Deformation Behavior of Titanium using FFT-EVP Simulations

Azdine Nail-Ali, Samuel Hémery, Mikael Gueguen

Effect of Microtextured Regions on the Deformation Behavior of Titanium using FFT-EVP Simulations

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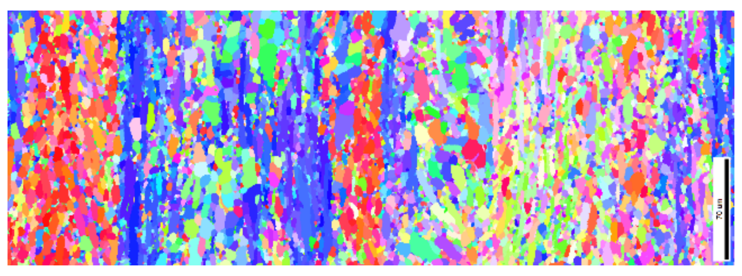
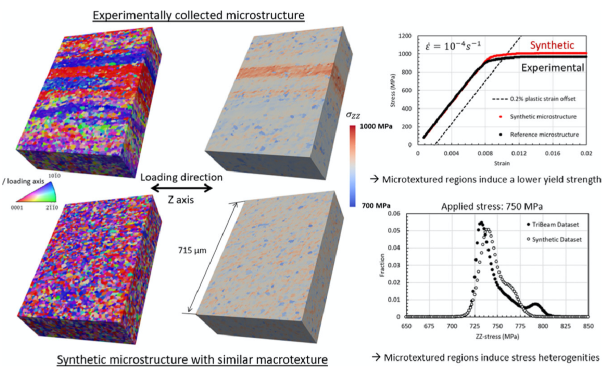
Contexte

- Generate 3D macro-zones while maintaining crystallographic texture and grain morphology.
- Study the influence of macro-zones on mechanical fields
- To study the influence of the morphology of the macro-zone on the macroscopic behavior.

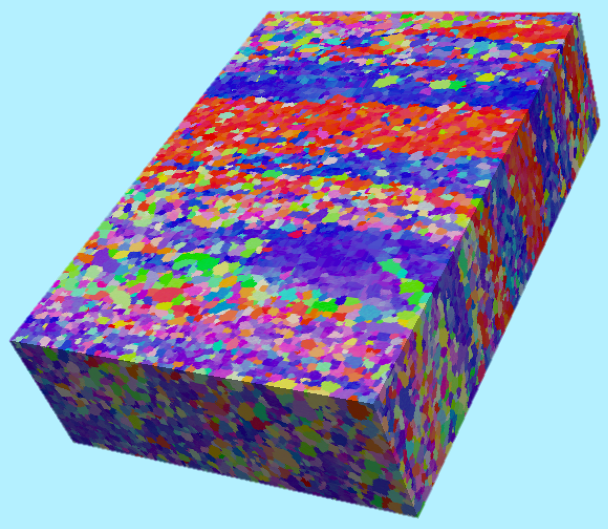




What is a Macrozone?

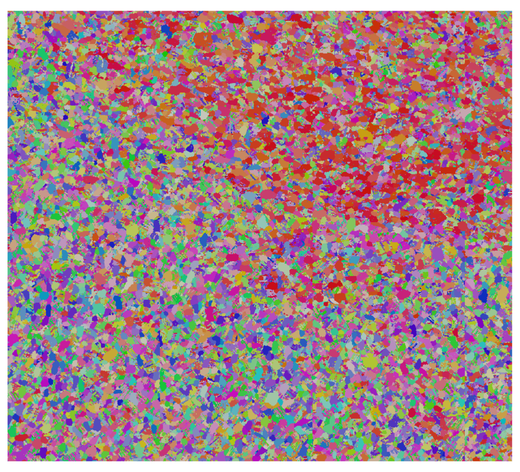
A Macrozone (or MTR) is a region with sharp texture…

Recent studies highlighted that the presence of micro-textured regions (MTRs), which result from the α/β processing step could have a major effect on the effective slip length.



Macro-Zone generation

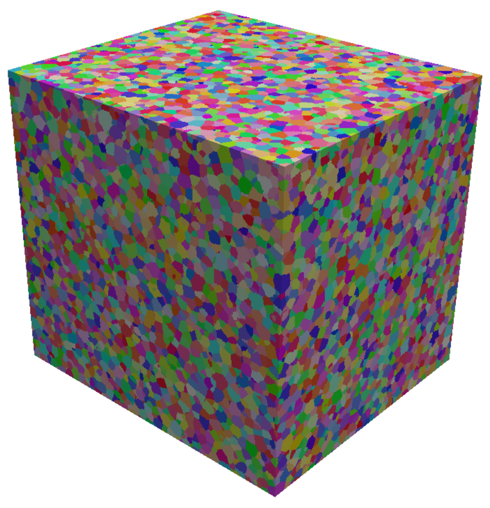
Reference material



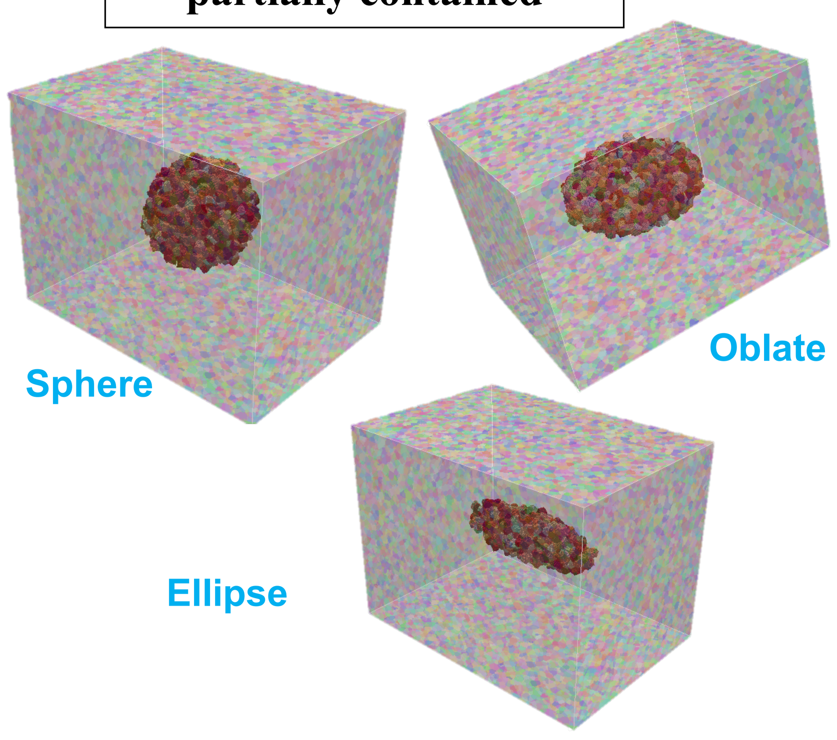
$\phi = (\phi_1, \Phi, \phi_2)$

Loading direction (Y)

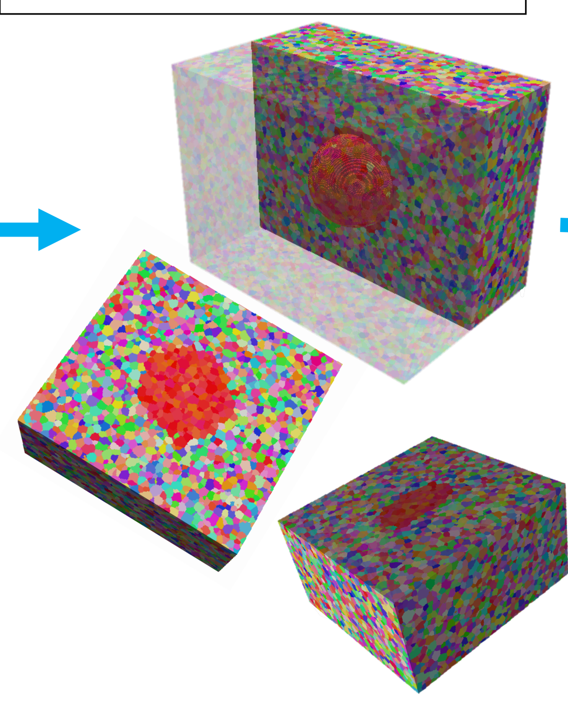
Generate 3d virtual aggregate and assigned euler angles



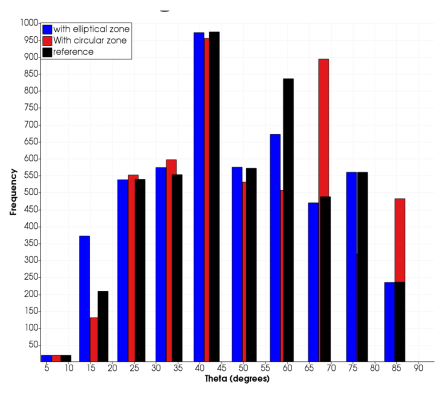
Fix a macrozone and redistribute grain fully or partially contained



Assign new orientations to all grains in macrozone



Optimization of theta histogram



Levenberg Markert algorithm based

$$Hist_{rand}(\phi+\alpha) \approx Hist_{rand}(\phi) + J\alpha$$

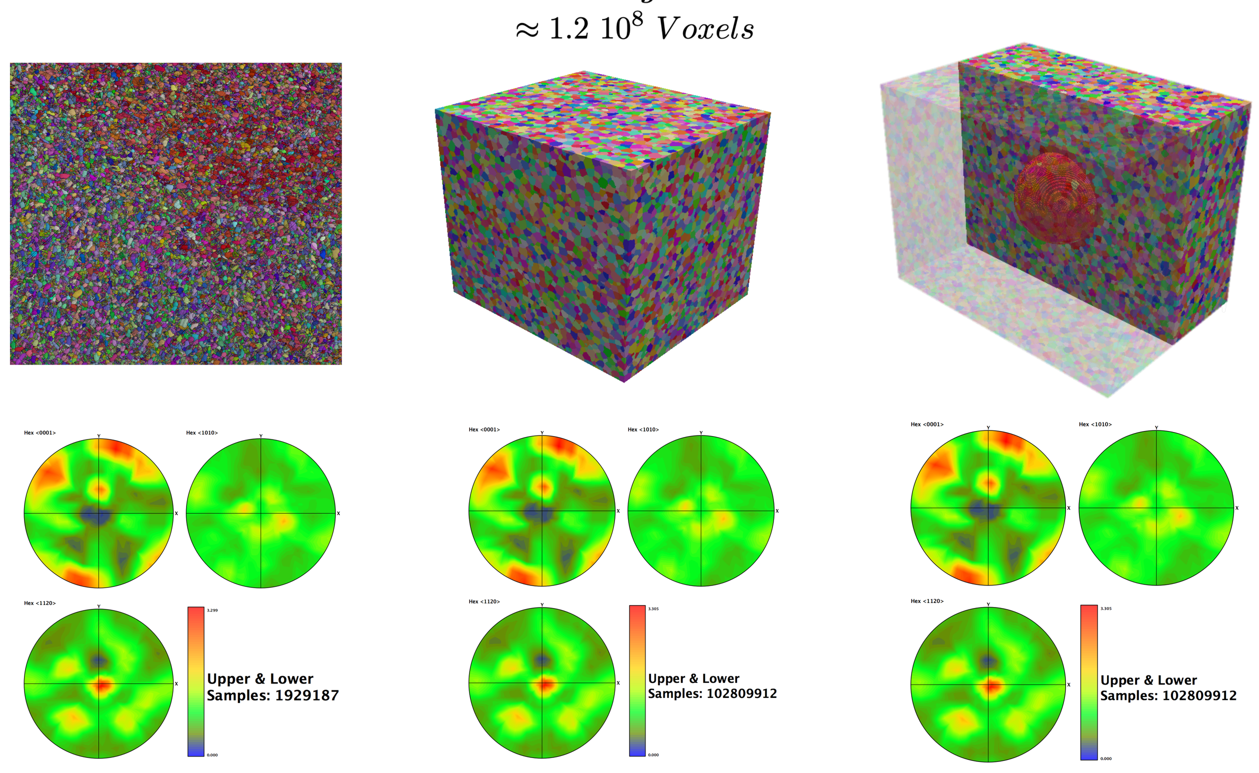
$$(\mathbf{J}^T\mathbf{J})\,\boldsymbol{\alpha} = \mathbf{J}^T\left[Hist_{ref} - Hist_{rand}(\phi)\right],$$

The algorithm is based mainly on the Gauss-Newton algorithm.

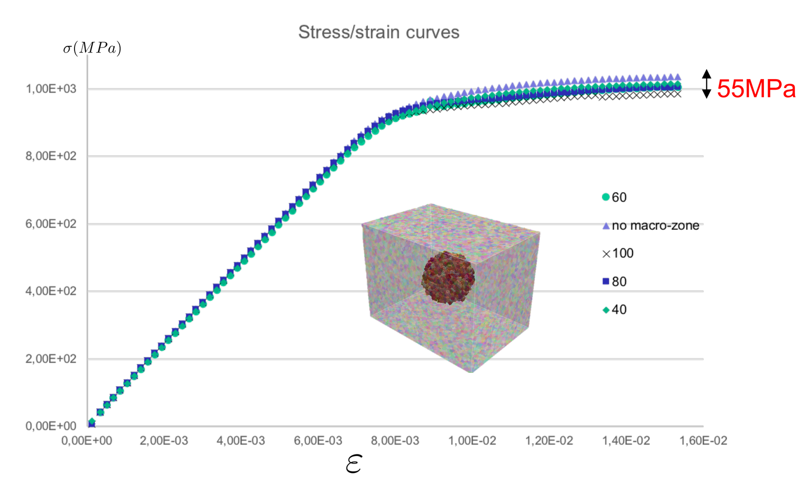
Macroscopic texture preserved

$\approx 1.4\ 10^4$ *grains*

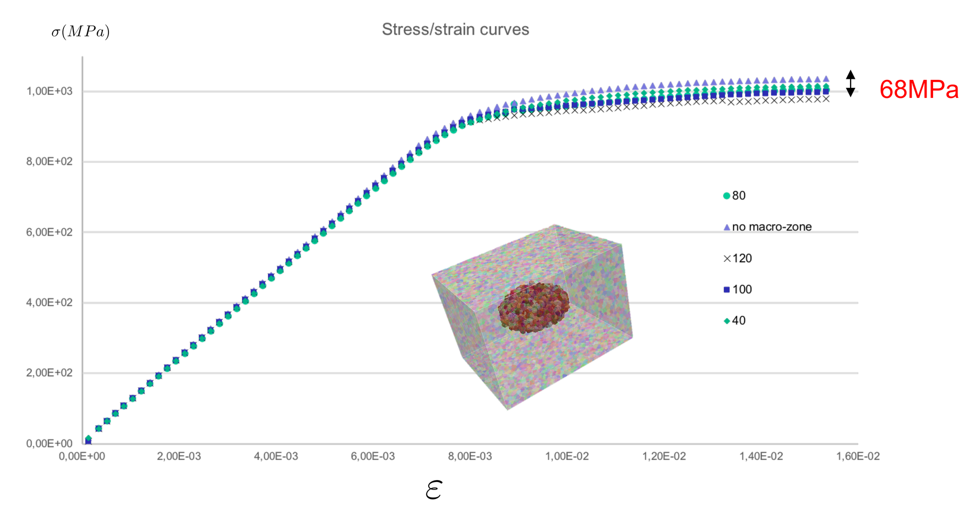
$\approx 8\ 10^4$ *grains*
$\approx 1.2\ 10^8$ *Voxels*



FFT-EVP computation



- Elastic-viscoplastic – Fast Fourier Transforms based CP calculations
  - In-house EVP-FFT code
  - Computationally efficient calculations
  - No meshing required
  - Periodic boundary conditions



- Crystal plasticity model

$$\dot{\boldsymbol{\varepsilon}}^{P}(\boldsymbol{x}) = \sum_{s=1}^{N} \boldsymbol{m}^s(\boldsymbol{x})\dot{\gamma}^s(\boldsymbol{x})$$

$$\dot{\gamma}^s(\boldsymbol{x}) = \dot{\gamma}_0 \left(\frac{|\boldsymbol{m}^s(\boldsymbol{x}):\boldsymbol{\sigma}(\boldsymbol{x})|}{\tau_0^s}\right)^n sgn(\boldsymbol{m}^s(\boldsymbol{x}):\boldsymbol{\sigma}(\boldsymbol{x}))$$

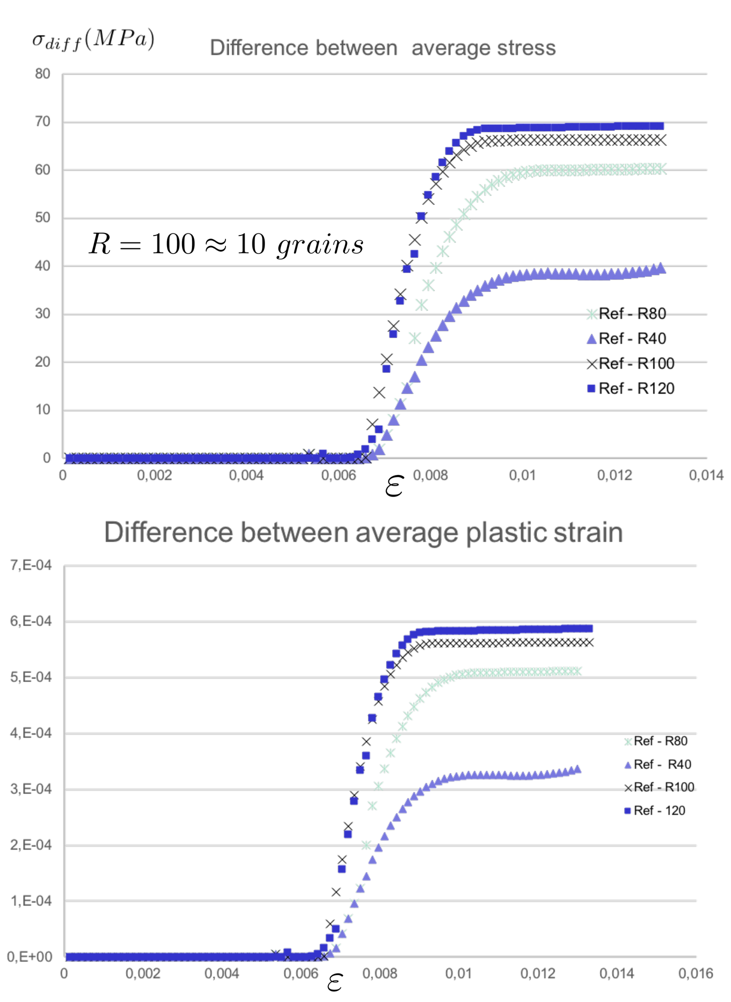
Elementary formulation
→ No fitted parameter
→ No hardening considered

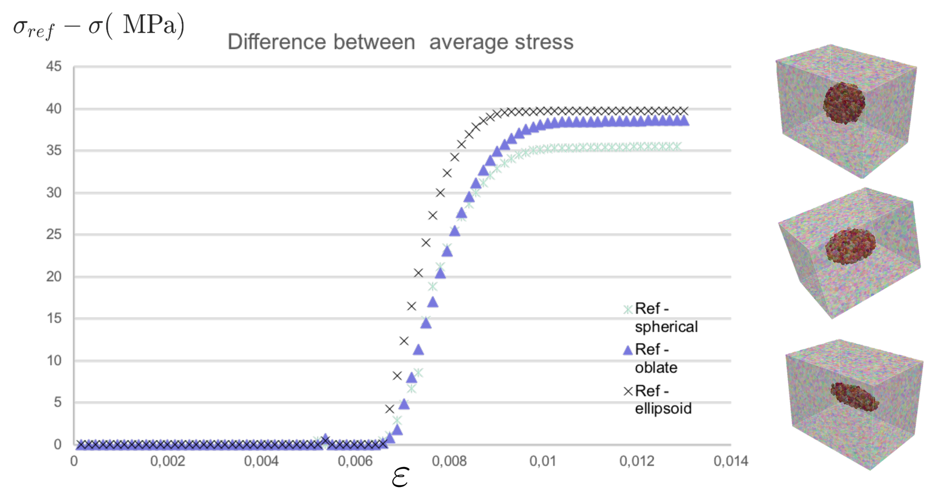
- Material parameters

Parameter	Value
Basal CRSS (τ_0^{Basal})	338 MPa
Prismatic CRSS ($\tau_0^{Prismatic}$)	352 MPa
Pyramidal CRSS ($\tau_0^{Pyramidal}$)	660 MPa
$\dot{\gamma}_0$	10^{-7} s^{-1}
n	0.02

Material parameters extracted from litterature data

Size and Morphology Effects





$V_f(ellipsoid) \approx V_f(oblate) \approx V_f(sphere)$

In summary

Various harmful effects of MTR

- Size effects of the MTR on the
- Morphology effects

Effects on the macroscopic stress-strain behavior

	Volum Fraction	500MPa σ_{max}	900MPa σ_{max}	900MPa ε_p	RP02 σ_{RP02}	RP02 σ_{max}	RP02 ε_p
No MTR	0%	602	1018	0.0078	996	1118	0.01
Sphere	0.5%	604	1022	0.0079	983	1140	0.0092
	3.6%	612	1036	0.0081	968	1227	0.0096
	7.0%	701	1186	0.009	953	1278	0.011
Oblate	0.3%	607	1027	0.0078	973	1202	0.0098
	1.0%	619	1048	0.0082	965	1216	0.0099
	1.9%	621	1052	0.0089	959	1256	0.0115
	3.7%	662	1121	0.0094	951	1282	0.0116
Elipse	3.4%	675	1143	0.0087	932	1189	0.0115

Table of the different effects of the Morphology of MTR on stress and deformation

Outlooks:

- Dwell / Fatigue effects?
- Comparison with self-consistent methods.
- Can we find a VER?

References

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