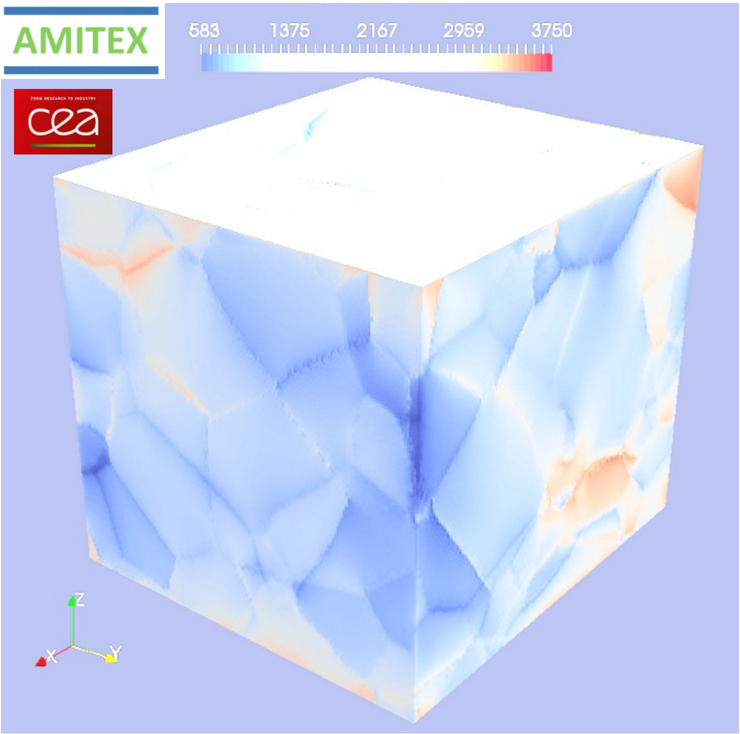
- Elements : Linear tetrahedral
- Loading : ε_{TOTAL} = 3 %
- Computation: 1.6G RAM, 4,120s on laptop
- Meshing convergence to be studied





Simulated data – FFT Simulations

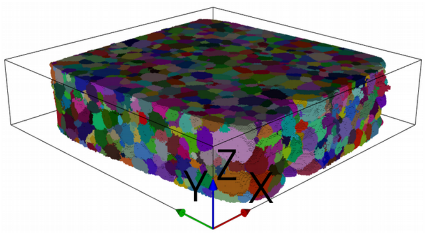
- Tested on data from previous ESRF DCT campaign : Anisotropic elasticity
- Actual behavior law to be coded with MFRONT



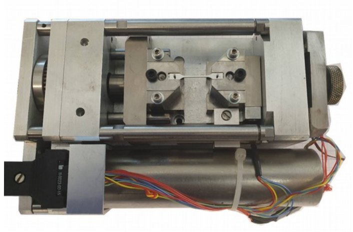
- 1 deformation increment
- 1 node on CRISTAL cluster
- Computation time : 8 min

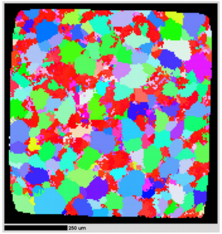
Achievements

- **Digital twin:**
  - 2 PSICHE scans merged (~ 3,200 grains)

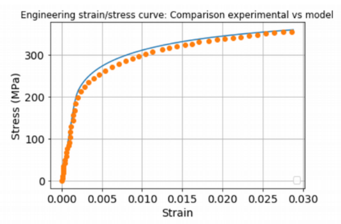


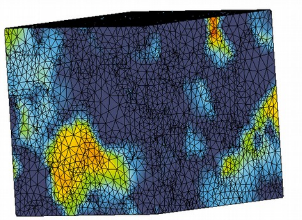
- **Experimental data:**
  - First reference stress/strain curves
  - Defined strategy for SEM in-situ campaign
  - First 3D Lab DCT results





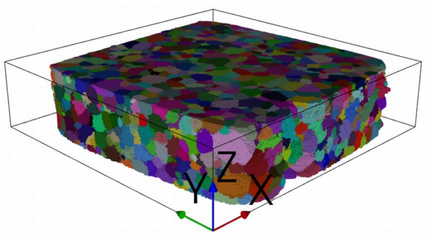
- **Simulation Data :**
  - First version of behavior model
  - Parameters identification initiated
  - FEA results on PSICHE data



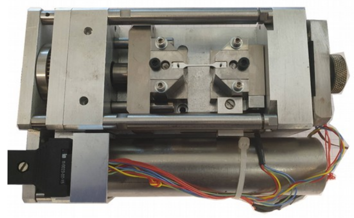


Outlook

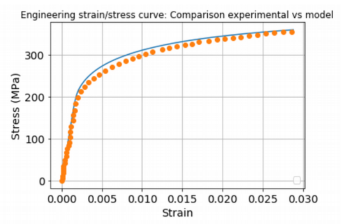
- **Digital twin:**
  - Complete reconstructions (~10,000 grains)
  - Update 6D DCT Rec algorithm for PSICHE



- **Experimental data:**
  - Perform SEM in-situ campaign (DMS student support)
  - Explore SEM-DIC potential
  - 3D Lab DCT: Travel to Lund



- **Simulation Data :**
  - Behavior model: Enrich model
  - Parameters identification: Enrich with new tests
  - Simulations on complete PSICHE volumes



- **Statistical learning:**
  - Extract physical data from structured dataset
  - Statistical analysis of plasticity mechanims

THANK YOU FOR YOUR ATTENTION.

ANY QUESTIONS ?