In situ multimodal experimental testing and simulations in volume for statistical analysis of crystal plasticity

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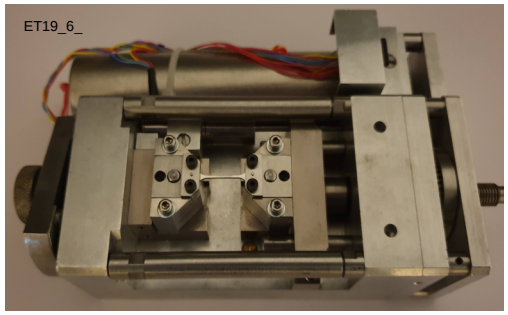
MINES ParisTech, PSL research university, Centre des Matériaux, Evry

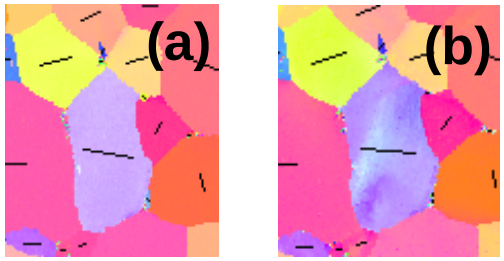
Agenda

- Previous status
- Experimental data:
  - SEM in situ test
  - New PSICHE campaign
  - Examples of mutlimodal hybrid dataset :
- Simulation data
  - Finite strain crystal plasticity model
  - Parameters identification
  - Simulation strategy
- Outlook

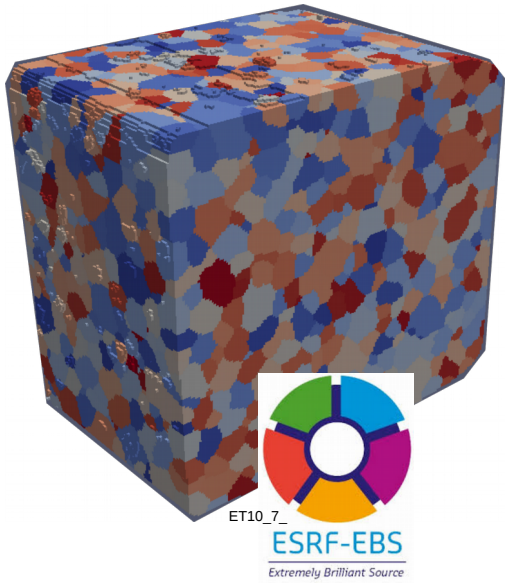
Previous status (04/15/21)

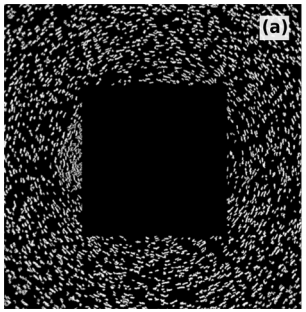
- Experimental priority : Hybrid in situ multimodal tests : initial DCT + EBSD in situ
- Digital twins :
  - Synchrotron ESRF EBS : Ready for meshing and simulation
  - LabDCT Lund : First conclusive results



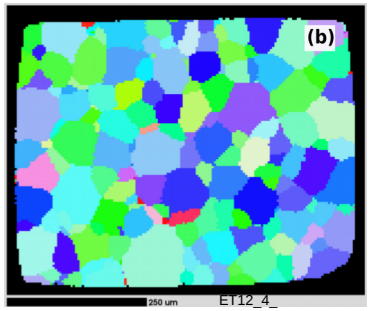


(a)Initial underformed state
(b) εp=2,36 %





(a) Lab DCT detector
1 image/201 - resolution 4µm

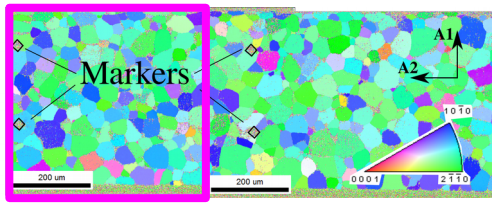


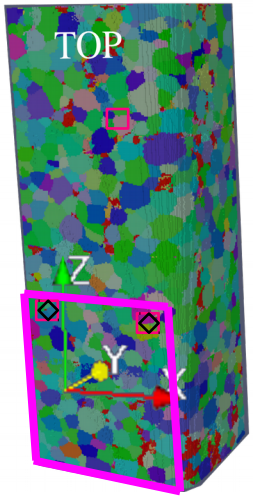
(b)Reconstructed grain map slice with GrainMapper (XnovoTech)

Multimodal data – Example 1

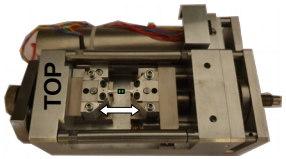
1st hybrid multimodal test

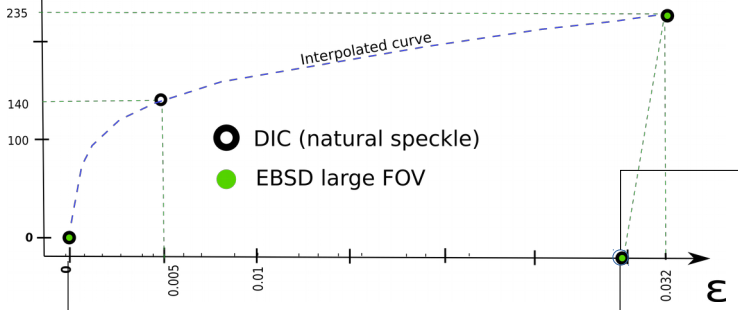
Ref SEM
Ref DCT (LabDCT + ESRF)



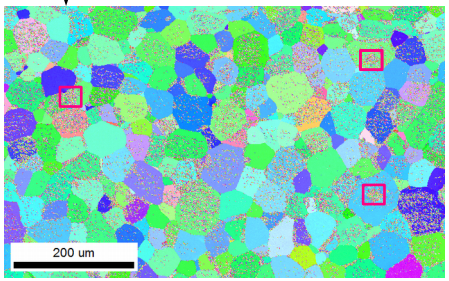


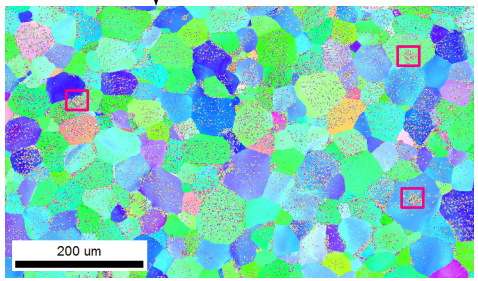
SEM in situ
06/17/21

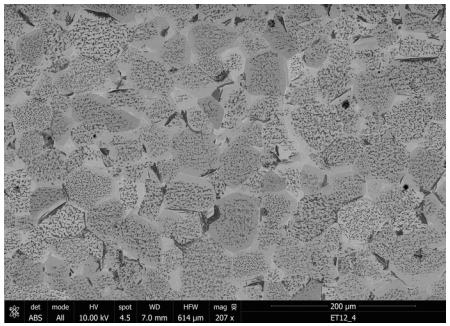


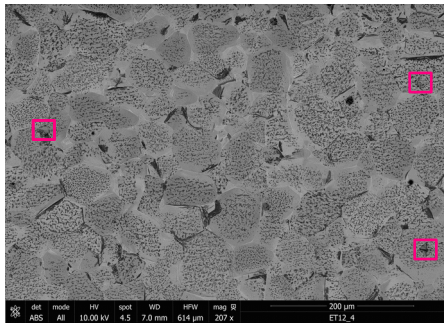


DCT Post Mortem
PSICHE July 21



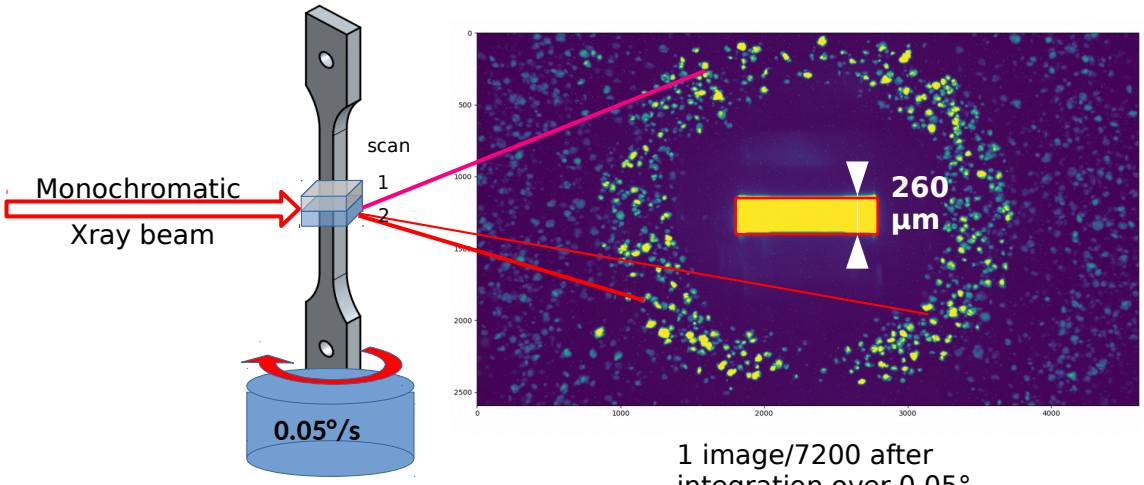




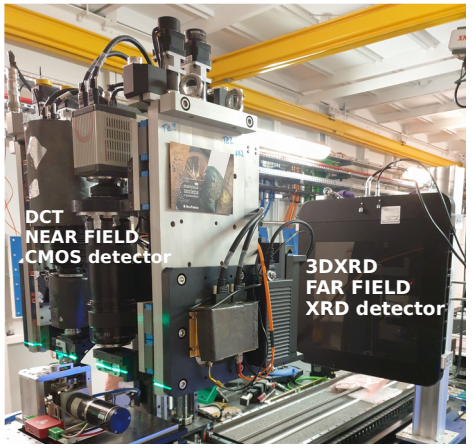


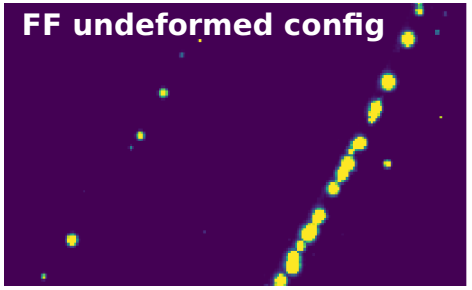
PSICHE July 21

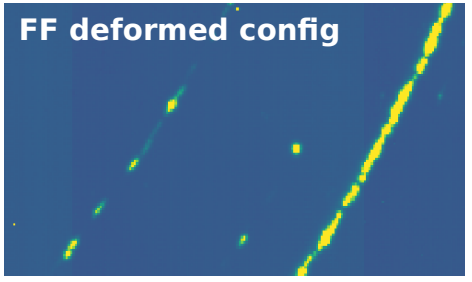
- Jul 2021 - SOLEIL synchrotron - PSICHE line
- Commissionning
- 1 DCT scan @ 1.085µm resolution → 2h, 150Go
- Undeformed DCT : 4 samples
- 4D interrupted DCT : 2 samples



1 image/7200 after integration over 0.05°







- Additional modalities: 3DXRD (Far Field), PCT
- Total data: 4.2 To data

CMOS : Complementary Metal Oxide Semiconductor

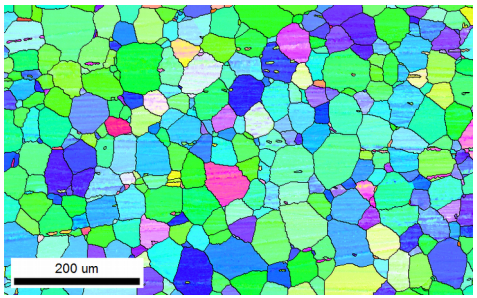
PCT : Phase Contrast Tomography
3DXRD: 3D X-ray Diffraction

Acknowledgment : Andrew KING (PSICHE), Wolfgang LUDWIG (ESRF)

Multimodal data – Example 2

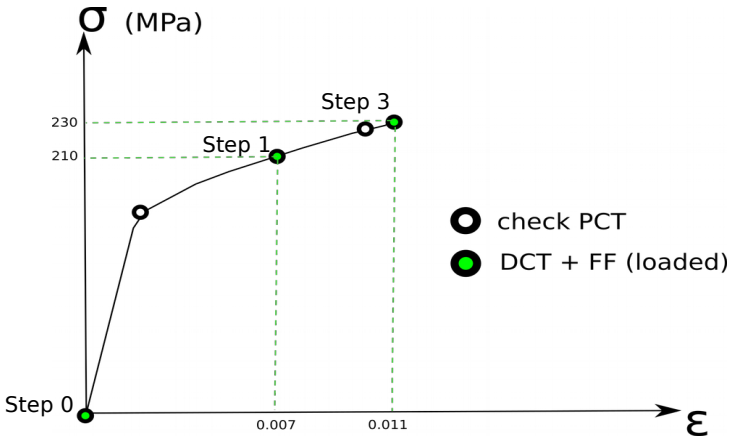
ET12_7

Ref SEM

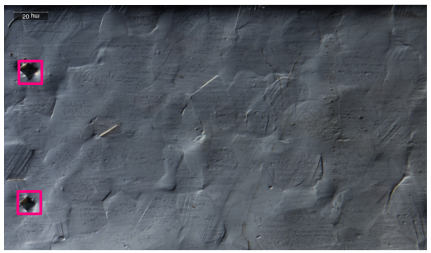


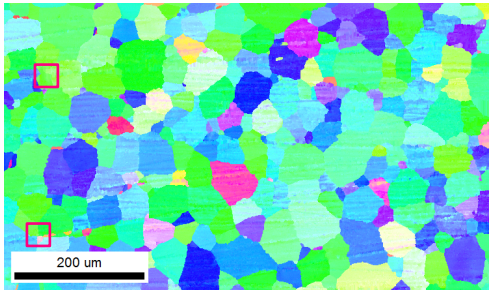
Synchrotron in situ

Single scan height	# load steps	# DCT/FF scans/step	Total height scanned
260µm	2	2	~540µm

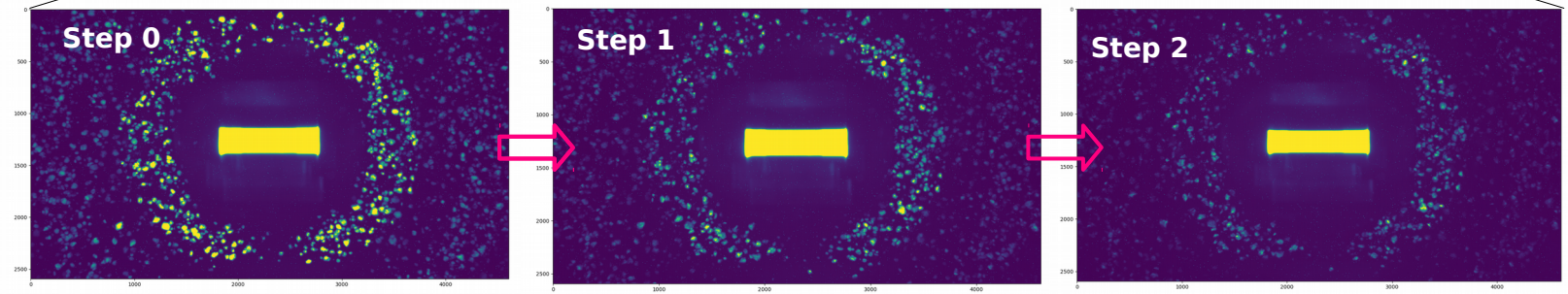


Post Mortem

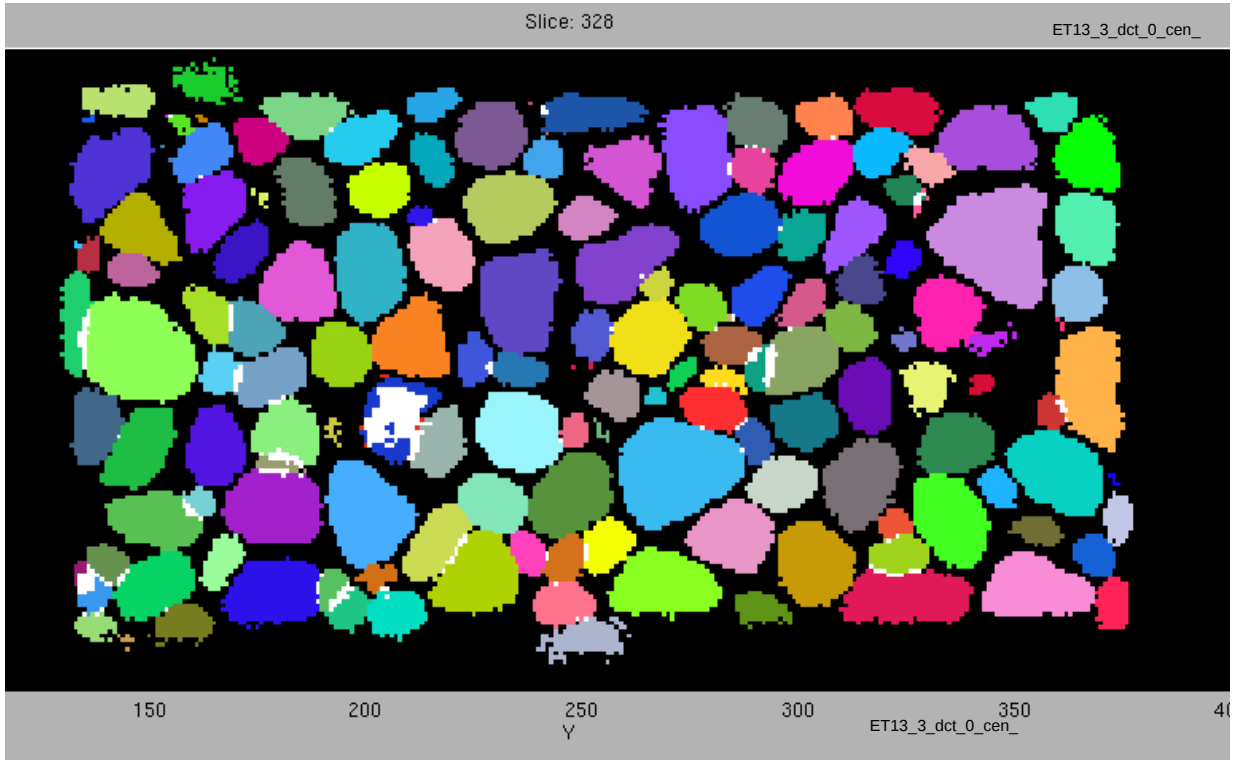




DCT images

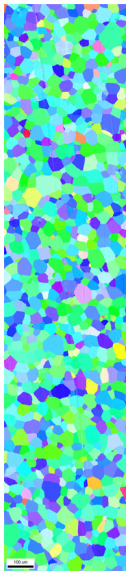


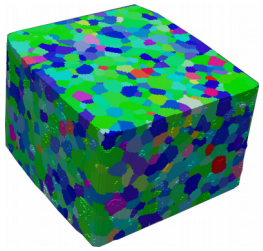
PSICHE July 21 – First DCT Rec



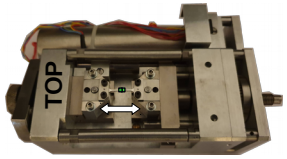
Multimodal data – Example 3

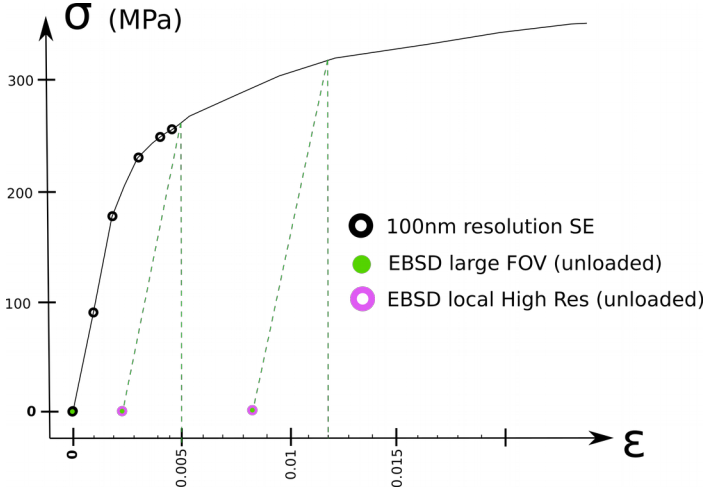
Ref SEM
Ref DCT





SEM in situ
Scheduled – 09/02/21





DCT
Post Mortem

To be scheduled
Options :
LabDCT, ESRF DCT, PSICHE DCT

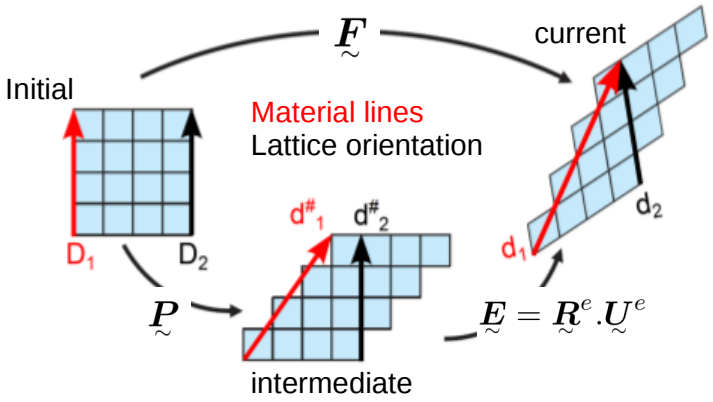
Simulations on digital twins

Finite strain crystal plasticity model

- Elastoviscoplastic continuum mechanics
- Kinematics :
  - $\underset{\sim}{F}(\underline{X}) = \underset{\sim}{E}(\underline{X}).\underset{\sim}{P}(\underline{X})$ (Mandel, 1973)
  - $\underset{\sim}{R}^e \rightarrow$ Lattice curvature evolution (SSA)

$$\underset{\sim}{\alpha} \simeq -\mathrm{curl}\,\underset{\sim}{R}^{eT}$$

$$\underset{\sim}{\kappa} = \underset{\sim}{\alpha}^T - \frac{1}{2}(\mathrm{trace}\,\underset{\sim}{\alpha})\underset{\sim}{1}$$



- Behavior law :
  - (Meric, Cailletaud, 1991)
  - Only isotropic hardening

$$\underset{\sim}{\Pi}^e = \underset{\sim}{C} : \underset{\sim}{E}^e$$

$$\dot{\gamma}^s = \mathrm{sign}(\tau^s)\left\langle \frac{|\tau^s| - \tau_c^s}{K} \right\rangle^n$$

$$\tau_c^s = \tau_c + q\sum_{r=1}^{N} h^{sr}(1 - \exp(-bv^r))$$

$$\underset{\sim}{C}^e := \underset{\sim}{E}^T \cdot \underset{\sim}{E}, \quad \underset{\sim}{E}^e = \frac{1}{2}(\underset{\sim}{C}^e - \underset{\sim}{1})$$

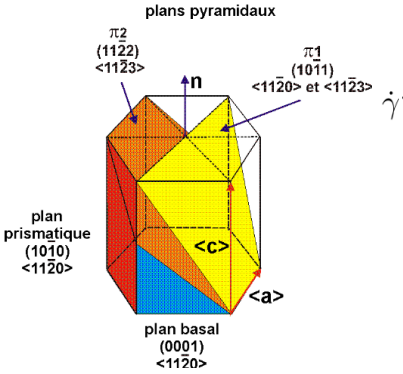
$$\tau^s = \underset{\sim}{M} : \underline{m}^s \otimes \underline{n}^s$$

Parameters identification

- RD monotonic tensile test input data
- Small strain crystal elastoviscoplastic scheme
- Breveiller-Zaoui homogeneization → Digital twin sub volume (580 grains)

$$\underset{\sim}{C} = \begin{pmatrix} 162000 & 92000 & 69000 & 0 & 0 & 0 \\ 92000 & 162000 & 69000 & 0 & 0 & 0 \\ 69000 & 69000 & 180000 & 0 & 0 & 0 \\ 0 & 0 & 0 & 46700 & 0 & 0 \\ 0 & 0 & 0 & 0 & 46700 & 0 \\ 0 & 0 & 0 & 0 & 0 & 35000 \end{pmatrix}$$

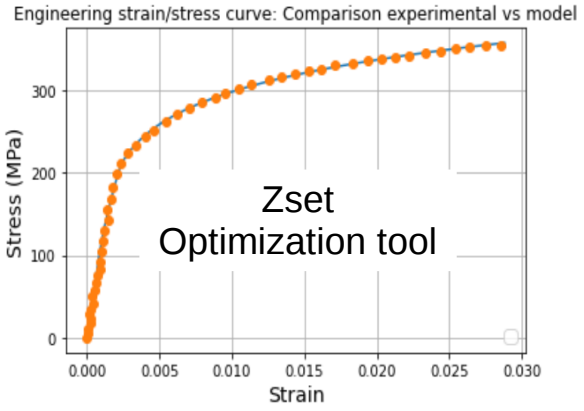
(Simmons et Wang, 1971)

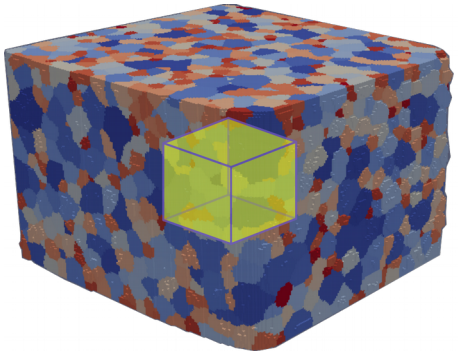


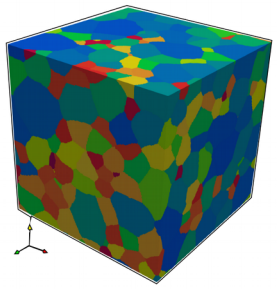
$$\dot{\gamma}^s = \mathrm{sign}(\tau^s)\left\langle \frac{|\tau^s| - \tau_c^s}{K} \right\rangle^n$$

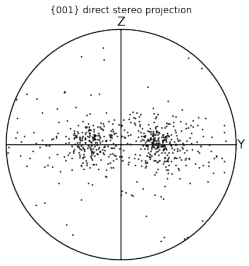
$$R = \mathrm{R0} + \cancel{\mathrm{Q}\left(1 - e^{-\mathrm{b}p}\right)}$$

SSA





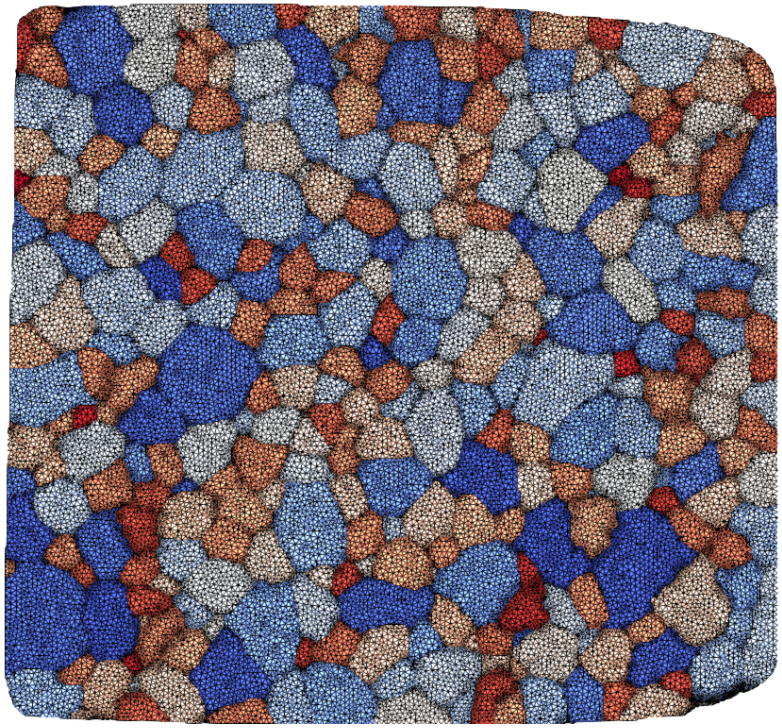


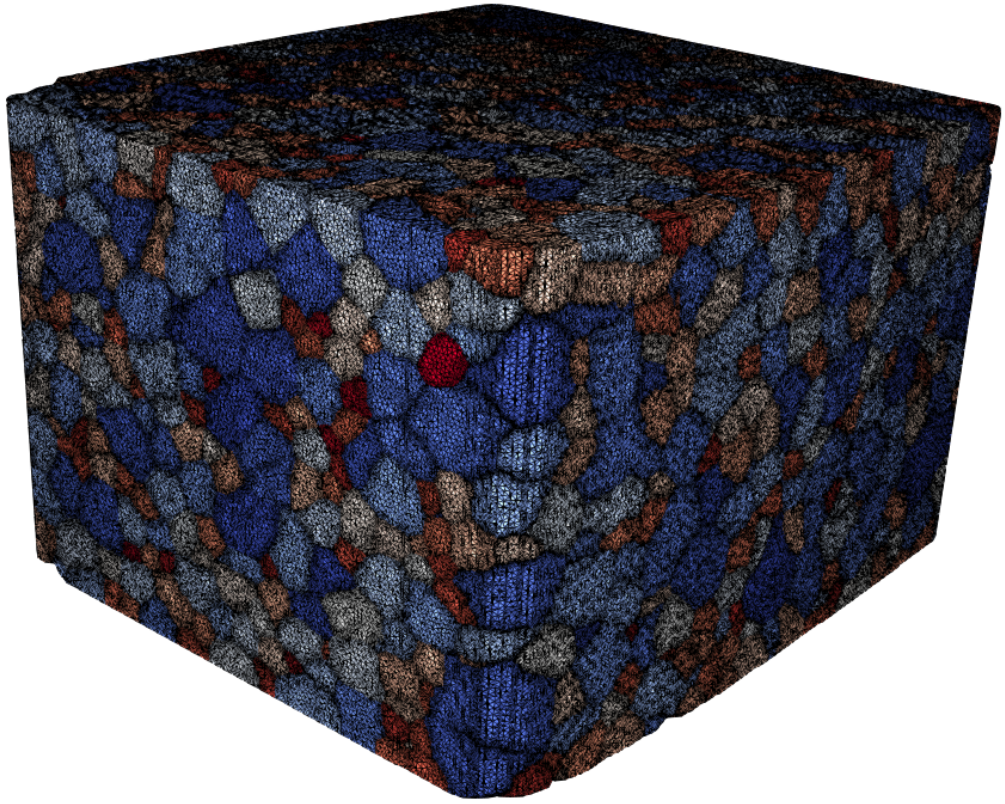


K = 40
n = 10
$R0_{prism}$ = 50 MPa
$R0_{bas}$ = 60 MPa
$R0_{pyr1}$ = 111 MPa

RD: Rolling Direction

Morphological meshing

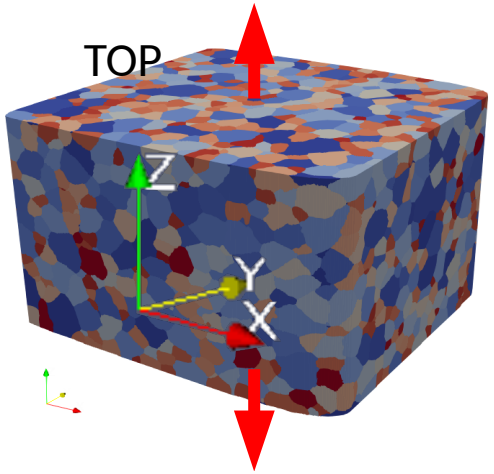


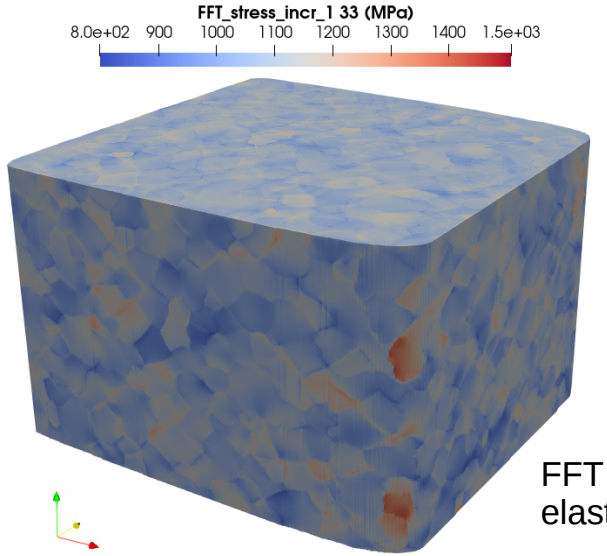


Acknowledgment :
Franck N'GUYEN , Aldo MARANO
(Centre des matériaux)

Simulations strategy

- Volume and surface
- FFT : Equivalent (AMITEX – CEA) = Priority
- FEM : Mandel Crystal (Zset)
- Monocyclic, based on real in situ test (SEM)





FFT anisotropic elasticity

FEM: Finite Element Modeling
FFT: Fast Fourier Transform

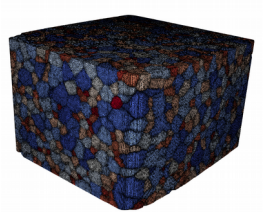
Acknowledgment :
Aldo MARANO
(Centre des matériaux)

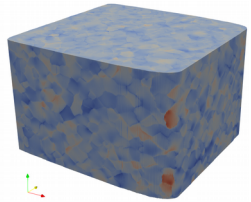
Outlook

Outlook

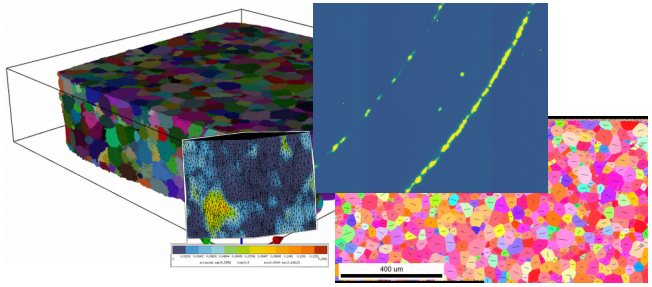
- **Experimental data:**
  - Considered completed as part of PhD
  - Opportunity for DFXM @ ESRF ID06

- **Simulation Data :**
  - Finalize parameters identification
  - Launch crystal plasticity simulations on digital twins

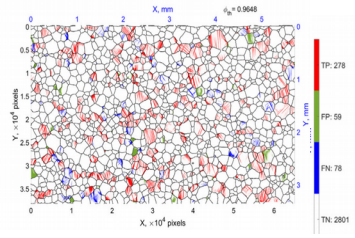


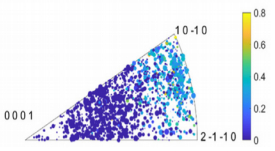


- **Data unification:**
  - Consolidate modalities to prepare ground for statistical analysis (leverage BIGMECA data plateform)



- **Satistical learning :**
  - Extract physical data from images and volumes.
  - Perform statistical analysis of plasticity mechanims.





THANK YOU FOR YOUR ATTENTION

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