06/09/2020

Statistical study of polycrystal plasticity using experimental and simulation data

BIGMECA COPIL

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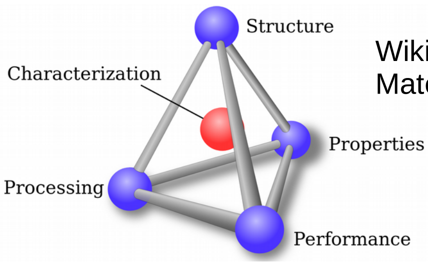
Agenda

- Background on crystal plasticity
- Problem vs Opportunity
- Objectives & Methodology
  - Multimodal data (Experimental, Simulated)
  - Data storage and structure
  - Machine Learning
- Conclusion

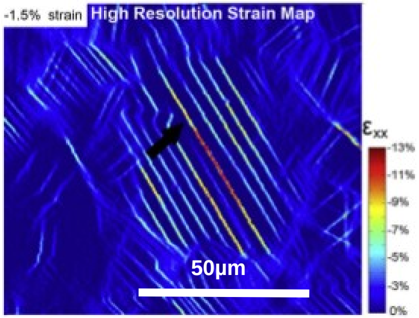
Background on crystal plasticity

- **Why**: Quest to improve knowledge in life duration, damage, manufacturing processes
- **Material Science Paradigm :**
  Establish Process-Structure-Properties (PSP) relationships

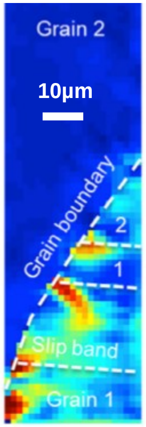


Wikipedia : Material Science

- **Scope for plasticity** : Microstructure scale
- **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)

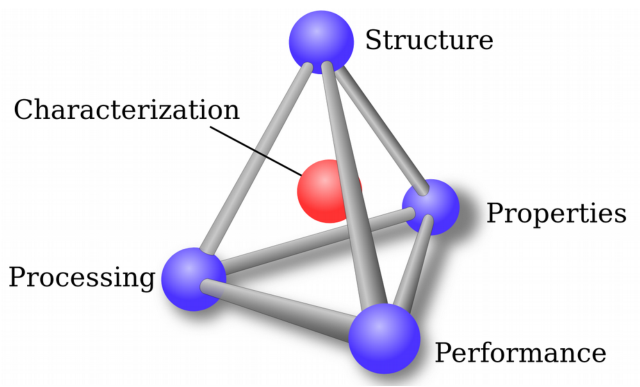
- **Long term vision** :
  - Derive physics based behavior laws
  - Relate them to macroscopic material properties
  - Adapt material design based on environment, properties requirements

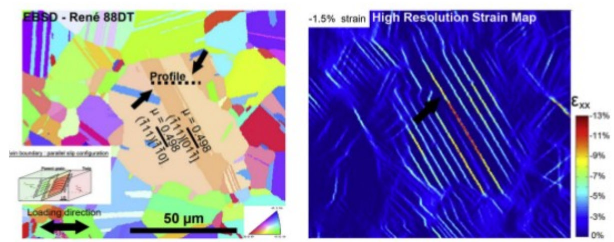
DAXM: Differential Apperture Xray Microscopy
In-situ = Measure of deformations during the test = adding temporal dimension
SEM: Scanning Electron Microscope

Background on crystal plasticity

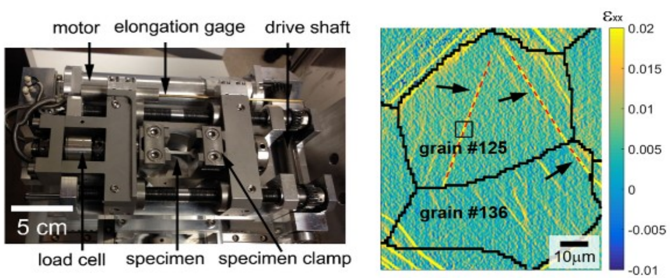
History & state of the art

- > 1950: Theoretical framework (Hill, 1950) (Mandel, 1972) (Germain, 1983)
- > 1970s: Characterization : non destructive 2D, destructive 3D

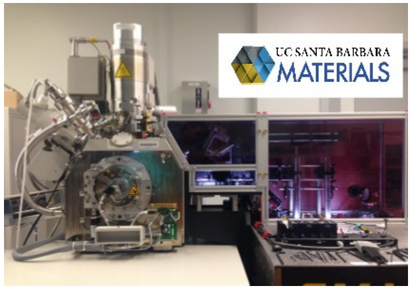


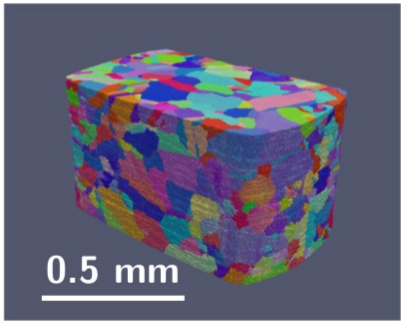


[Stinville et al., 2016]



[Chen and Daly, 2016]



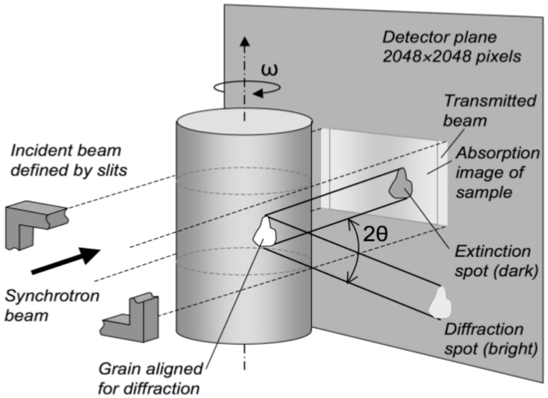


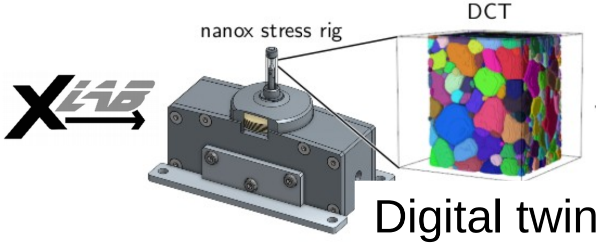
(Echlin et al., 2015)

Background on crystal plasticity

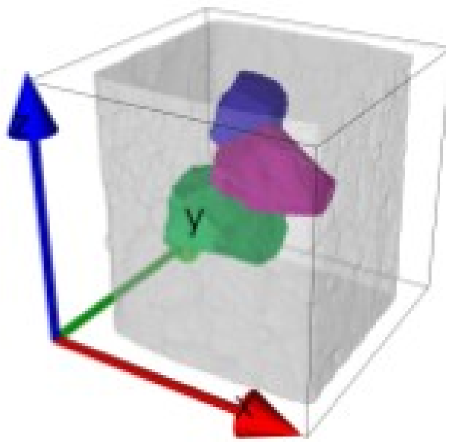
History & state of the art

- ~2000: New era of non destructive volumic techniques : 3DXRD (Poulsen)
- > 2010: DCT at ESRF (Ludwig et al., 2009) (Reischig et al., 2013)
- > 2010: DCT compatible in-situ stress rigs (Xlab) development at CDM
- 2014 : ESRF : in-situ DCT + TT (Guéninchault, 2017)

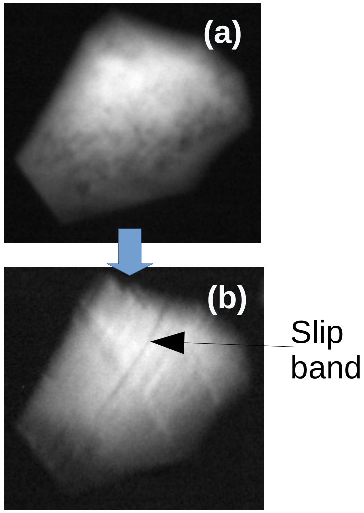




Digital twin



Grains selection + TT



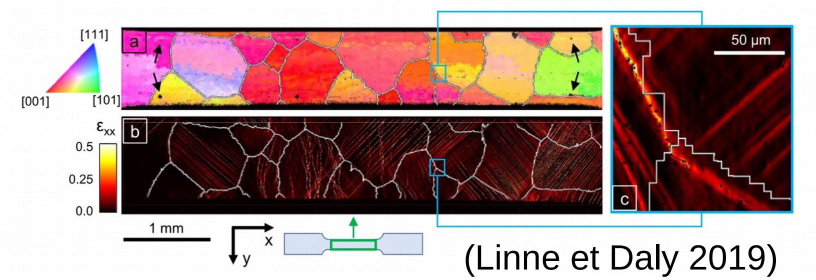
(a) Undeformed grain
(b) Plastified grain

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

In-situ = 4D = Measure of deformations during the test = adding temporal dimension
TT: Topotomography

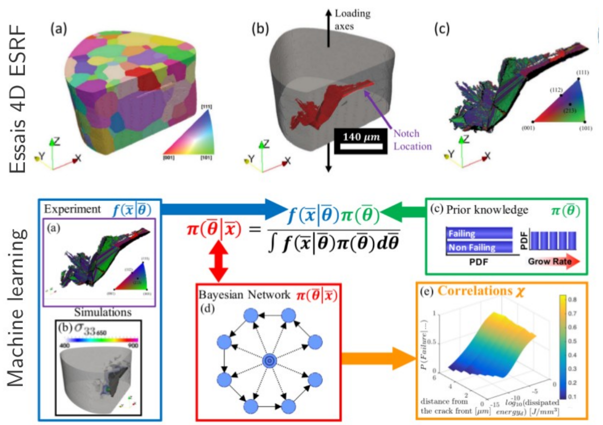
Problems vs Opportunities

- **Problem**: Complexity of mechanical mechanisms at mesoscopic scale (~10^3 grains)
  → Current approaches limited to derive realistic models in realistic time frame.



(Linne et Daly 2019)

- **Opportunities**:
  - Machine learning applied to mechanics :
    - Extract physics based statistical data
    - Derive microstructural behavior laws
  - TT results (Guéninchault, 2017)
  - CDM expertise: characterization, simulation
  - Deployment of DCT technique at SOLEIL

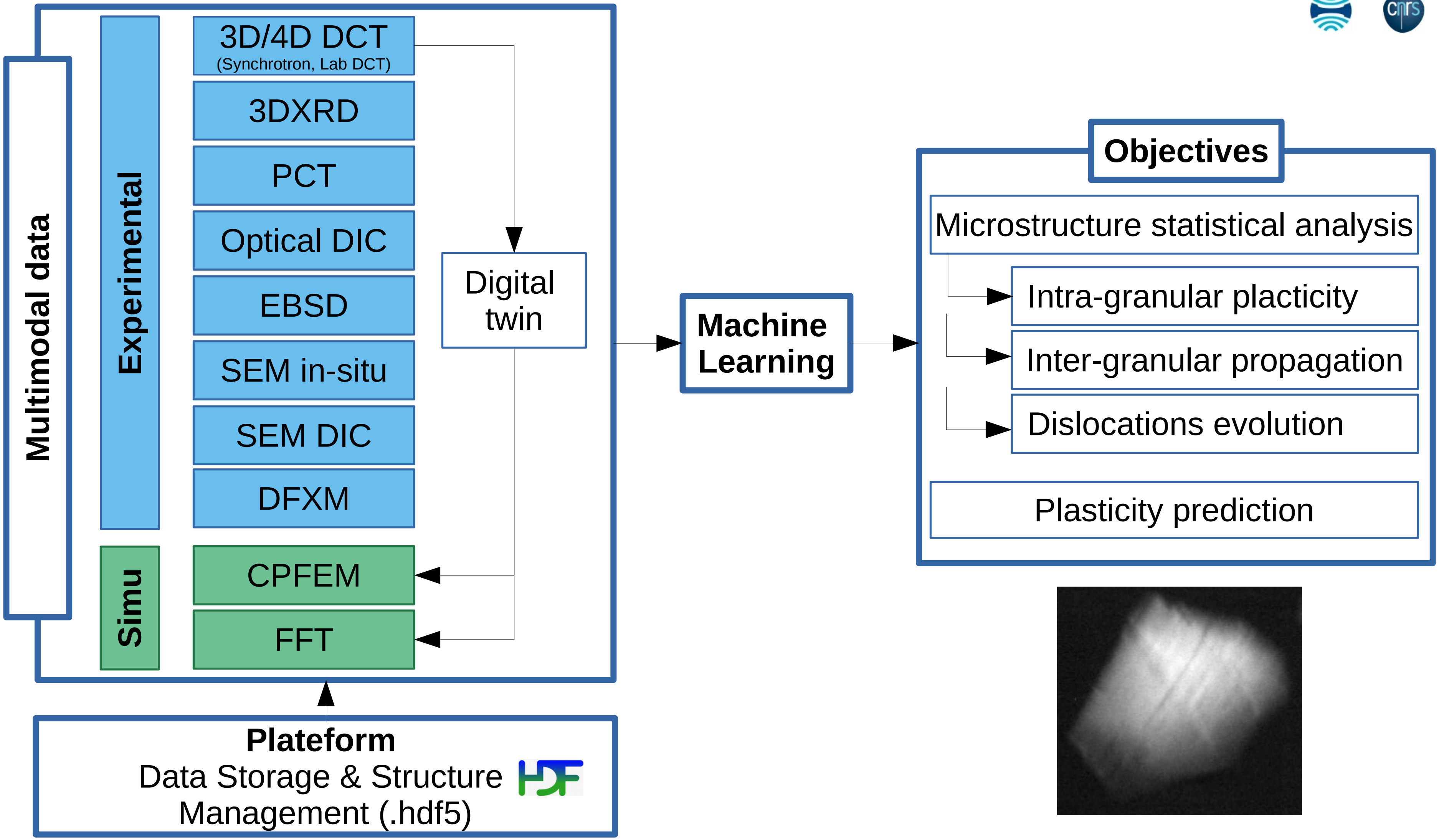


(Rovinelli et al. 2018)

- **Several applications → BIGMECA Research initiative**
  Plasticity, damage and fracture, crack propagation, twinning

SOLEIL : Synchrotron at Plateau de Saclay (Paris Area)

Objectives & Methodology - Overview



3DXRD : 3D Xray Diffraction
CPFEM : Crystal Plasticity Finite Element Modeling
DIC : Digital Image Correlation

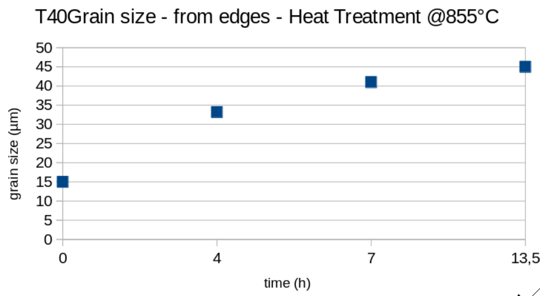
DFXM : Dark Field X-ray Microscopy
EBSD : Electron Back Scattering Diffraction
FFT : Fast Fourier Transform

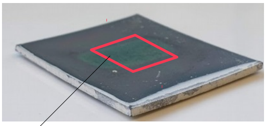
PCT : Phase Contrast Tomography
SEM: Scanning Electron Microscope

Methodology – Experimental data

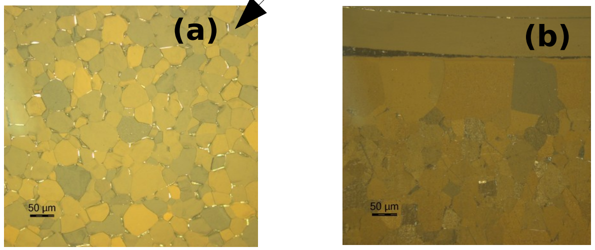
Synchrotron campaign - Preparation

- **Material** :
  - Titanium phase-α (T40)
  - Hexagonal lattice
  - Transus 913°C
  - Raw material : sheet 1.6mm thick
  - Manufacturer : TIMET
  - Initial average grain size : 15µm
- **Heat Treatment** :
  - Target grain size : 60µm
  - AET oven
  - Oven T°C mapping & calibration (855°C)
  - Cycle : Duration screening, 855°C, argon (10 L/min)
  - Representative sheet treated : 30x35mm
- **Micrographies** :
  - Main face + Through thickness cut
  - Pre-polishing (respectivly electrolytic, mechanical)
  - Chemical etching (Kroll)
  - Cross validation with EBSD
- **Outcome :**
  - Cycles selected : 17h (+1 backup 24h cycle)
  - **Actual average grain size : ~50µm**

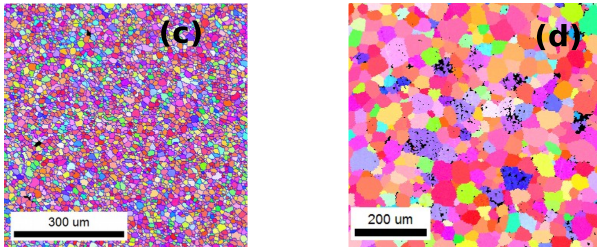




Sheet 35x30mm



Micrographies Bright Light, Polarized, x200, 17h:
(a) Main face, (b) Through thickness cut

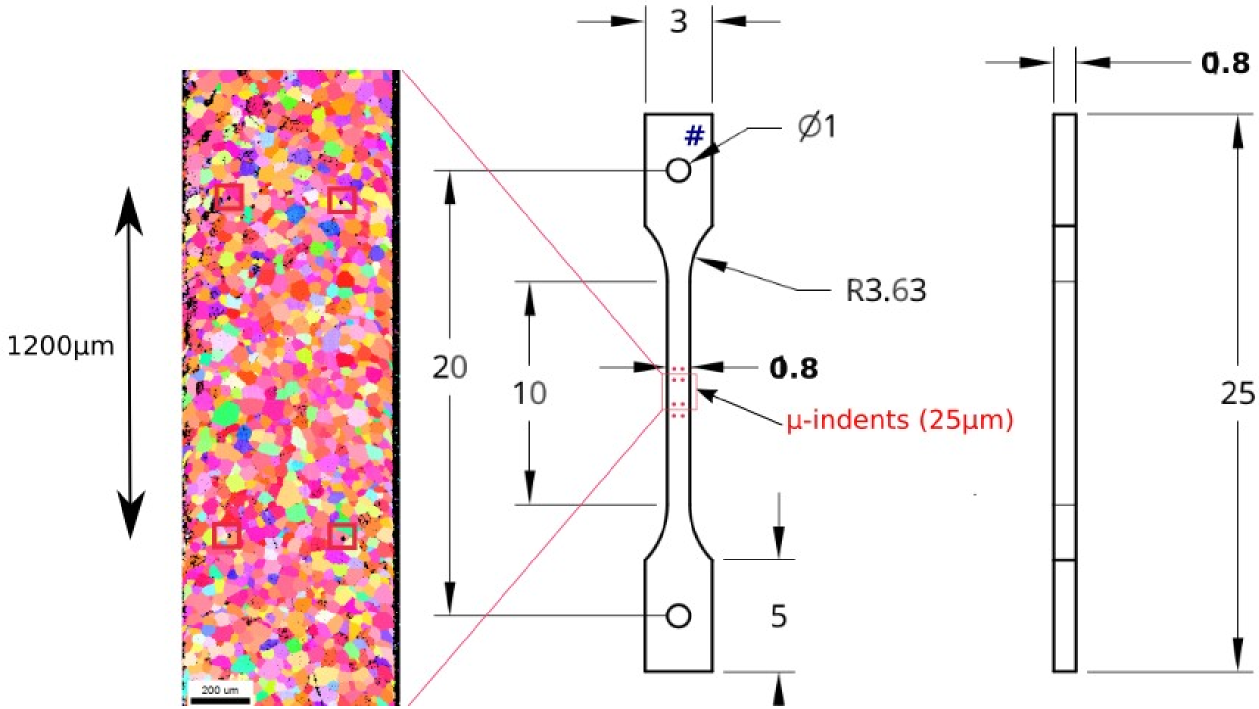


EBSD : (c) Initial grain size ~ 15µm,
(d) after heat treatment (855°C, 17h, 24h) ~ 50µm

Methodology – Experimental data

Synchrotron campaign - Preparation

- 28 dog-bone samples (7 samples/sheet) by EDM machining
- Preparation of reference scans (SEM-mapping + EBSD):
  Pre-polishing 1200 → 4000 grit abrasive → 12h OPS → 8 μ-indents Vickers (virtual extenso)
- Opposite face + edges: 1200 grit abrasive by hand



EBSD – 2μm resolution

Methodology – Experimental data

Synchrotron campaign

- SOLEIL - PSICHE line : 4-9 March 2020
- Scale of interest : Slip systems
- 5 samples scanned ~ 2 To data
- 4D DCT in-situ by steps – 2.85µm resolution, 1h/scan

Sample	Approx section	# DCT scans	1 scan height	# load Steps	Total height scanned
ET11_2_	850x850µm	7	400µm	3	1000µm

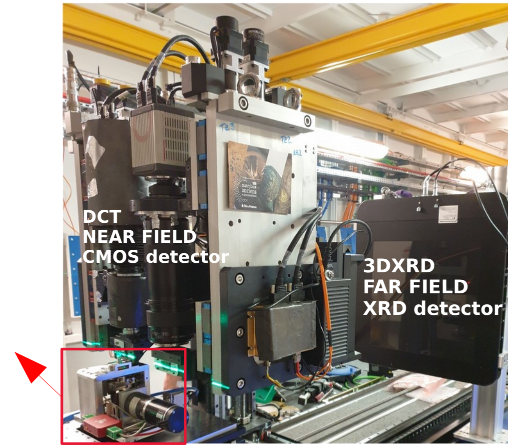
- 3D DCT – 2.85µm resolution, 1h/scan

Sample	Approx section	# DCT scans	1 scan height	# load Steps	Total height scanned
ET8_6_	800x800µm	3	200µm	NA	560µm
ET11_3_	800x800µm	9	120µm	NA	920µm

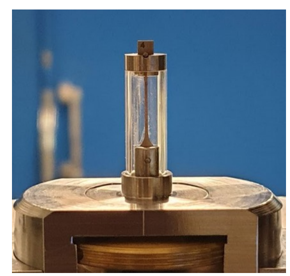
- 4D DCT in-situ by steps – 1.3µm resolution, 2h/scan

Sample	Approx section	# DCT scans	1 scan height	# load Steps	Total height scanned
ET11_4_	600x600µm	12	~285µm*	2	~700µm (TBC)
ET11_5_	600x600µm	8	~400µm*	3	750µm

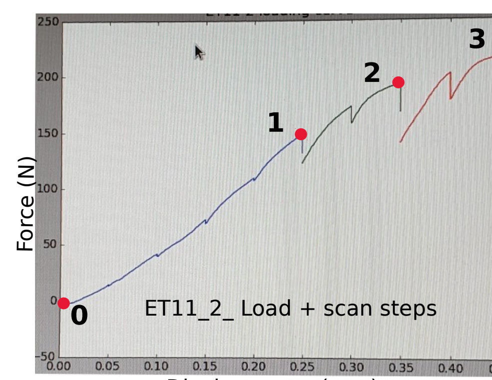
- Extra data: 3DXRD (Far Field), Absorption tomography, PCT
- Extra samples tested : Ti7Al, HEA (for VTT)



VIDEO :
Sample on Bulky stress rig
with DCT setup, Near Field



DCT setup on Bulky



CMOS : Complementary Metal Oxide Semiconductor
HEA : High Entropy Alloy
PCT : Phase Contrast Tomography

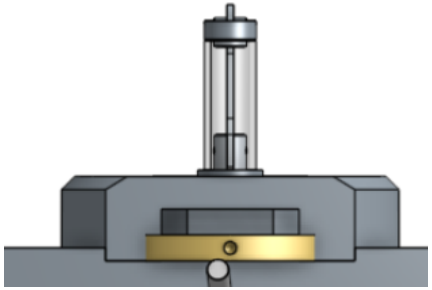
XRD: X-ray Diffraction
VTT : Teknologian tutkimuskeskus University (Finland)

*Height adapted depending on load step

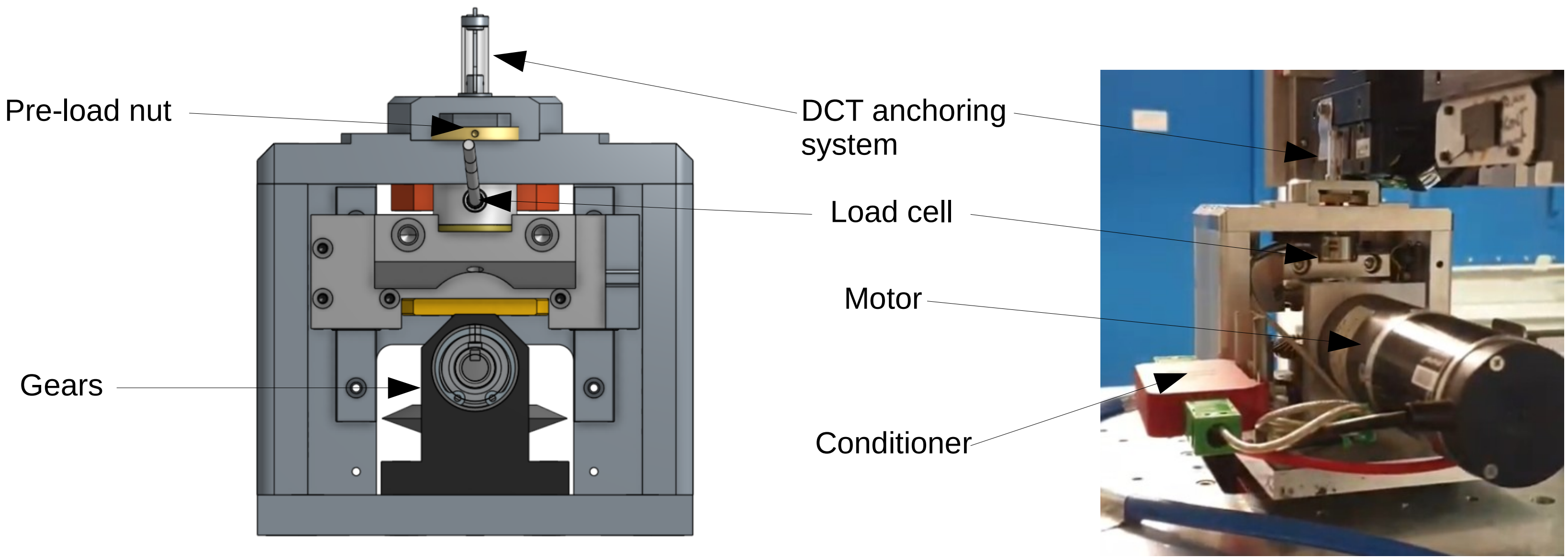
Methodology – Experimental data

Bulky in-situ test rig

- Existing rig (developed by CDM) with design improvements :
  - New anchoring system compatible with DCT experiment
  - Specific integration on PSICHE line
- User friendly + valid load range for current experiment
- Calibration before campaign : Load cell (500 lbs) + conditioner



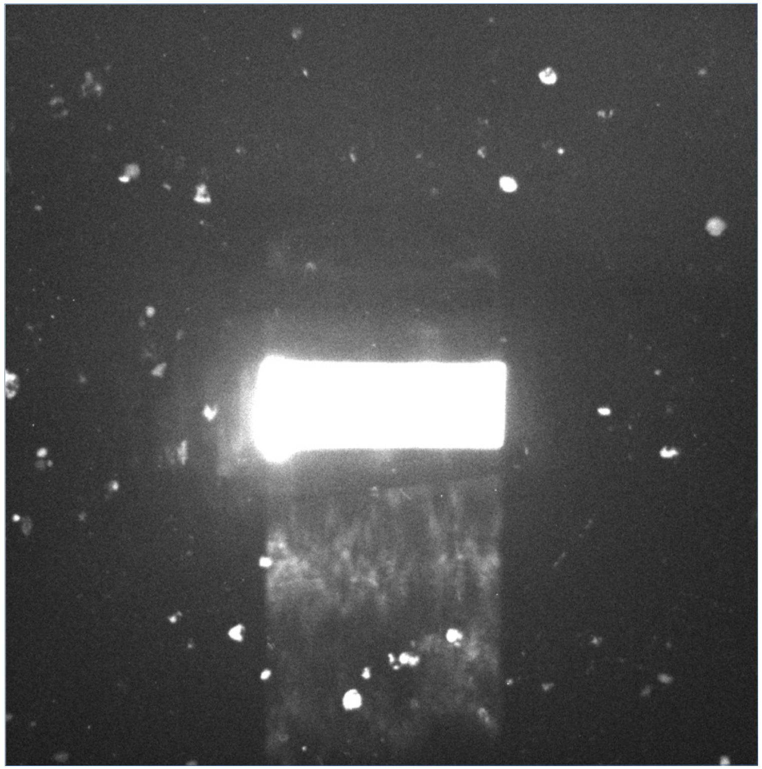
DCT anchoring system



Methodology – Experimental data

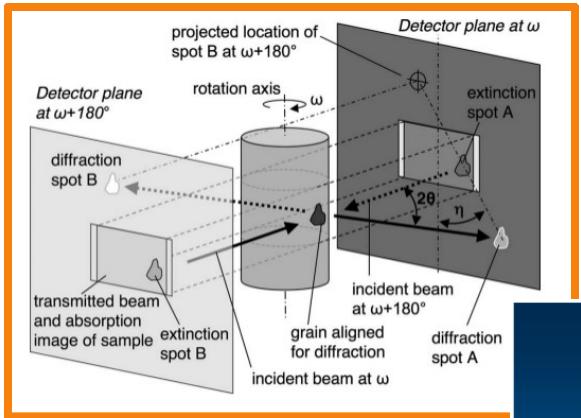
Synchrotron campaign

1 projection/3600 on detector 2.85µm.
sample ET11_3_ Beam height 120µm.
→ 1 scan = 1800 grains



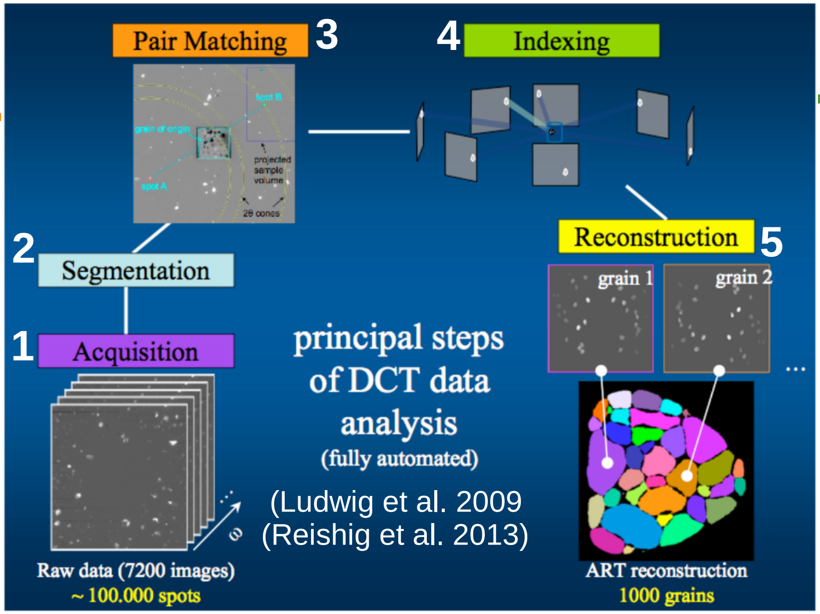
1 projection/3600 on detector 1.3µm.
sample ET11_4_. Beam height 285µm.
→ 1 scan = 2100 grains

Methodology – Image reconstruction

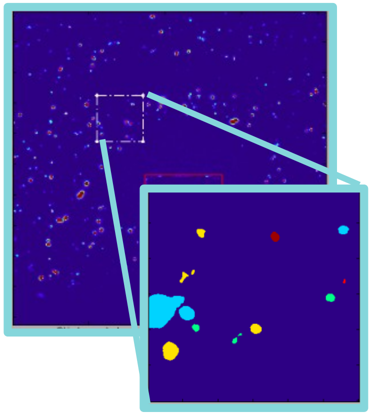


- **Indexing :**
  Assign pairs to specific grains

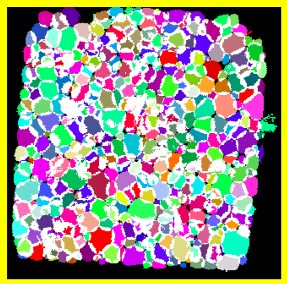
- Criteria : spot shape-size-area ; {hkl} planes ; distance between diffracted beams ; > 5 pairs.



Spots **segmentation**



- Grains 3D **reconstruction** (SIRT)
- Grains **segmentation**
- Absorption mask **reconstruction**
- Data **cleaning**
- Grains **dilatation**



SIRT: Simultaneous Iterative Reconstruction Technique

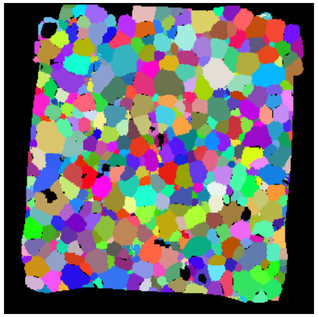
Methodology – Image reconstruction

- **Pushing the limits of DCT reconstruction algorithm:**
  - 3D DCT

Sample	Approx section	# DCT scans	1 scan height	# load Steps	#grains /scan	Total height scanned	Total # grains estimate
ET8_6_	800x800µm	3	200µm	NA	4000	560µm	**~8,000 grains**
ET11_3_	800x800µm	9	120µm	NA	1800	920µm	**~10,000 grains**

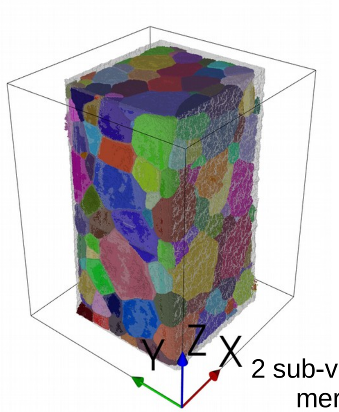
  - 4D DCT

Sample	Approx section	Load step	#scans /step	1 scan height	#grains /scan	Total height scanned	Total # grains estimate
ET11_4_	600x600µm	0	3	285µm	2100	~700µm (TBC)	**~5,000 grains**
		1	3	260µm*	on-going		on-going
		2	6	200µm	on-going	1080µm	on-going



XY slice of PSICHE reconstructed DCT sub-volume ET11_3_dct_0_z4_

- **Sub-volumes merging**:
  - First sub-volumes merged
    (from previous ESRF campaign on Ti7Al)

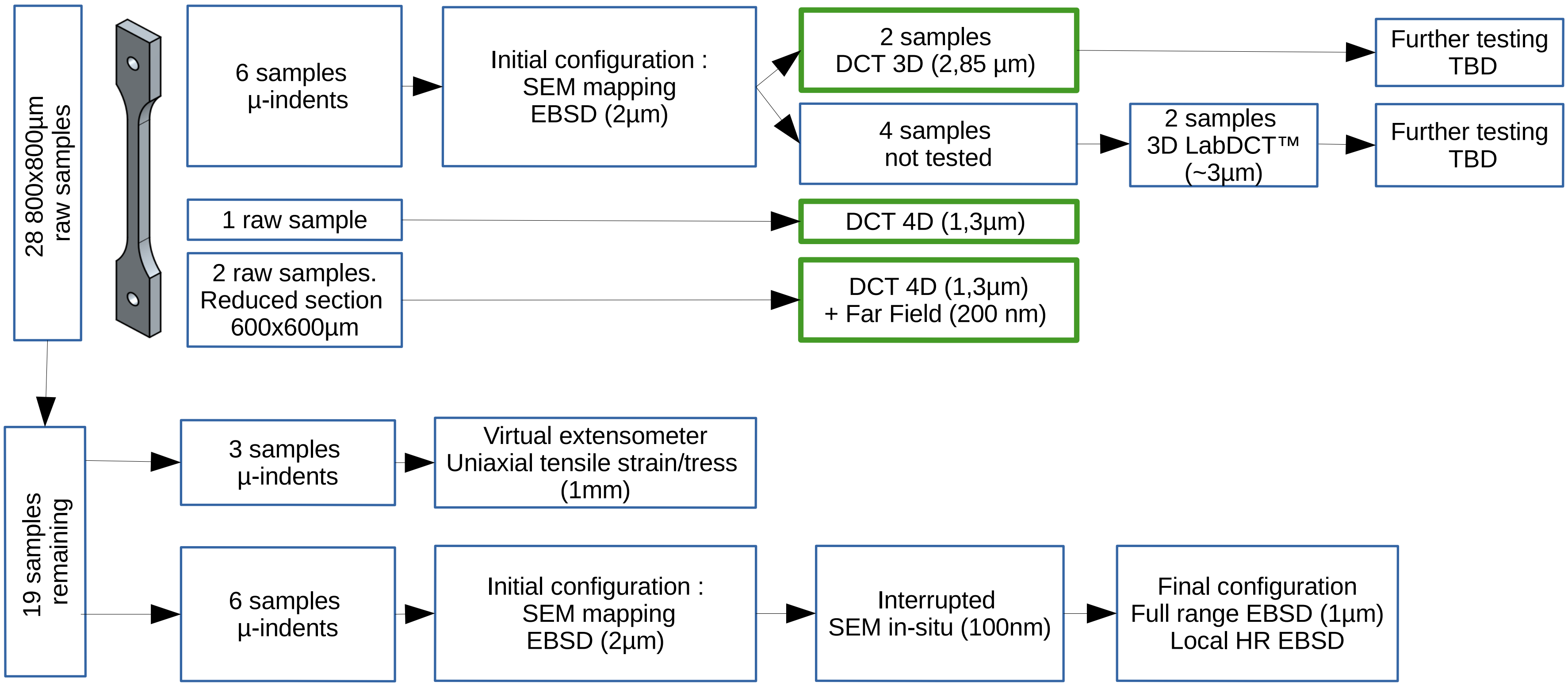


2 sub-volumes merged

*Average

Methodology – Experimental data

Multimodal dataset construction strategy

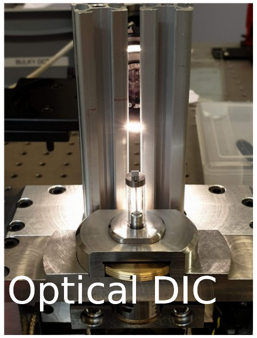


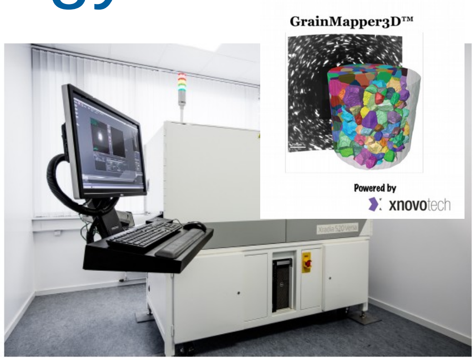
4D = interrupted in-situ testing
HR = High Resolution
TBD = To Be Determined

Methodology – Experimental data

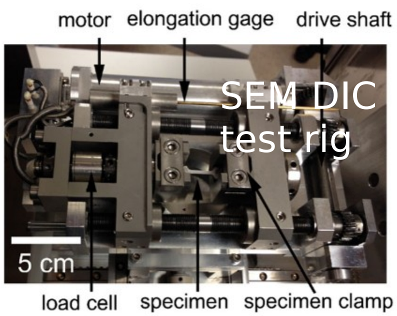
Multimodal dataset construction strategy

- Short term :
  - 3DXRD (Far Field)
  - 3D LabDCT™
  - EBSD
  - SEM mapping
  - Optical DIC (virtual extenso)
  - In-situ SEM
- Long term :
  - SEM DIC (20 nm)
  - PSICHE 2
  - DFXM (100 nm)

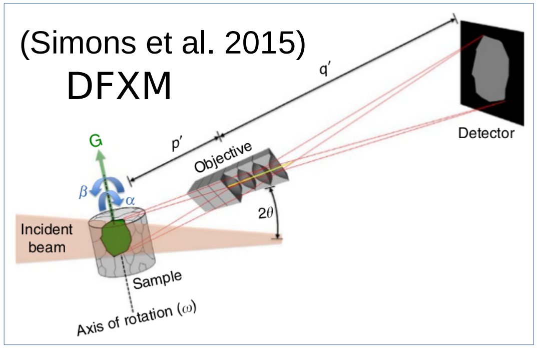


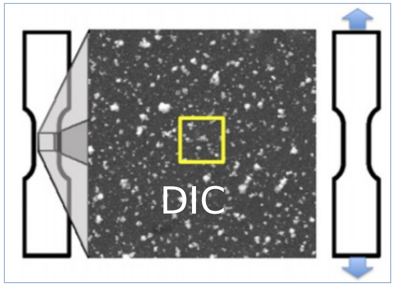


Zeiss Xradia Versa X-ray Microscope with LabDCT



(Kammers et Daly 2013)





3DXRD = 3D X-ray Diffraction
DIC : Digital Image Correlation
DFXM : Dark Field X-ray Microscopy

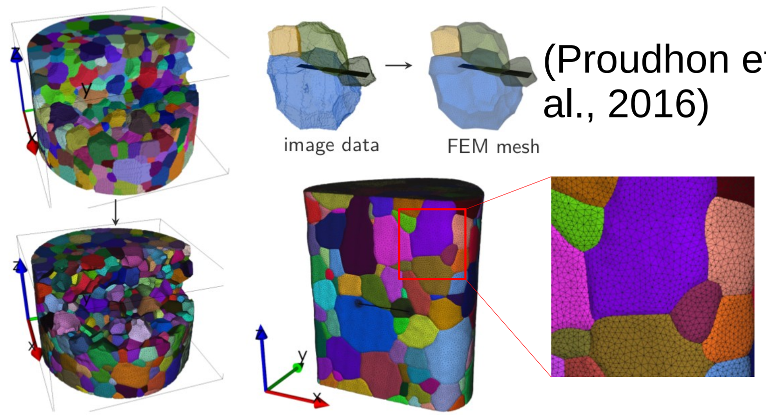
EBSD : Electron Back Scattering Diffraction
PCT : Phase Contrast Tomography
SEM: Scanning Electron Microscope

Methodology – Simulation data

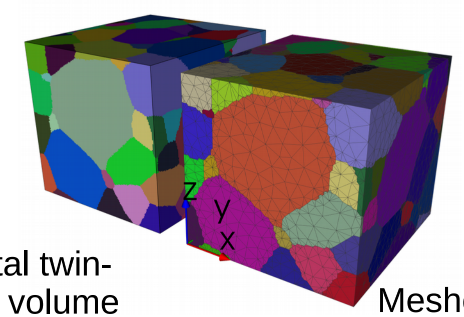
- Simulate directly with digital twin

- **FEA** (Zset):
  - New approach : Morphological meshing (N'Guyen, 2014) on test volume fromprevious DCT campaign (Ti7Al - 105 grains)
  - Improvement on-going (coarsening)
  - Anisotropic elasticity → Plasticity

- **FFT** (Amitex) :
  - No need for meshing
  - Anisotropic elasticity → Plasticity



(Proudhon et al., 2016)



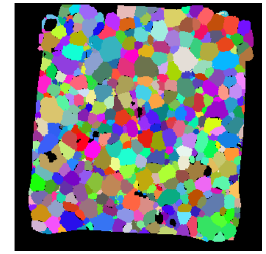
First digital twin-
DCT test volume

Meshed volume for FEA - morphological method

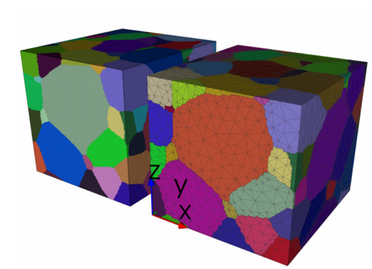
CPFEM = Crystal Plasticity Finite Element Modeling
FEA : Finite Element Analysis
FFT = Fast Fourier Transform

Conclusion

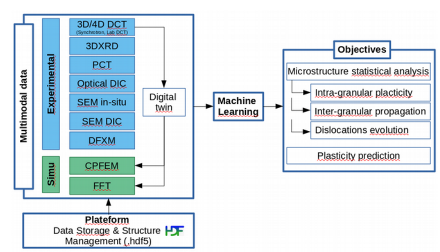
- **First milestones achieved :**
  - Data statistically representative for study of polycrystalline plasticity : **10^4 grains/sample**
  - First 3D volumes reconstructed (digital twins)

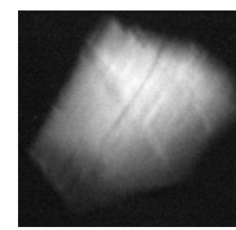


- **Current focus**:
  - Merge sub-volumes of PSICHE data
  - Perform first **simulations** on test volume
  - Build **data plateform** (Aldo MARANO)



- **Future work** :
  - Perform simulations on PSICHE samples
  - Complete multimodal dataset
  - Implement **Machine learning to help us understanding key plasticity mechanisms**





THANK YOU FOR YOUR ATTENTION.

ANY QUESTIONS ?

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