Meshing and Finite Element Analysis from EBSD data

MTEX workshop – March 8th to 17th, 2021

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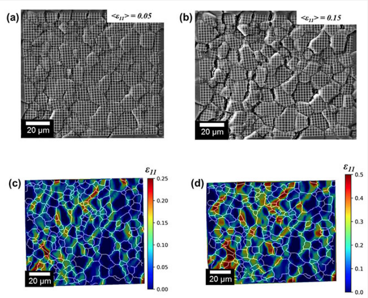
Strain localization in grains



In situ full field measurement using microgrid on AZ31 alloy[1].

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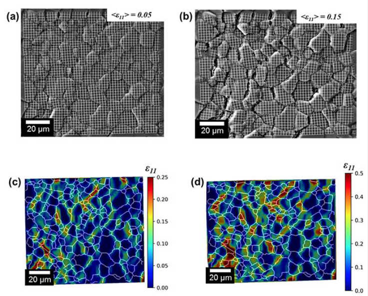

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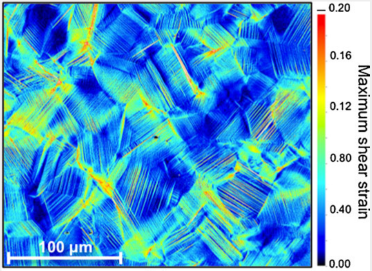
Shear bands



Shear localization in 304 stainless steel[2]

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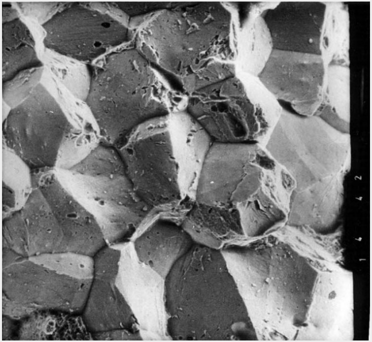
Fracture in steel



Intergranular fracture of Fe–0.35C–1.5Mn–0.1P[3]

[3] A. Kovalev and D. L. Wainstein (2003). In: *Modeling and Simulation for Material Selection and Mechanical Design*

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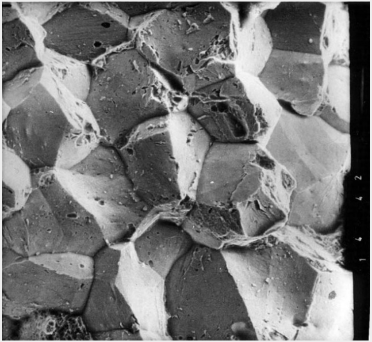

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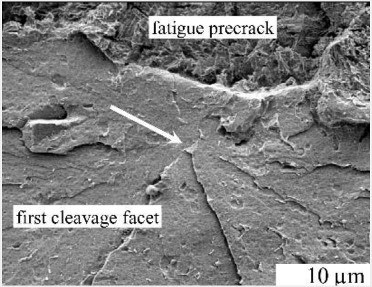

Crack initiation in HSLA steel after thermal cycle and fatigue test[4]

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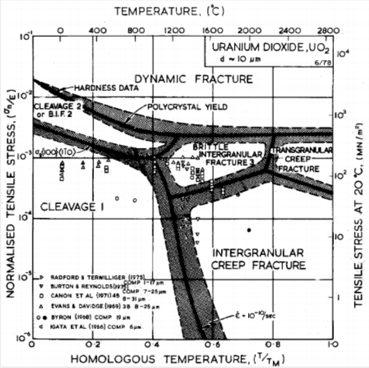
Ceramics

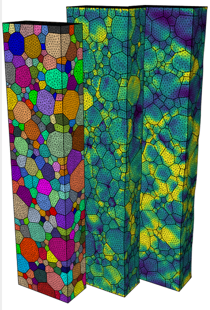


Fracture map for UO_2[5]

Cracks in nuclear fuel pellet[6]

5 C. Gandhi and M.F. Ashby (1983). In: *Perspectives in Creep Fracture*
6 J. Soulacroix (Oct. 2014). Thesis. Ecole Nationale Supérieure d'Arts et Métiers

Representative material



NEPER + FEPX

- ✓ Full 3D
- ✓ Require reduced informations about the material
- ✗ Local fields cannot be compared with experiment

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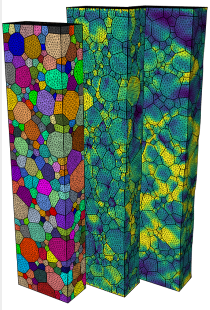

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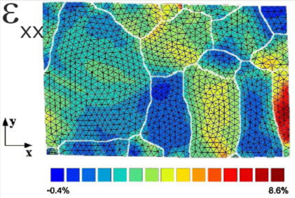
Imaged material



CPFEM on γTiAl[7]

- ✗ Only in 2D
- ✗ Require whole EBSD map
- ✓ Use realistic grain shapes

7 E. Héripré et al. (2007). In: *International Journal of Plasticity* 23.9

Objectives

Provide a tool for generating meshes from EBSD data leading to:

- high-fidelity grain shape,
- smooth description of GBs,
- customizable and flexible configuration.

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Gmsh

- Open source software[a]
- Works from command line or GUI
- Allows scripting

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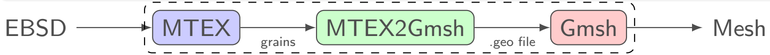

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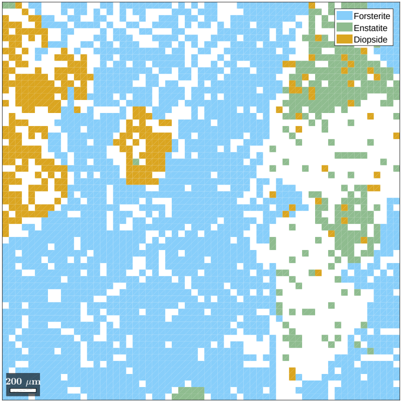
The *small* example



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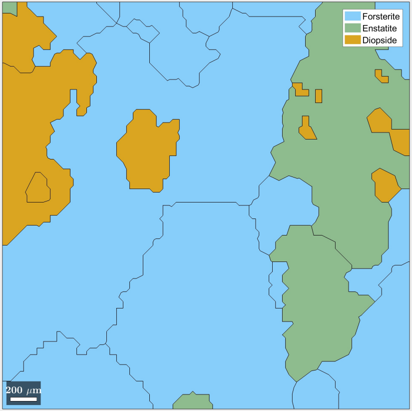

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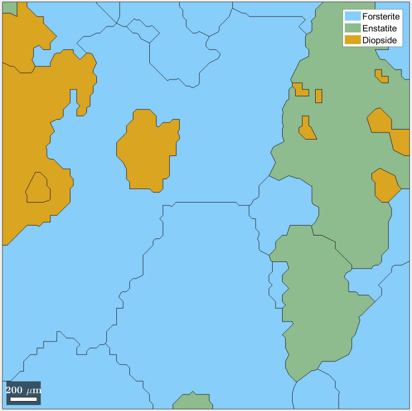

- Non-convex grain shapes
- Some nested grains
- Serrated grain boundaries

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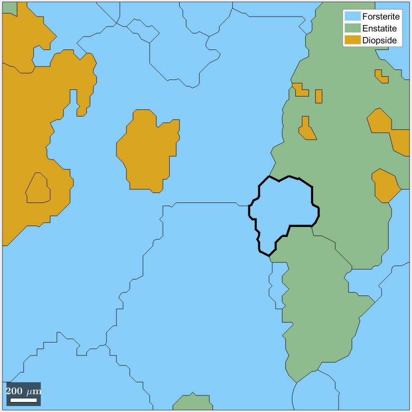

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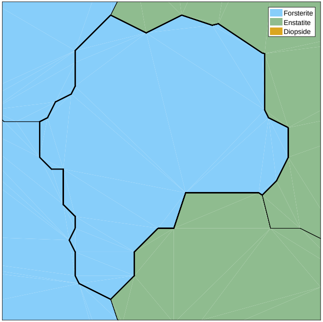
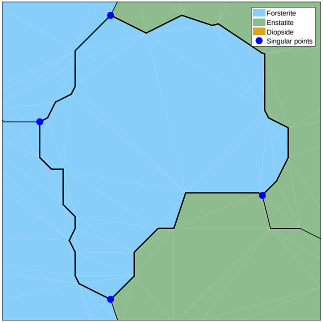
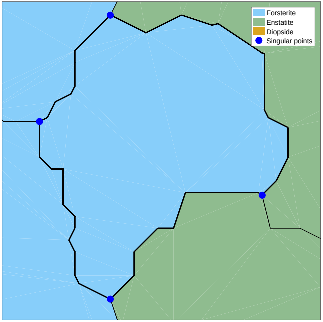
1. Get enclosing GB



1. Get enclosing GB
2. Track triple points (TP)



1. Get enclosing GB
2. Track triple points (TP)
3. Split GB into TP-to-TP segments



1. Get enclosing GB
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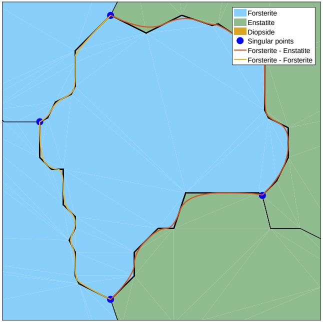
3. Split GB into TP-to-TP segments
4. Approximate each segment with B-Spline



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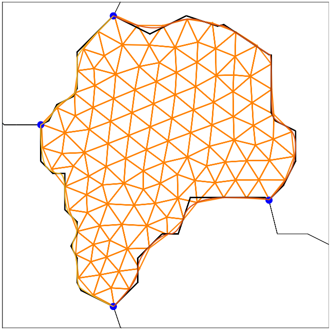
5. Mesh enclosed surfaces



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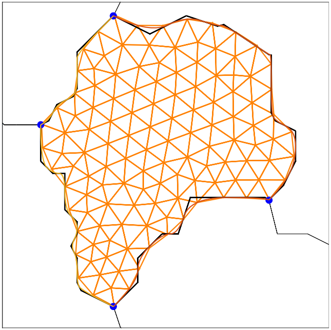
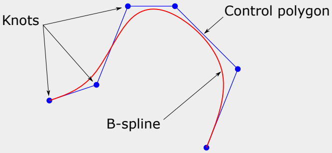
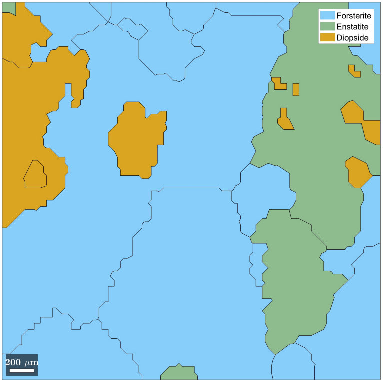


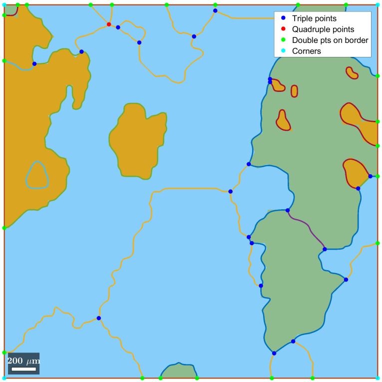
Cubic B-Splines

Properties:

- Variation diminishing (no extraneous undulations)
- $\mathcal{C}^2$ continuity
- End knots belong to the curve

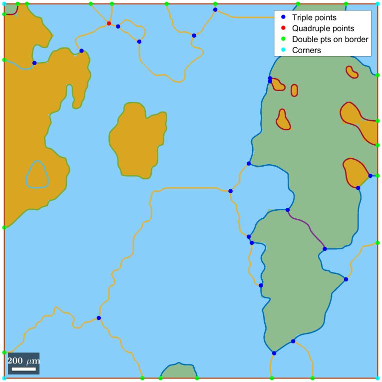



Forsterite
Enstatite
Diopside
200 μm



Mesh properties

- Grain boundaries are well-defined
- Singular points at their exact location
- Each grain is mesh independently



Meshing strategy

- 0D Nodes at singular points
- 1D Nodes at GBs
- 2D Populate grain area

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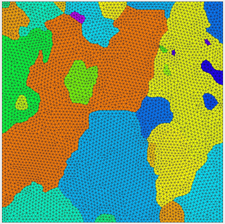
Default



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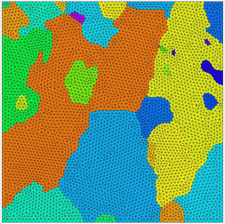
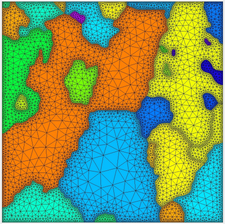


Size gradient



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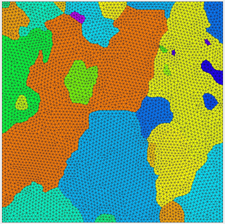

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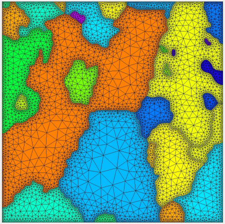
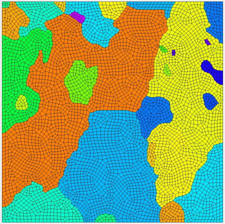


Hexahedrons



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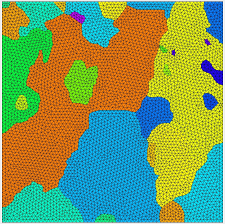

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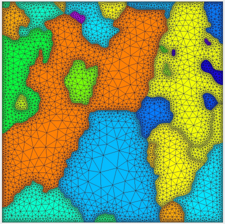

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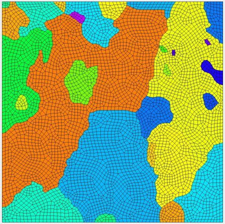
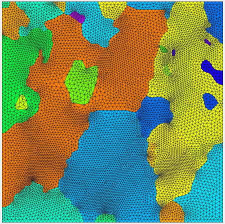


Size from curvature



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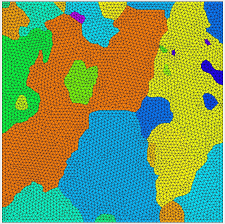

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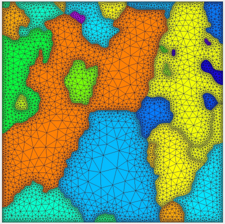

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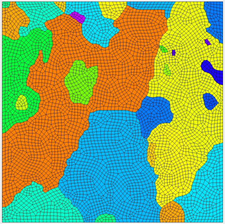

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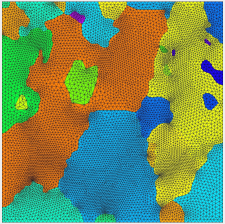
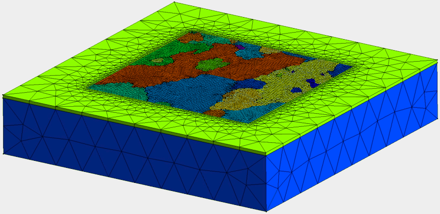
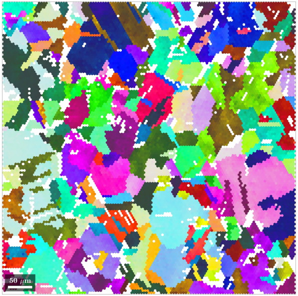


Embedded in a medium



Material

Pure copper (248 grains)



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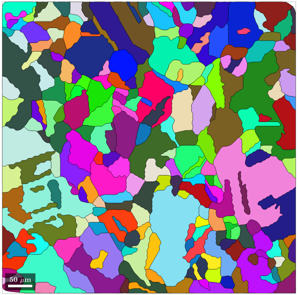

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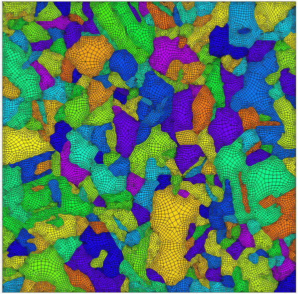

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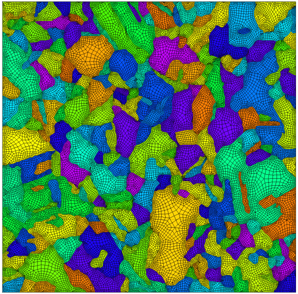
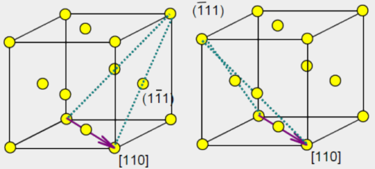


Crystal plasticity



12 slip systems in FCC: $\{111\}\langle 100\rangle$

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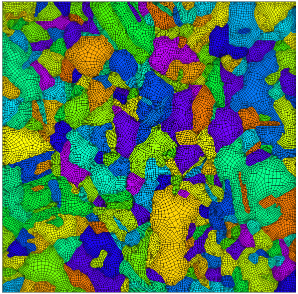

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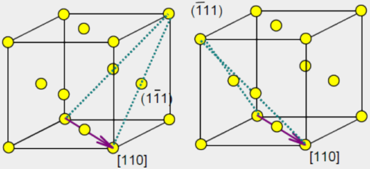

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Constitutive laws

Deformation gradient tensor $\boldsymbol{F} = \boldsymbol{F}_\mathrm{e}\boldsymbol{F}_\mathrm{p}$

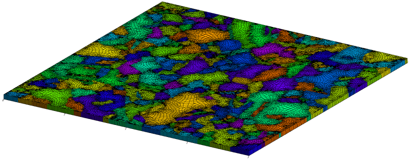
PKII stress tensor $\boldsymbol{S} = \boldsymbol{C} : \left[\frac{1}{2}\left(\boldsymbol{F}_\mathrm{e}^T\boldsymbol{F}_\mathrm{e} - \boldsymbol{I}\right)\right]$

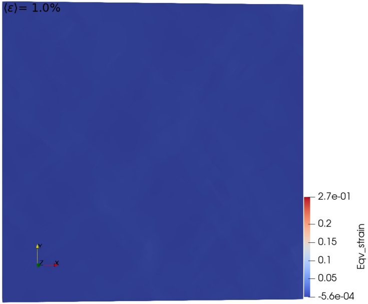
CPFEM simulation

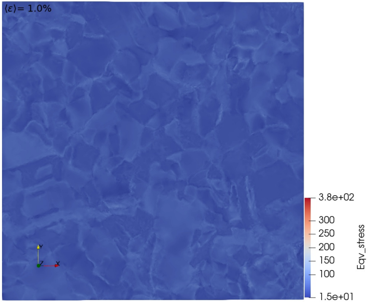
Code PRISMS-Plasticity[8]

Mesh 37k hex elements
75k nodes

Comp. 87 hours on 8 cores







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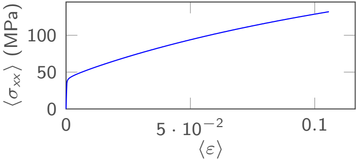

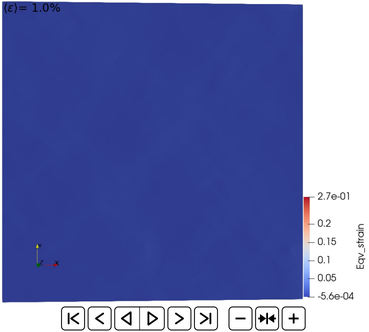

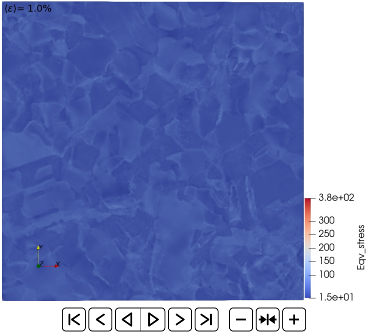

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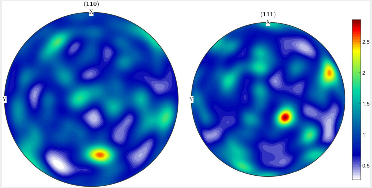
Texture at $\langle \varepsilon \rangle = 0$



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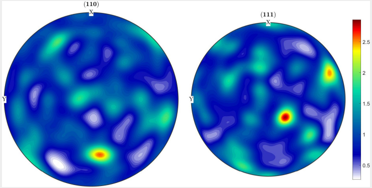
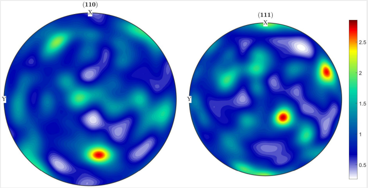


Texture at $\langle \varepsilon \rangle = 0.1$



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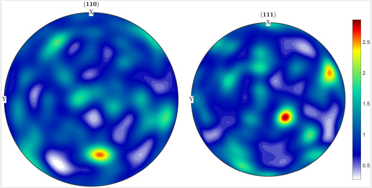
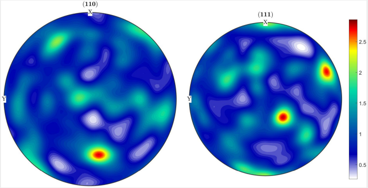
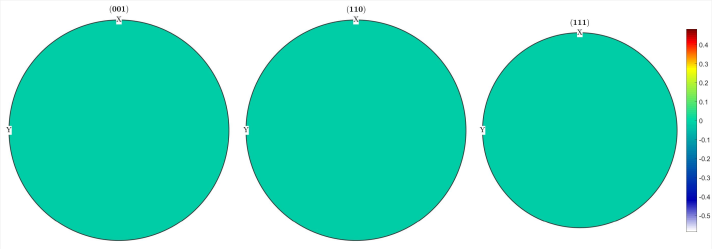


Texture at $\langle\varepsilon\rangle = 0.1$



$\Delta\mathrm{odf} = \mathrm{odf} - \mathrm{odf}_0$ (tensile direction: out-of-plane)



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Uranium dioxide (610 grains)

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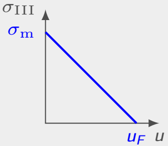

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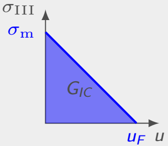

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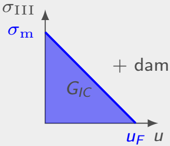

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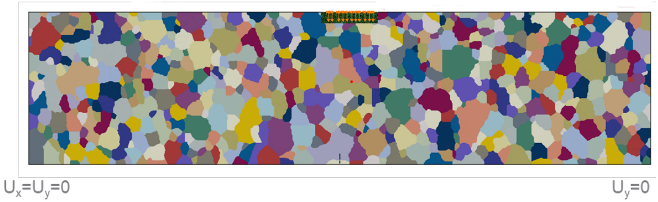

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3-point bending test

Notched sample

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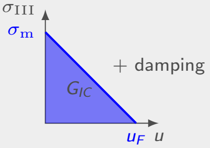
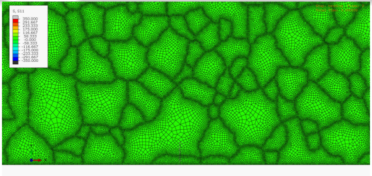


FEM code

Abaqus 2019 implicit

Mesh

378k hex elements, 766k nodes



Results

- Stress concentration at crack tip
- Changes of crack propagation direction depending on the grains

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- ✓ High-fidelity description of GBs
- ✓ Smooth approximation of GBs
- ✓ Works on multi-phased materials even with complex grain shapes
- ✓ Flexible integration (element types, surrounding medium...)

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Data availability

`https://doriandepriester.github.io/MTEX2Gmsh/`[a]

[a] Dorian Depriester and Régis Kubler (2020). In: *Journal of Open Source Software* 5.52.