



Textures Simulation – Crystal Plasticity

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www.atex-software.eu

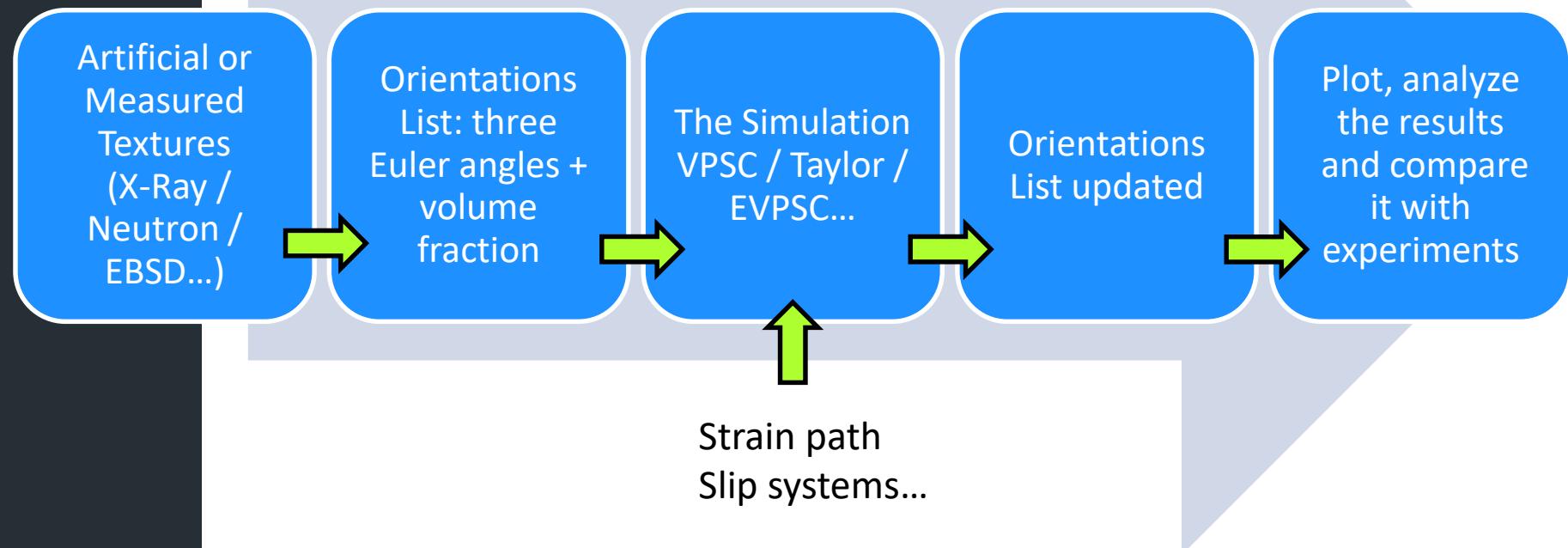
www.atex-software.eu/help.html

Youtube channel “atex software”

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The process



1. Here is written the list of what to do
2. This hand tells you where to click



Content



1. Input Data
 1. Generate textures
 2. X-Ray measurements
 3. Orientations Maps (EBSD)
2. Simulations (VPSC)
3. Simulations vs Experiments
 1. Ideal Orientations
 2. Correlation
4. Simulations On Orientations Maps

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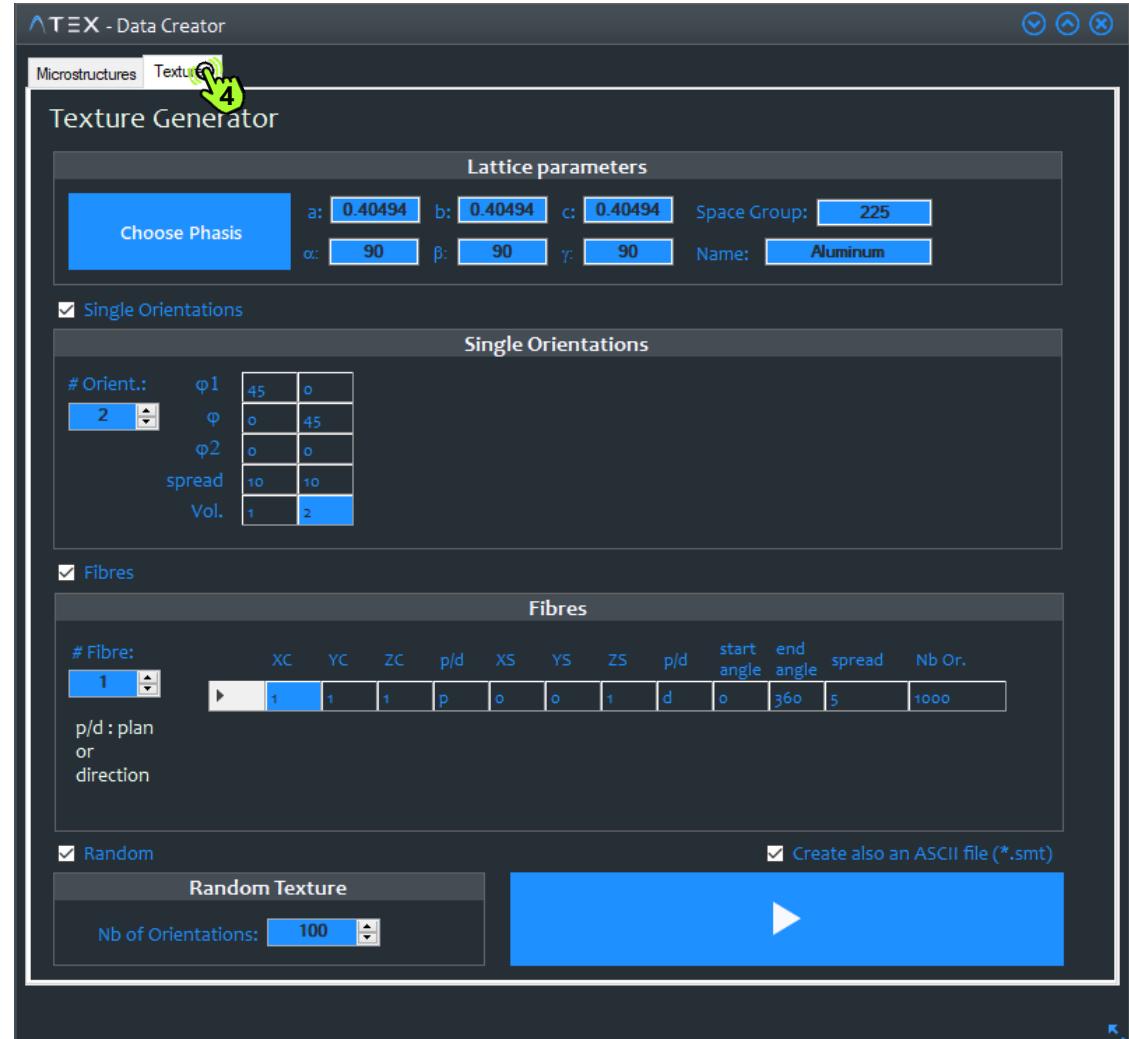
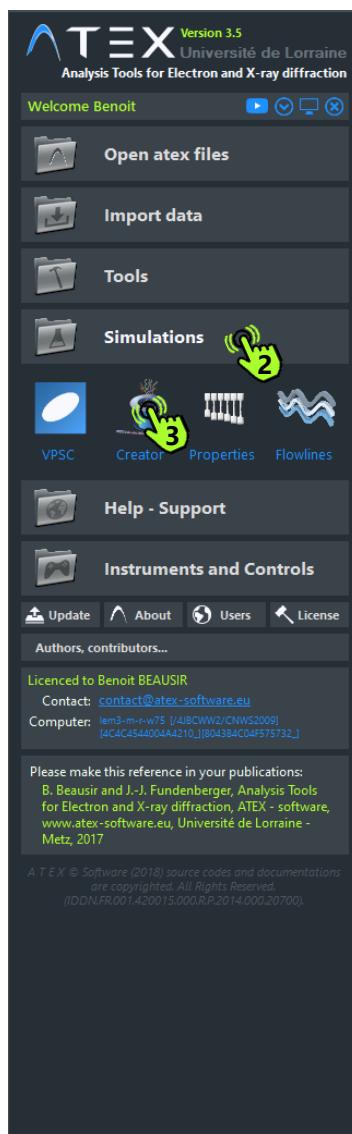
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TUTORIAL Textures Simulation – Crystal Plasticity

→ Generate textures

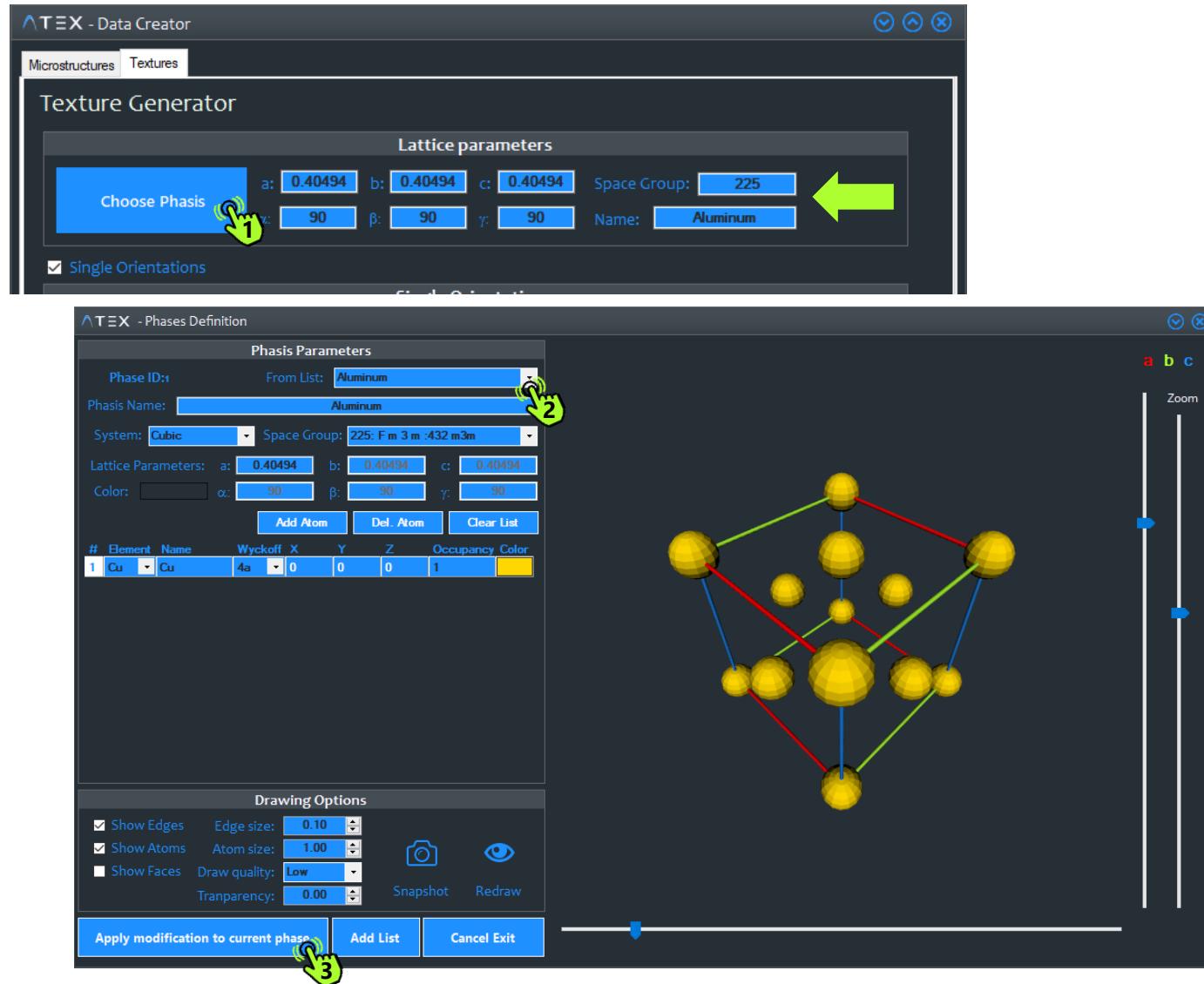
1. Open ATEX
2. Click on the “Simulations” button
3. Select “Creator” module
4. Select the “Textures” tab



→ Generate textures

1. Define the material by clicking on “Choose Phases” button to open the phases definition window
2. Select “Aluminium” for instance
3. Click on apply button to validate.

The lattice parameters, the space group and the name of the phase appears in the data creator window

ATEX - Data Creator

Texture Generator

Lattice parameters

Choose Phasis  a: 0.40494 b: 0.40494 c: 0.40494 Space Group: 225
γ: 90 β: 90 γ: 90 Name: Aluminum

Single Orientations

ATEX - Phases Definition

Phasis Parameters

Phase ID: From List: Aluminum 
Phasis Name: Aluminum 
System: Cubic Space Group: 225: F m 3 m :432 m3m
Lattice Parameters: a: 0.40494 b: 0.40494 c: 0.40494
Color: α: 90 β: 90 γ: 90
Add Atom Del. Atom Clear List

#	Element	Name	Wyckoff	X	Y	Z	Occupancy	Color
1	Cu	Cu	4a	0	0	0	1	

Drawing Options

Show Edges Edge size: 0.10
Show Atoms Atom size: 1.00  
Show Faces Draw quality: Low Transparency: 0.00 Snapshot Redraw

Apply modification to current phase  Add List Cancel Exit

3D Lattice Visualization: A 3D rendering of a crystal lattice structure. It consists of several yellow spheres representing atoms, connected by red and green lines representing edges and faces. The lattice is shown in perspective, with a vertical zoom slider on the right side of the visualization area.

→ Generate textures

- Now choose the kind of orientations you want to add to your texture
 - Single Orient.
 - Fibre
 - Random

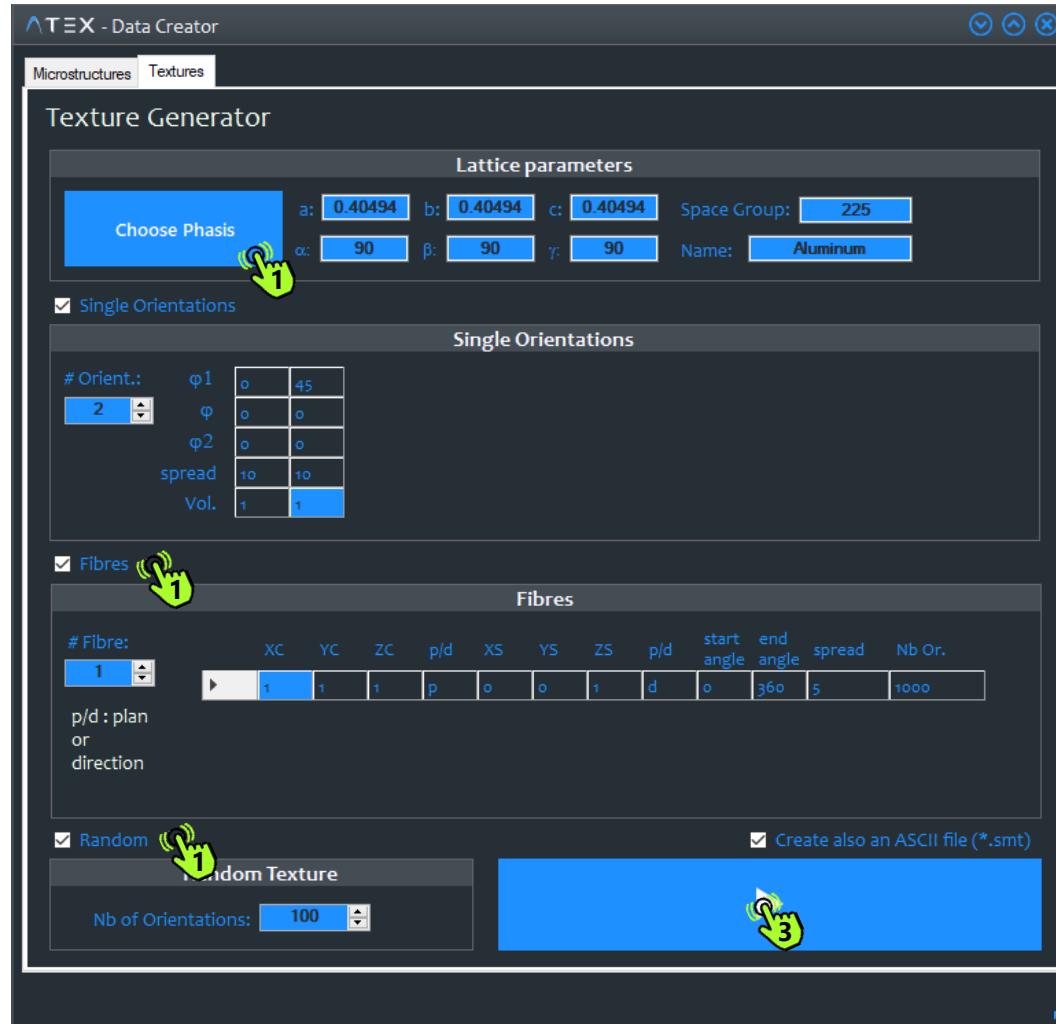
- You can also mix them

- Click on the generate button

An *.orli.atex file will be created (ORLI meaning Orientation List)

note that if the checkbox “Create ASCII...” is checked you will also get the orientation list in a text format file

- ATEX will ask you if you want to open your generated texture to plot it for instance, answer YES”



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→ Generate textures

- Once you said "YES" the ORLI module opens.

Here the texture is composed by two orientation (0,0,0) and (45,0,0) with the same weight

- Click on "pole figures" button to plot it

The (111) pole figures shows the projection of the four equivalents planes (111) of each orientation (0,0,0) in green, (45,0,0) in orange

- YOU NOW HAVE AN ORIENTATION LIST READY FOR THE SIMULATIONS



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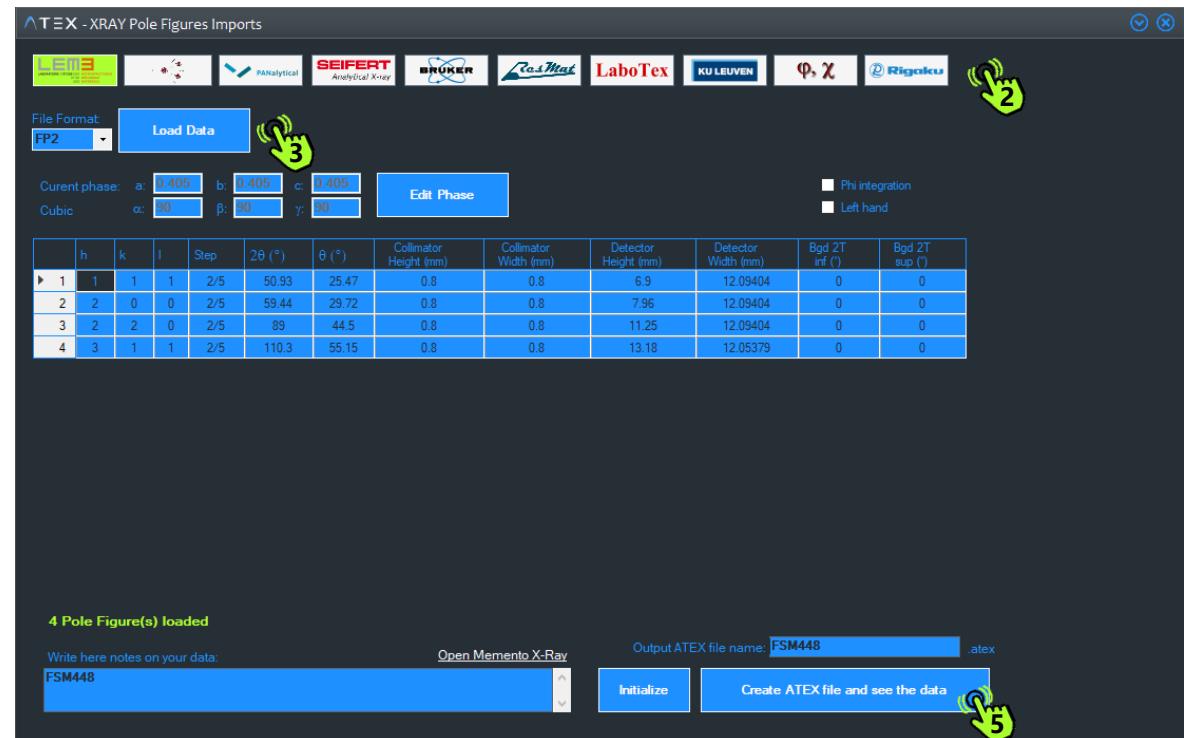
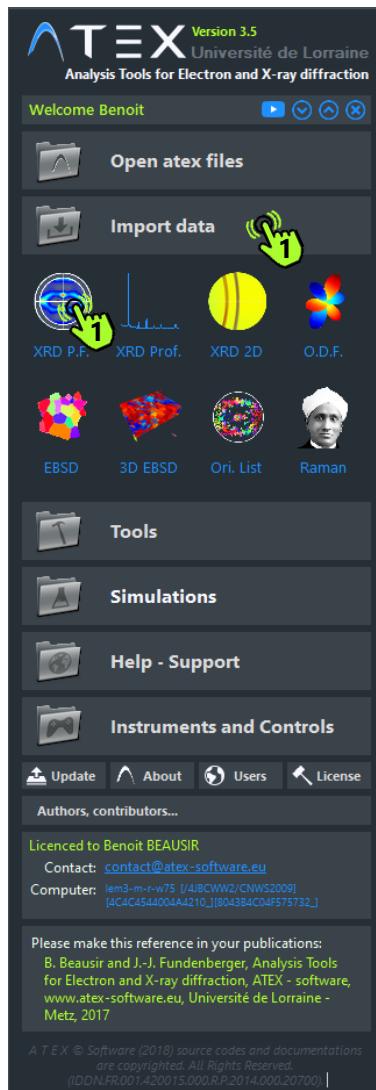
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→ Orientation list from X-Ray measurements

1. Select Import data tab, then click on “XRD-PF” button
2. Select your manufacturer
3. Select then the kind of data file format
4. Fill the missing information if needed (depending on the manufacturer file)
5. Click on “Create ATEX file” button
6. You will get a “.xipf.atex” file



XIPF meaning Xray Incomplete Pole Figures

TUTORIAL Textures Simulation – Crystal Plasticity

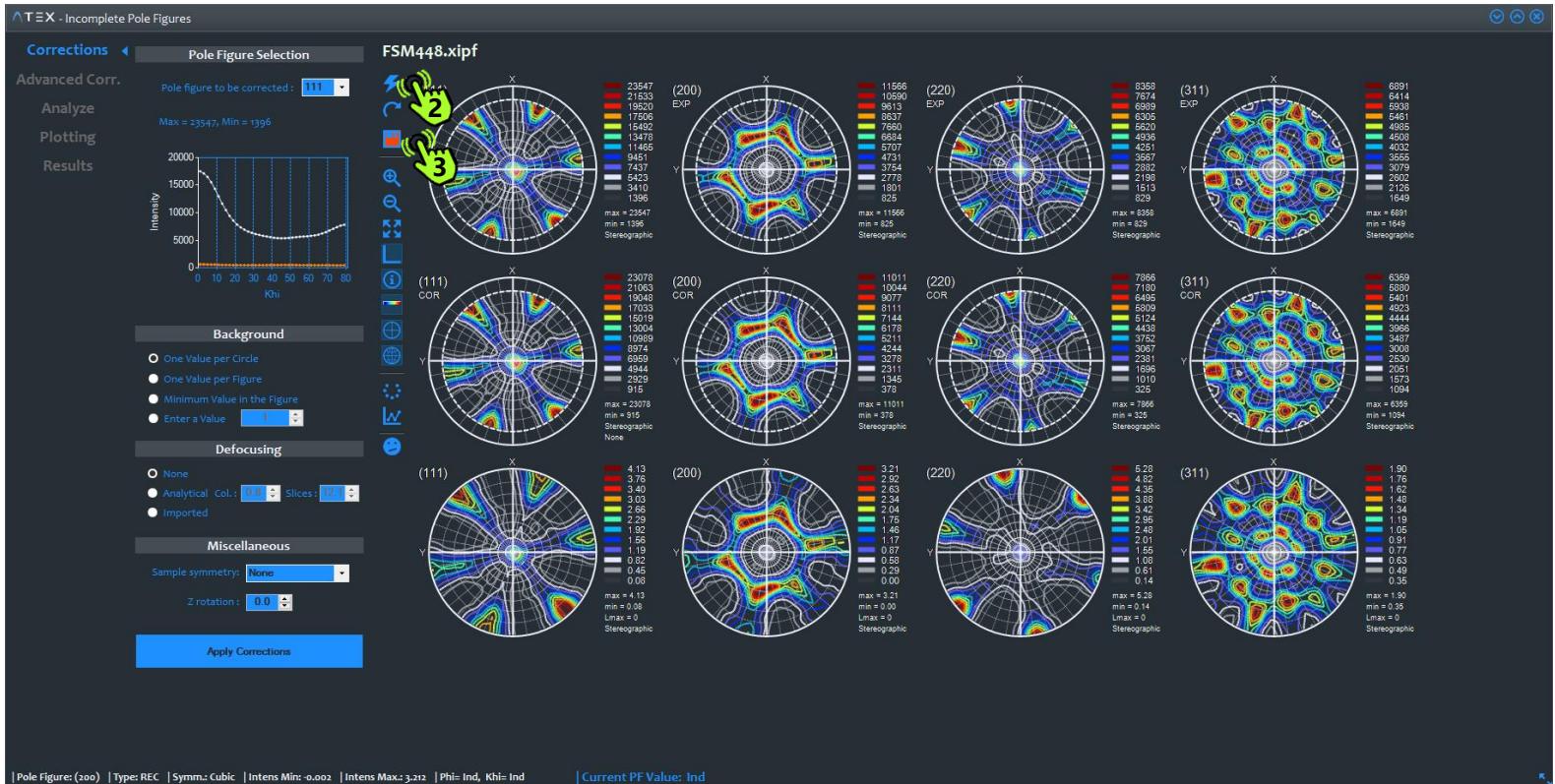
→ Orientation list from X-Ray measurements

1. The XRAY incomplete pole Figure module open automatically

2. Select your correction if needed then calculate the ODF by clicking on the “spark execute” button

3. Once your ODF is calculate, click on the red floppy button to save it, you will get an “*.CODF.ATEX” file

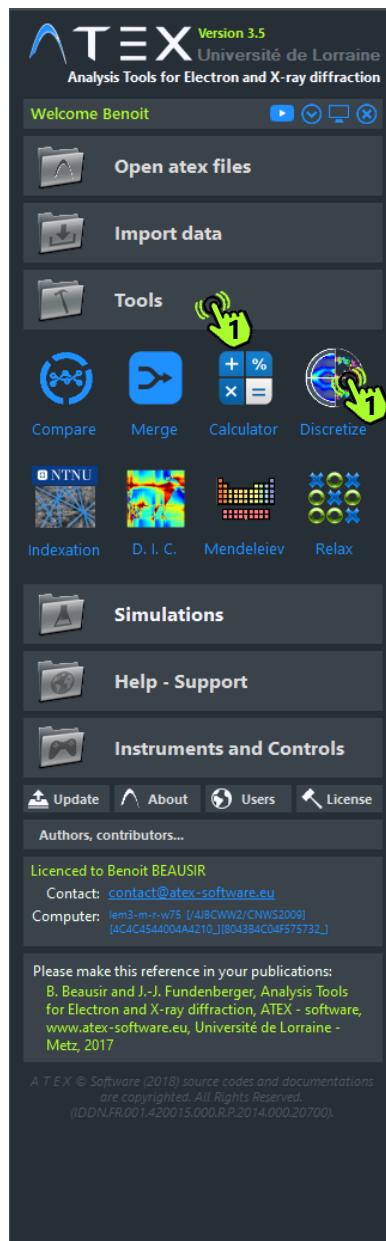
C as C-coefficient + ODF as Orientation Density Function



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Once you have your ODF, you have to discretize it to produce a list of single orientation

1. Select the “TOOLS” tab and click on the discretize button to open the discretization module
2. Load your ODF (*.codf.atex) file
3. Choose your discretization method and click on the “RUN DISCRETIZATION” button
4. You will get a new file “ori.atex” file containing the orientation list for the simulations



→ Discretize an ODF

The screenshot shows the "Textures Discretization" dialog box. It has a "Load Data" button with a green callout "2" pointing to it, and a "Run Discretization" button with a green callout "3" pointing to it. Below these are several configuration options:

- Random Distribution - Number of Orientations: 1000
- Fixed Number of Orientations: 1000 (selected)
- Regular Grid - Angular Resolution (°): 10
- Random Distribution - Minimum Disorientation Angle (°): 10
- Constant Weight - Angular Resolution (°): 10, 2916

A checkbox "Create also a ASCII file" is checked. The bottom right of the dialog has a "Run Discretization" button with a green callout "3".

Tools

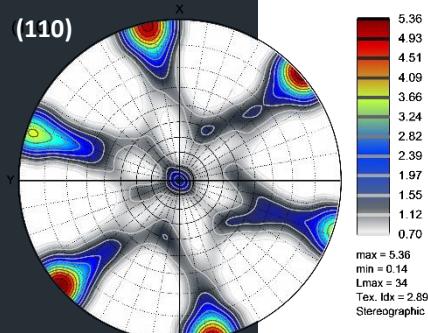
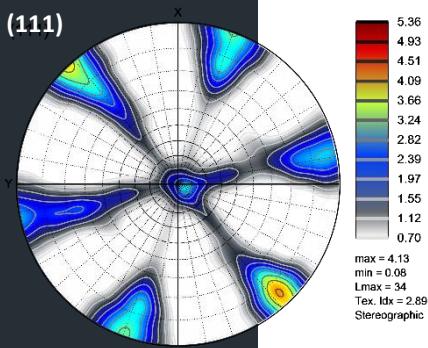
Methods of discretization:

- Random distribution - Number of orientations
- Fixed number of orientations
- Regular Grid
- Random distribution - Disorientation
- Constant weight

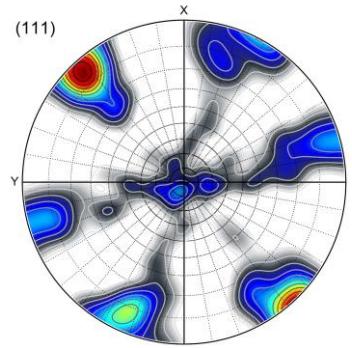
The bottom of the dialog box displays the URL www.atex-software.eu/help.html.

→ Discretize an ODF

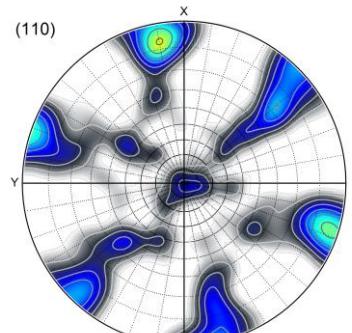
X-Ray measurements



100 Orientations

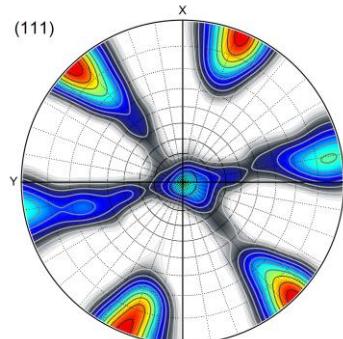


max = 5.56
min = 0.01
Lmax = 22
Stereographic

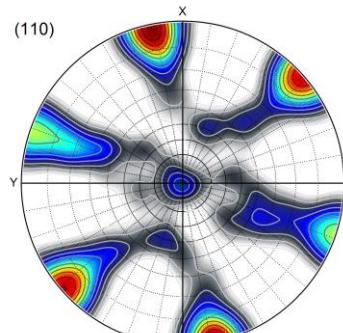


max = 5.56
min = 0.00
Lmax = 22
Stereographic

1000 Orientations

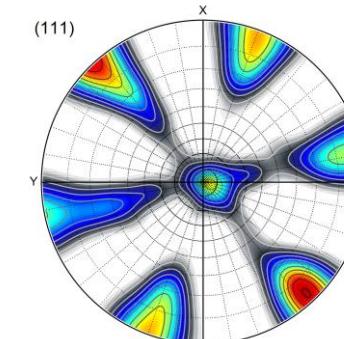


max = 3.77
min = 0.02
Lmax = 22
Stereographic

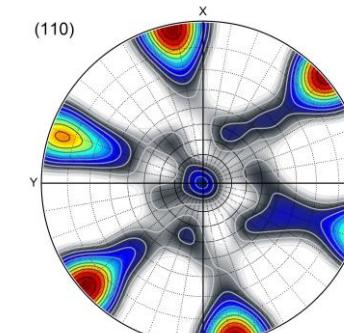


max = 4.24
min = 0.00
Lmax = 22
Stereographic

10000 Orientations



max = 3.86
min = 0.03
Lmax = 22
Stereographic



max = 4.14
min = 0.04
Lmax = 22
Stereographic

ODF discretized → ODF re-calculated

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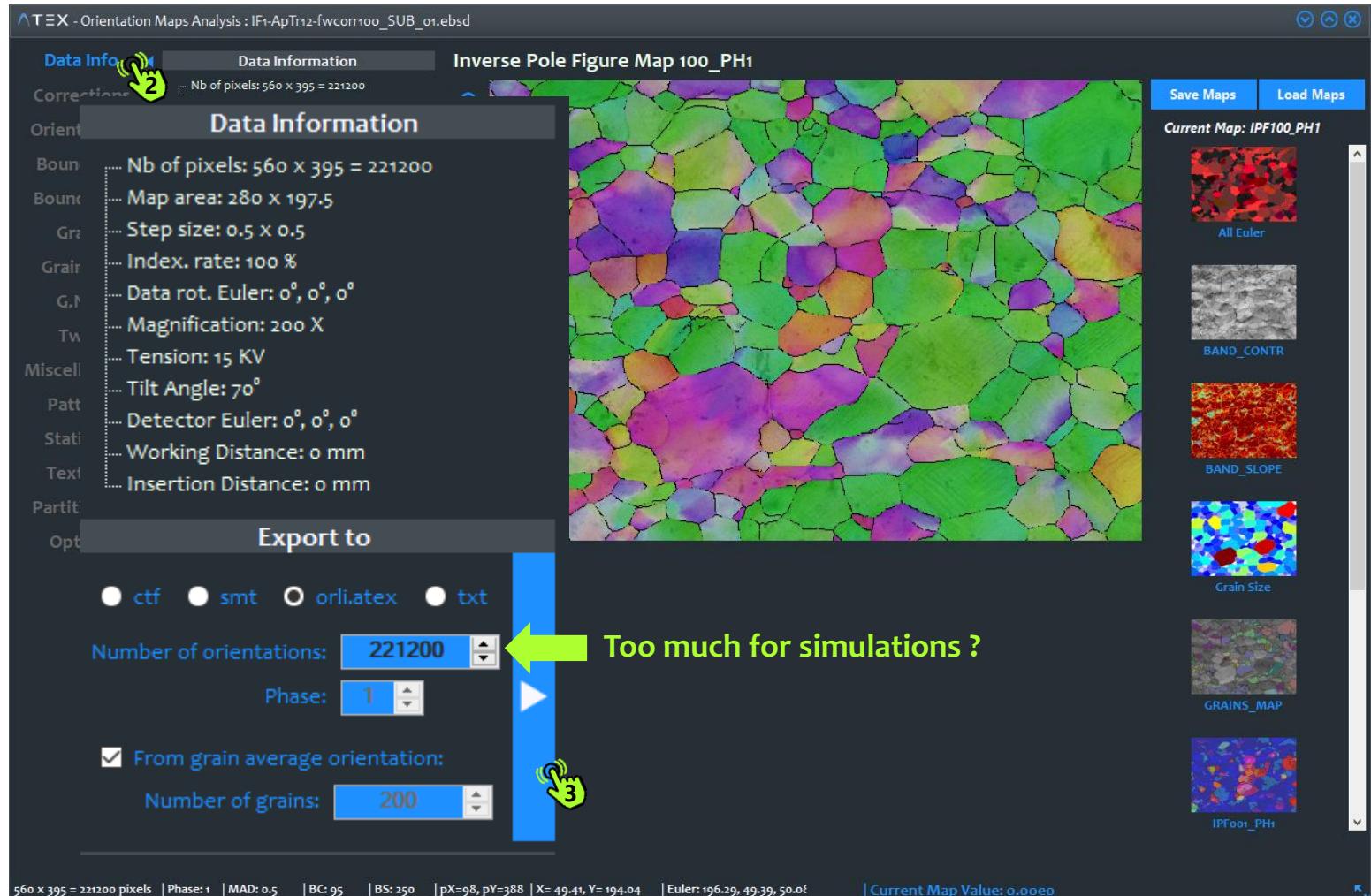
→ EBSD to Orientation List

1. Open an EBSD map (*.ebsd.atex)
2. In the tab “Data Info” several options to export your data are available:

- 1 – SMT and TXT
- 2 – ORLI.ATEX
- 3 – CTF

3. Question: From what my orientation list should be composed ?

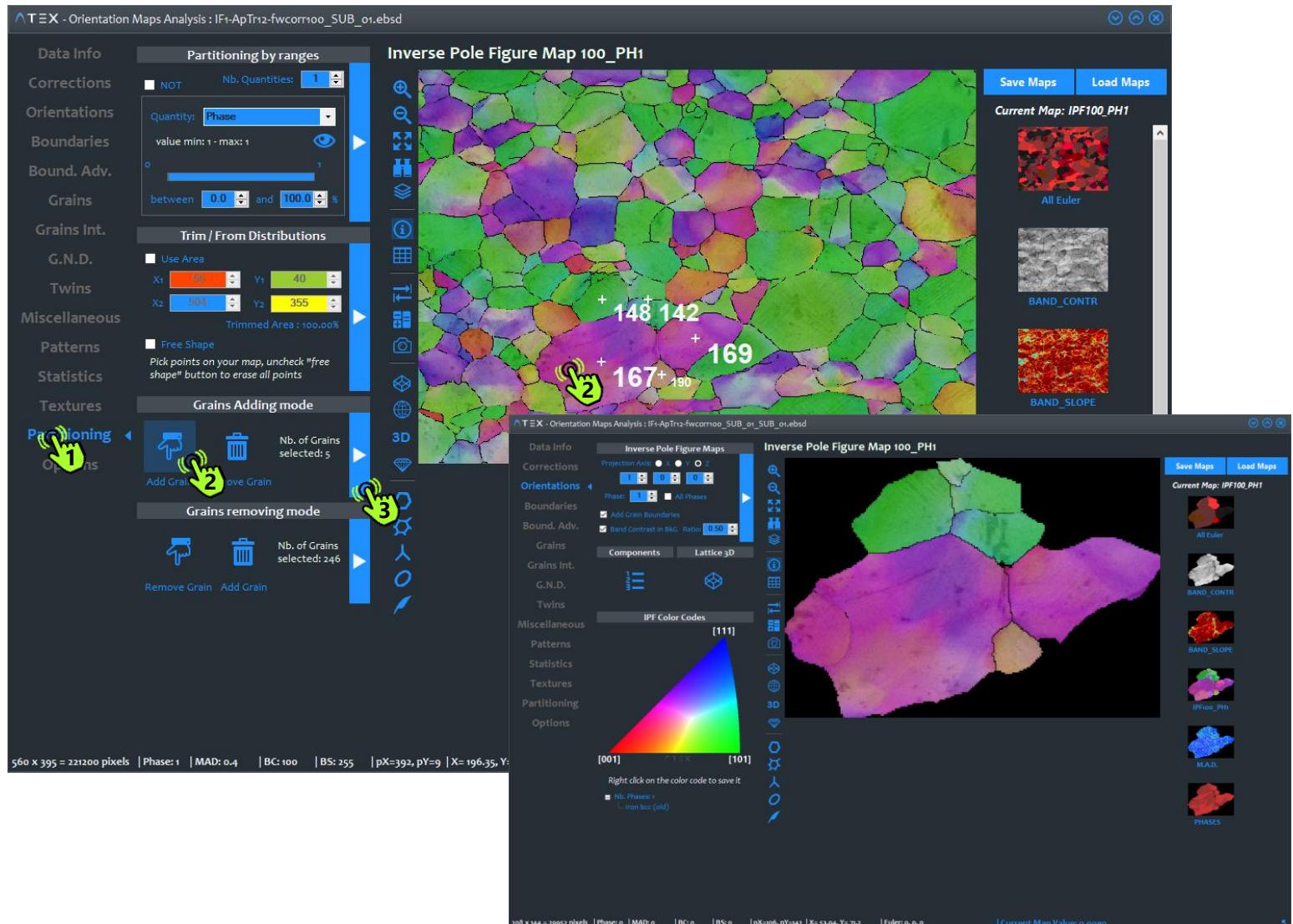
- Export full map
- part of map
- one orientation per grains
- selected grains (see next slide partitioning)



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→ EBSD to Orientation List, Partitioning

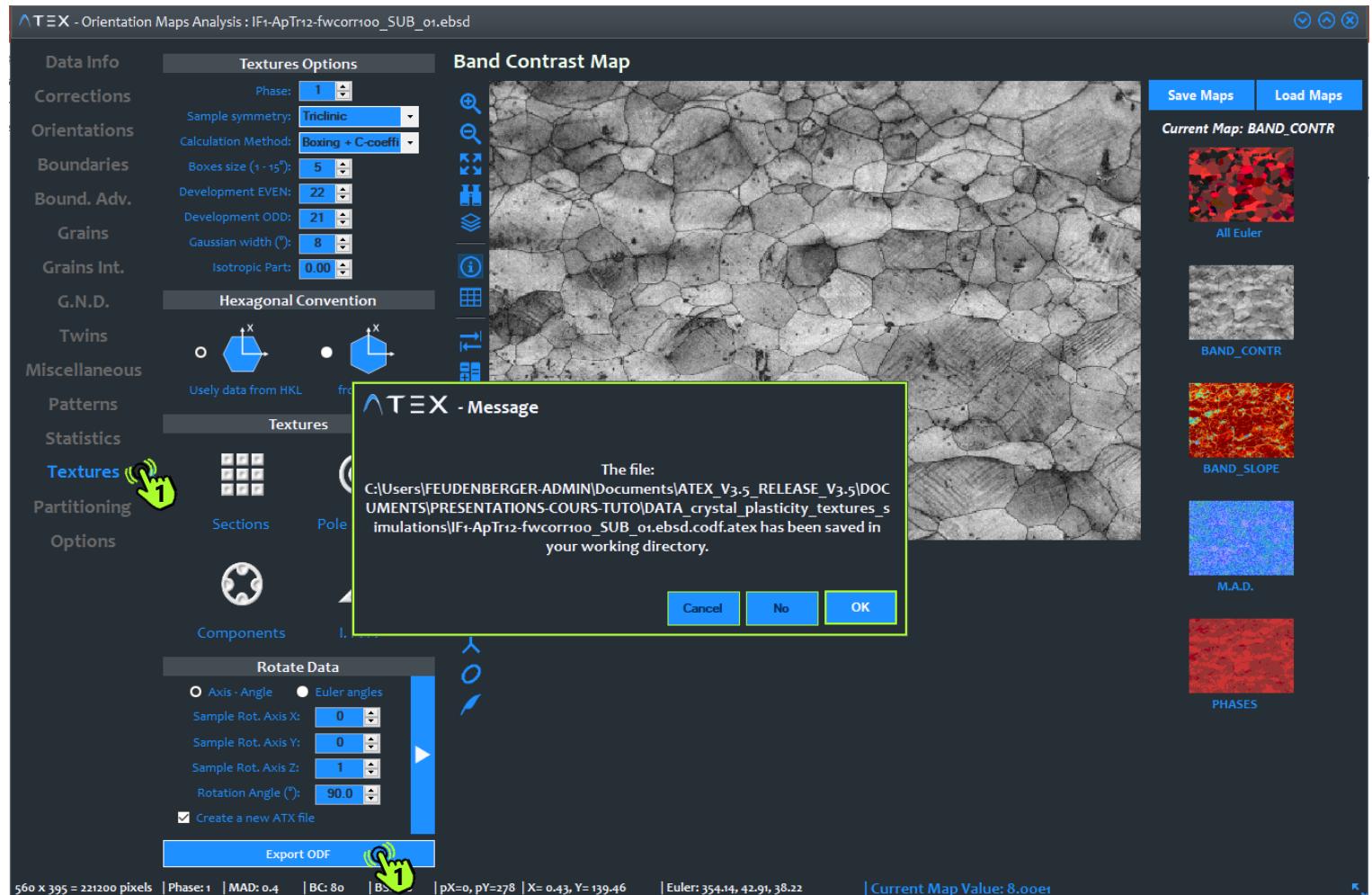
1. Go to tab "partitioning"
2. Select the "Grains Adding mode" for instance and pick few grains in the map
3. Click on execute button to generate the corresponding map
4. Then repeat the previous slide to export your data for simulation



→ EBSD → ODF → Discretization

You can also calculate the ODF from your EBSD measurements and then discretize it

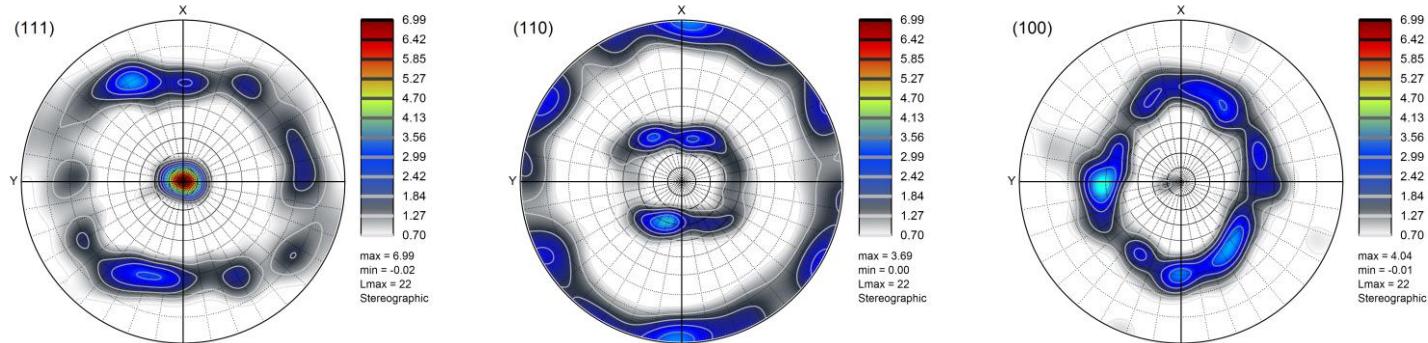
1. Go on tab “TEXTURES” and just export your ODF by clicking on the “Export ODF” button
2. See the slide “Discretization” to prepare your data for simulation



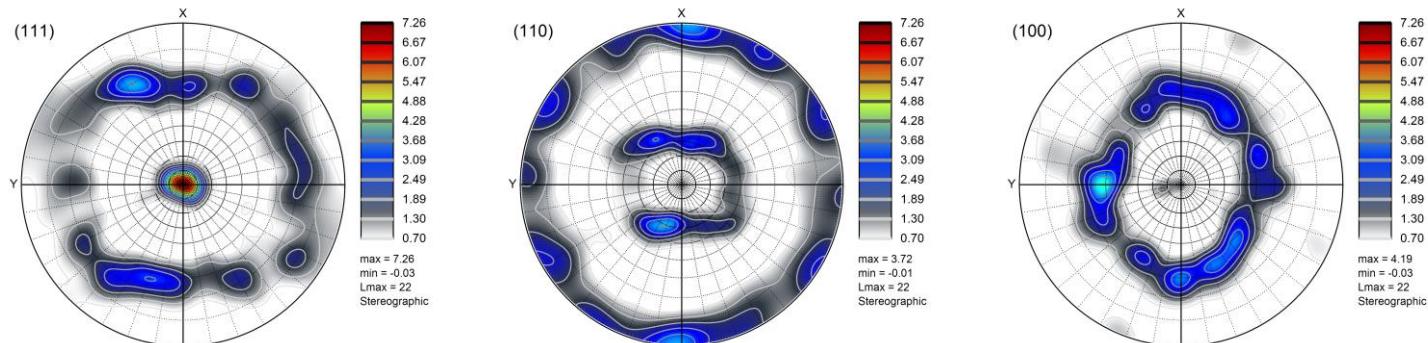
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→ Examples of orientation list with the different methods

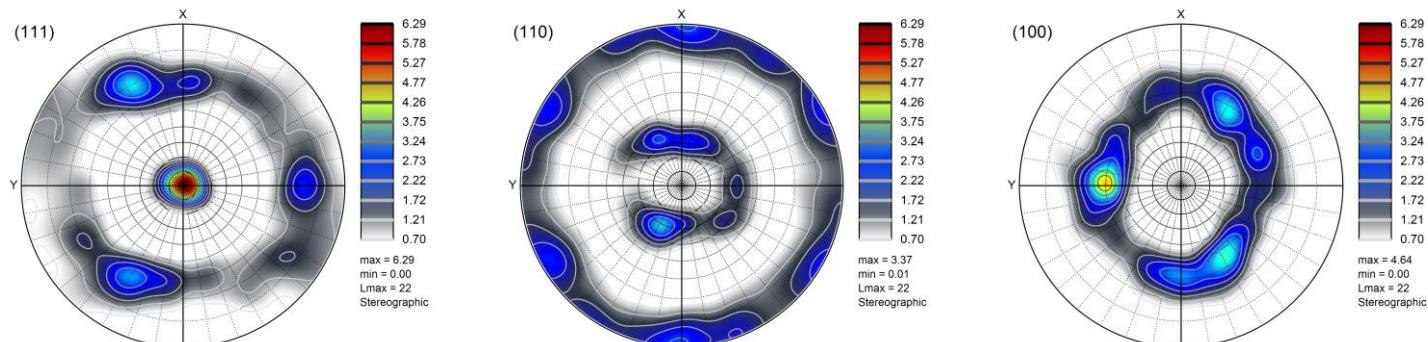
EBSD → full texture ODF calculated from all the 221000pixels



EBSD → one orientation per grain (the average orientation), 246 grains (>1 pixel)



EBSD → ODF → Discretization 1000 orientations



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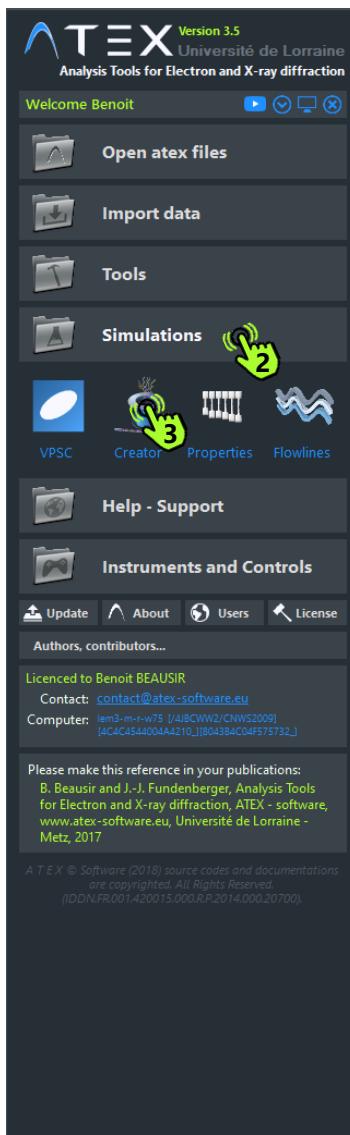


Content

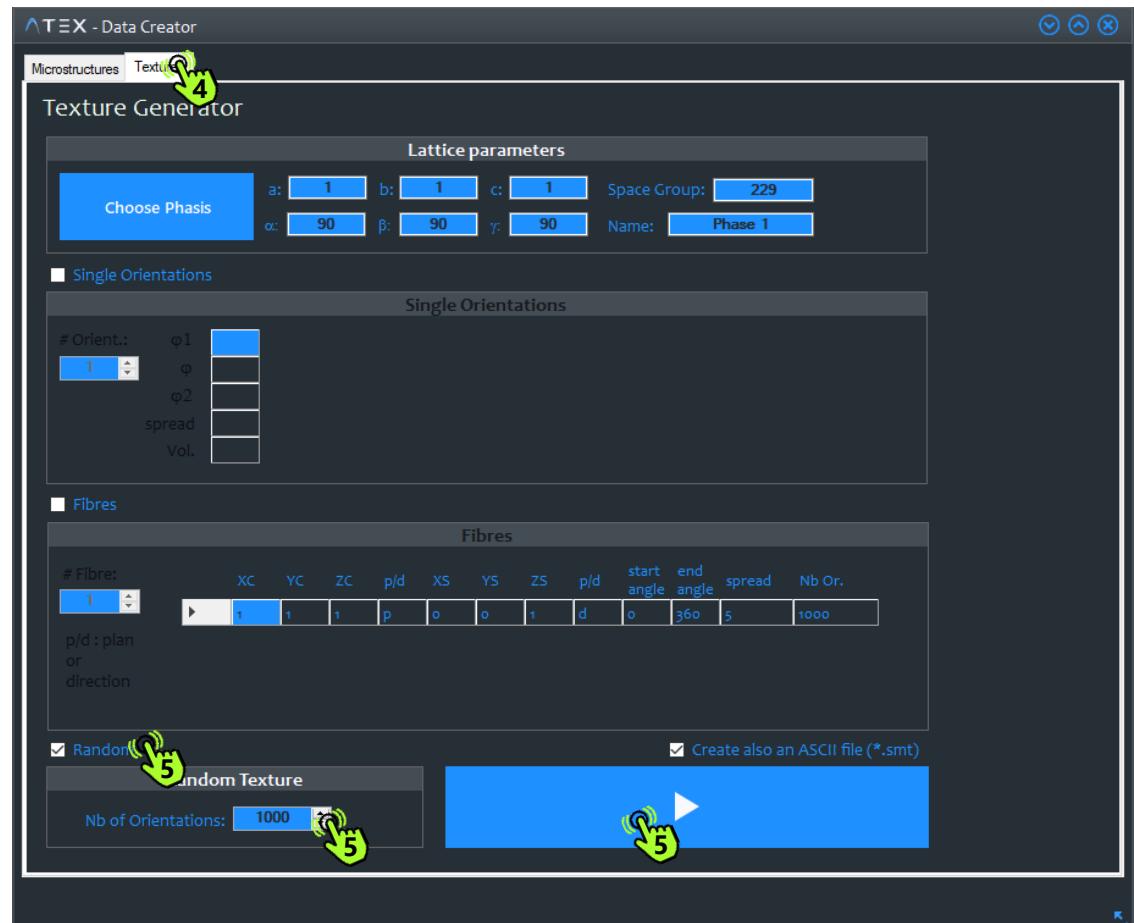
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TUTORIAL Textures Simulation – Crystal Plasticity

1. Open ATEX
2. Click on the “Simulations” button
3. Select “Creator” module
4. Select the “Textures” tab
5. Click the “Random check box”, select 1000 orientations and execute



→ Simulations (VPSC) generate 1000 random orientations



TUTORIAL Textures Simulation – Crystal Plasticity

Check the
generated
texture

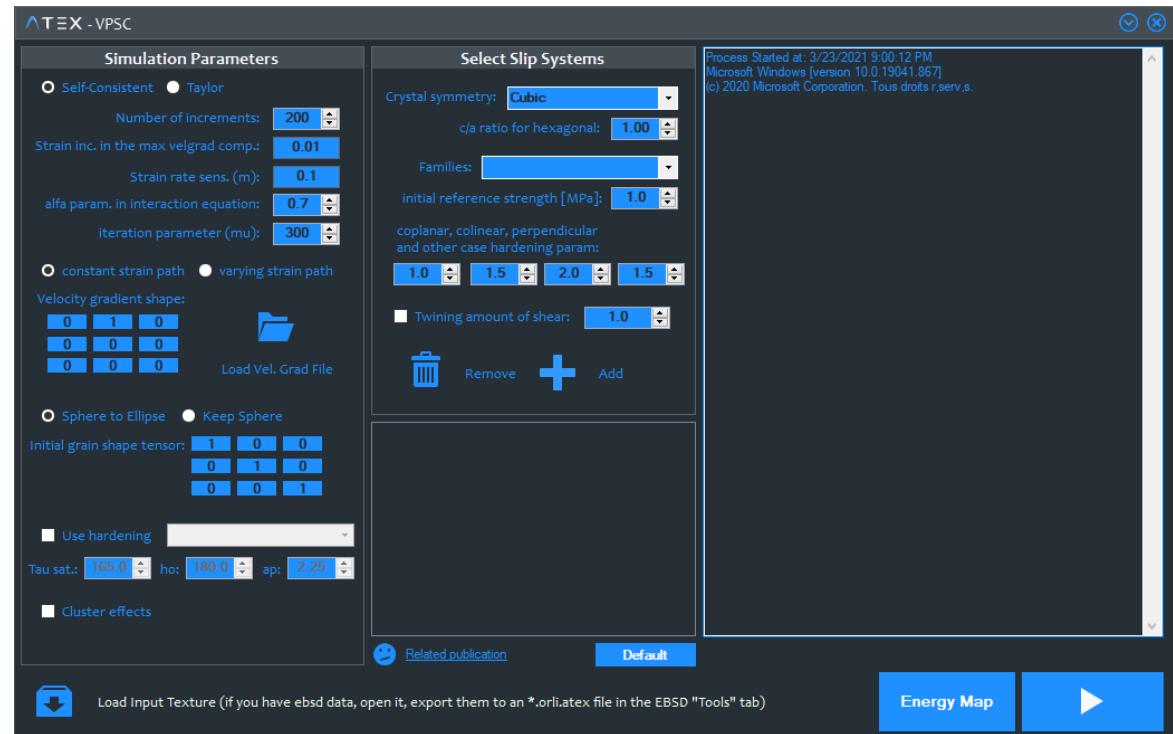
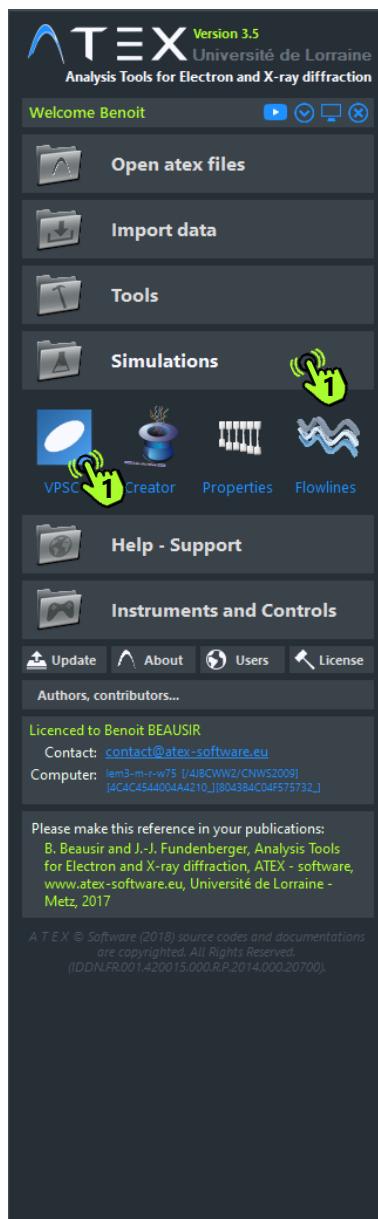
1000 random
orientations



TUTORIAL Textures Simulation – Crystal Plasticity

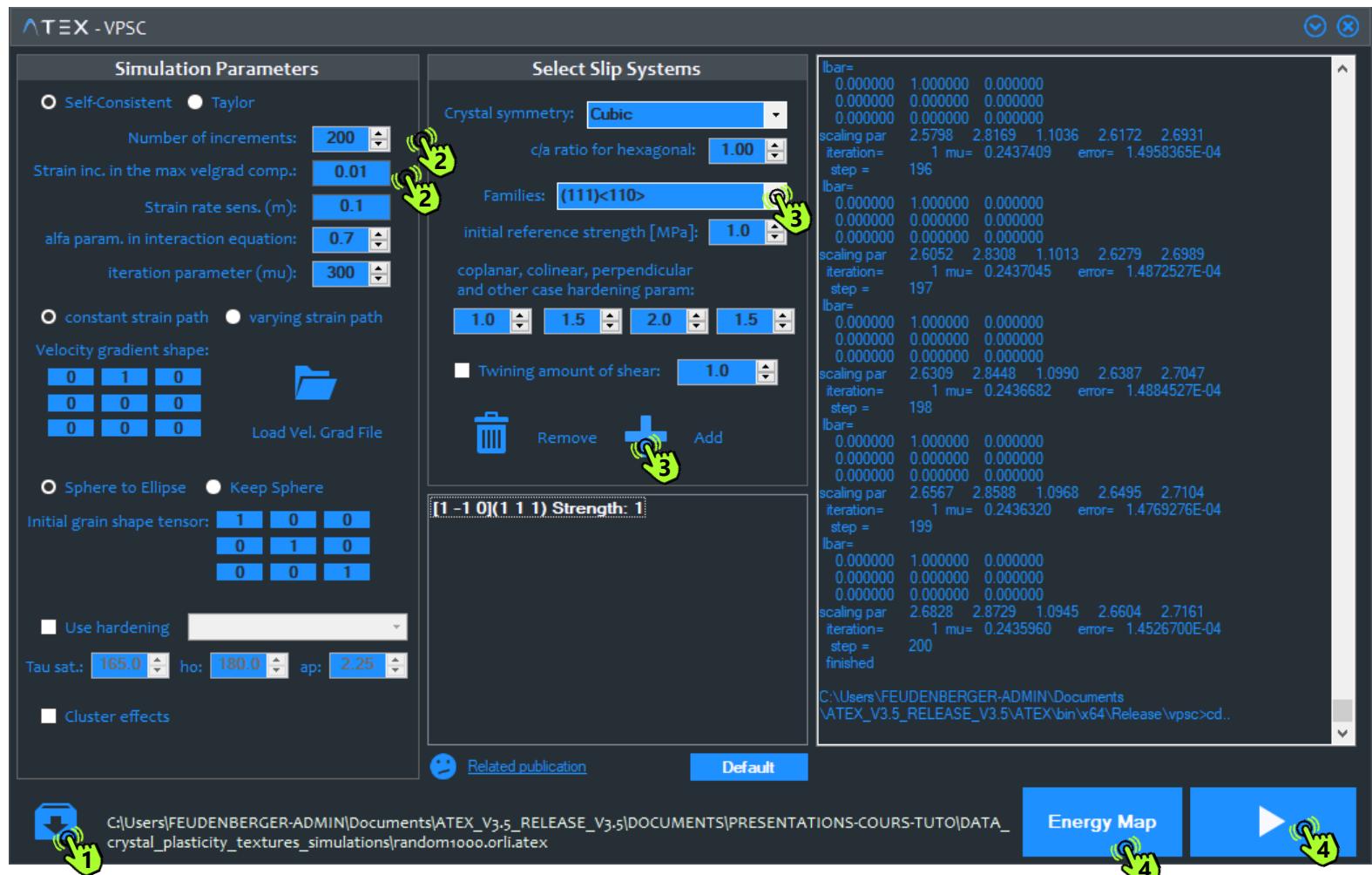
→ Simulations (VPSC)

- Select the “SIMULATIONS” tab and click on VPSC button to open the VPSC module



→ Simulations (VPSC)

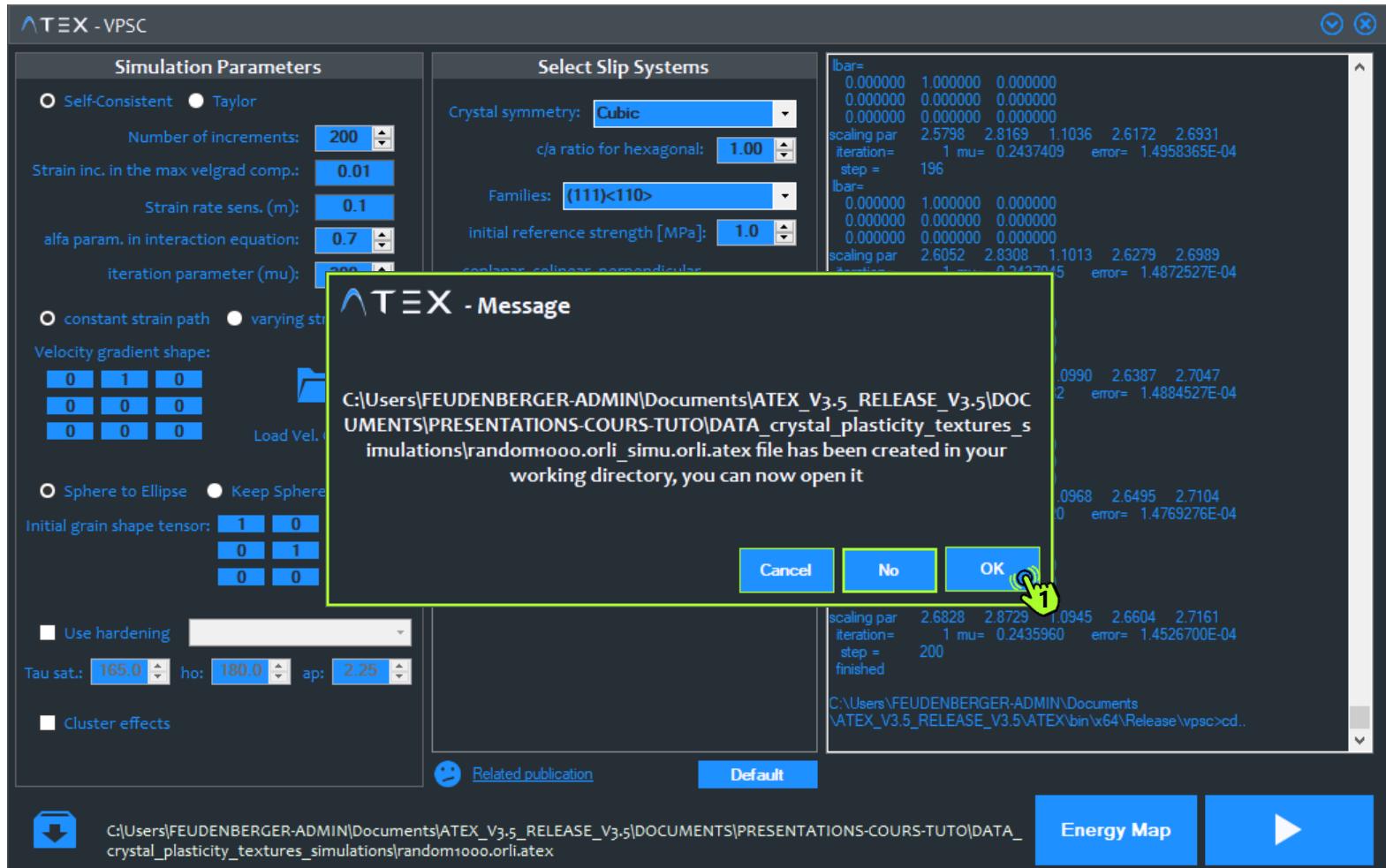
1. Select your input data file (orli.atex file)
2. Select the Simulation parameters
3. Select your slip system(s) family(ies) and if needed twins families
4. Run the simulations. You can also obtain the plastic energy by clicking on the “Energy Map” button,



Shear = 2, Aluminium

→ Simulations (VPSC)

- Once the simulations are finished an new file *_simu.orli.atex is created in your working directory, answer OK to open it



TUTORIAL Textures Simulation – Crystal Plasticity

→ Simulations (VPSC)

1. If you answer "OK" the ORLI module will open automatically your simulated texture
2. Click PF, IPF or Euler space Sections to draw it

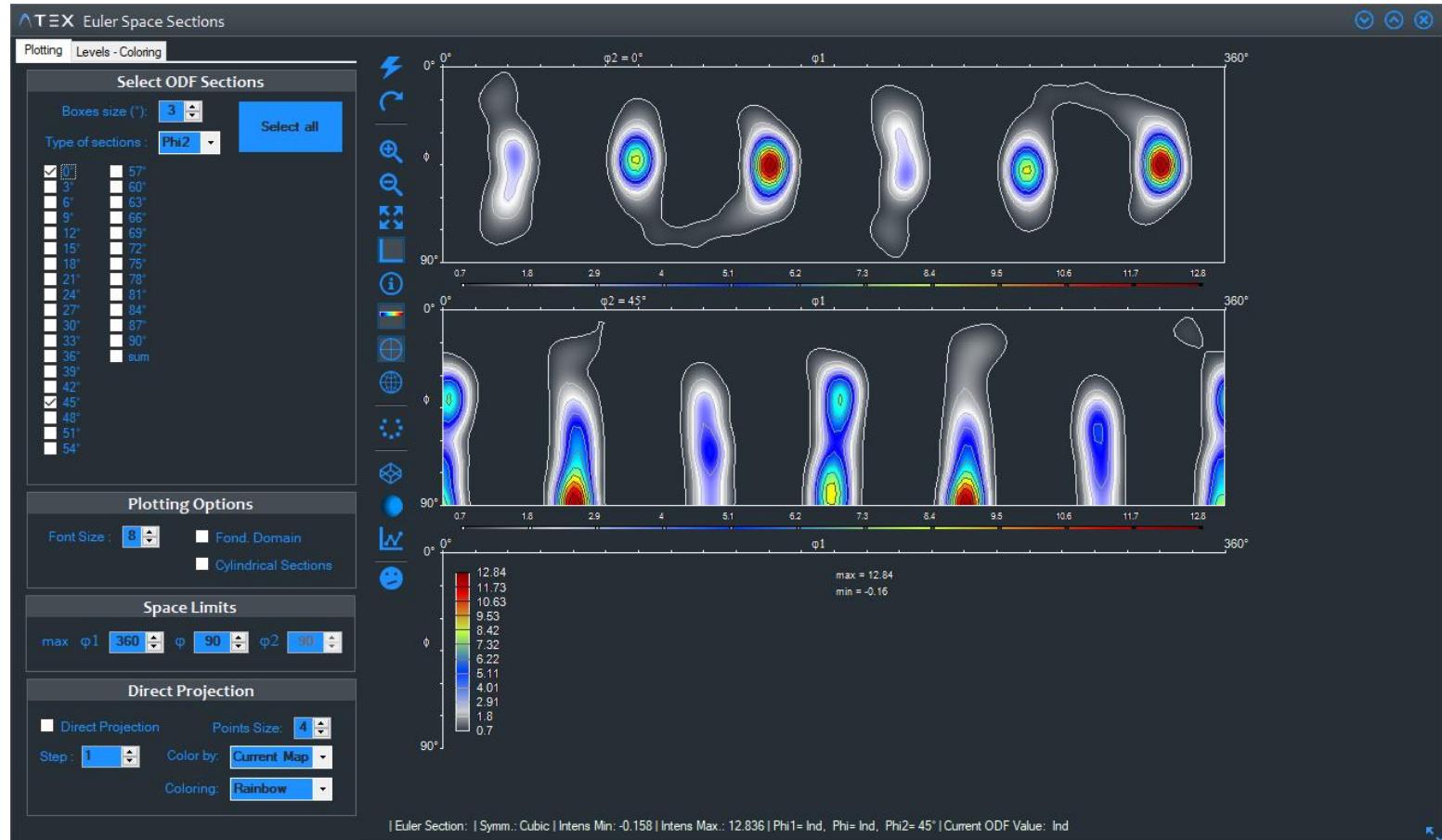


id (IDDN.FR.001.420015.000.R.P.2014.000.20700)
placed on public Web servers without permission.

→ Simulations (VPSC)

- Euler space
Sections of the simulated texture, here $\phi_2=0^\circ$ and 45°

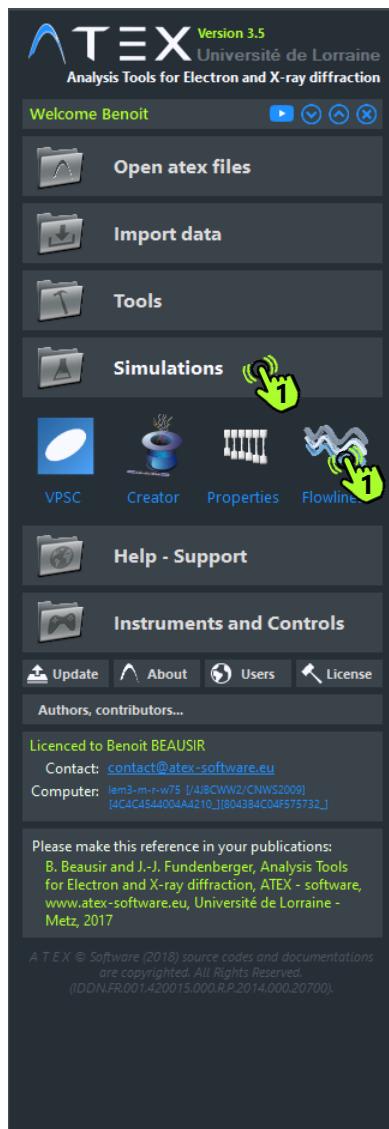
Typical representative sections cubic materials under simple shear



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→ Simulations (VPSC) - varying strain path

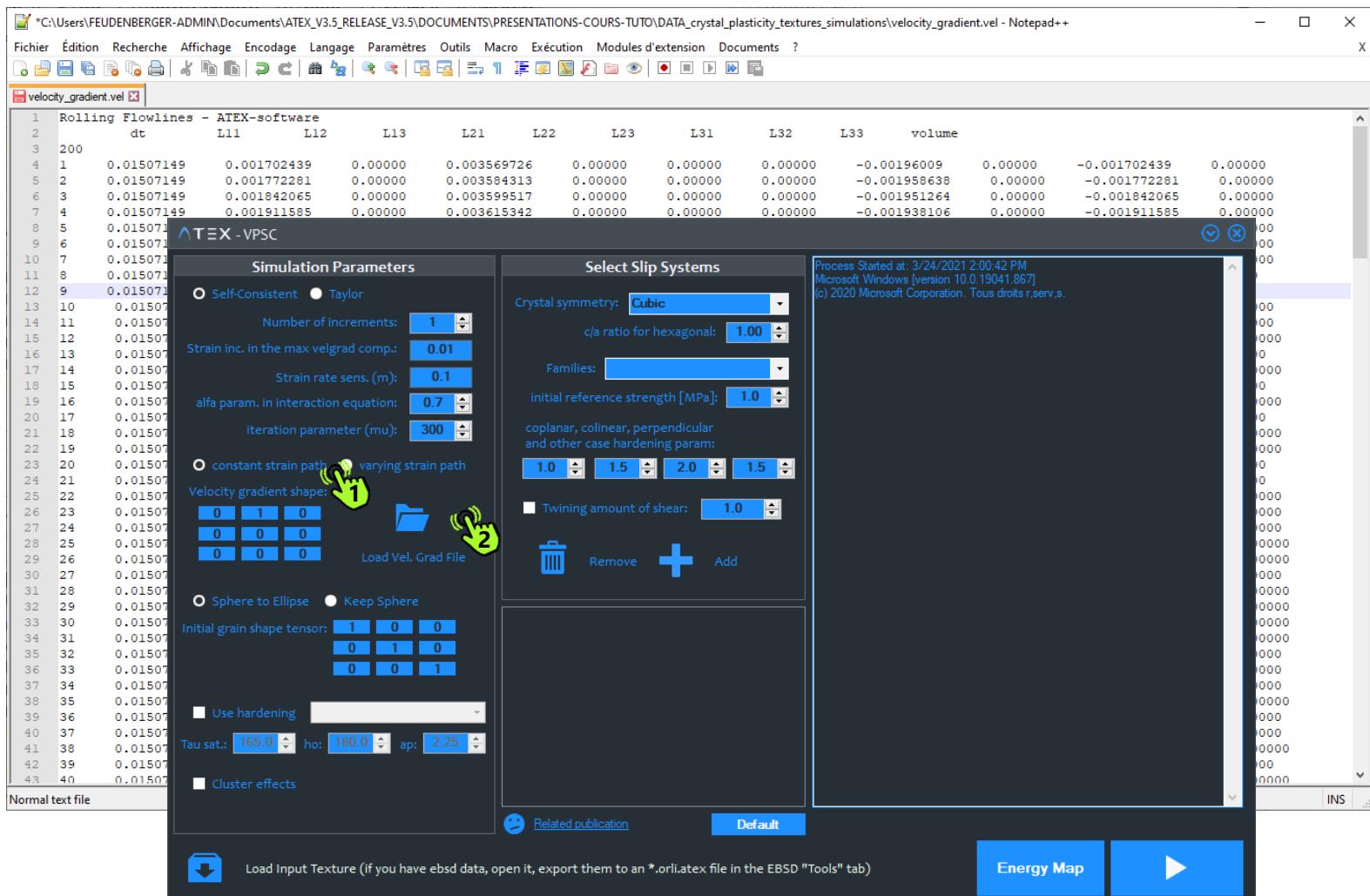
1. Select the “SIMULATIONS” tab and click on “Flowlines” button to open corresponding module
2. Select either ECAP or ROLLING tab
3. Set your parameters and click on “Export velocity gradient...” button



TUTORIAL Textures Simulation – Crystal Plasticity

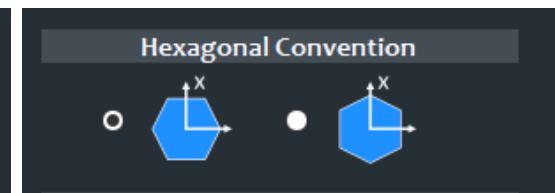
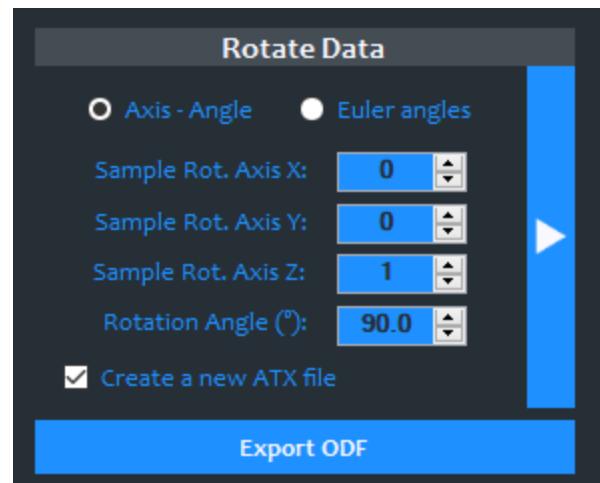
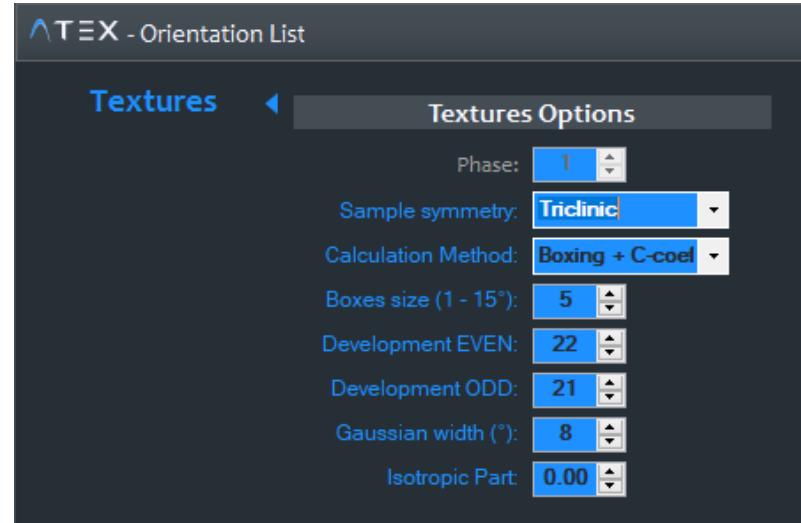
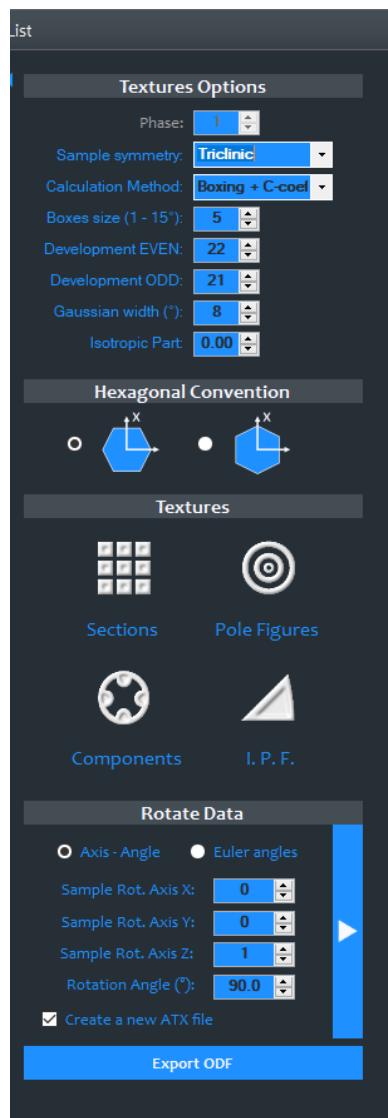
→ Simulations (VPSC) - varying strain path

1. Select “varying strain path”
2. Choose your *.vel” file



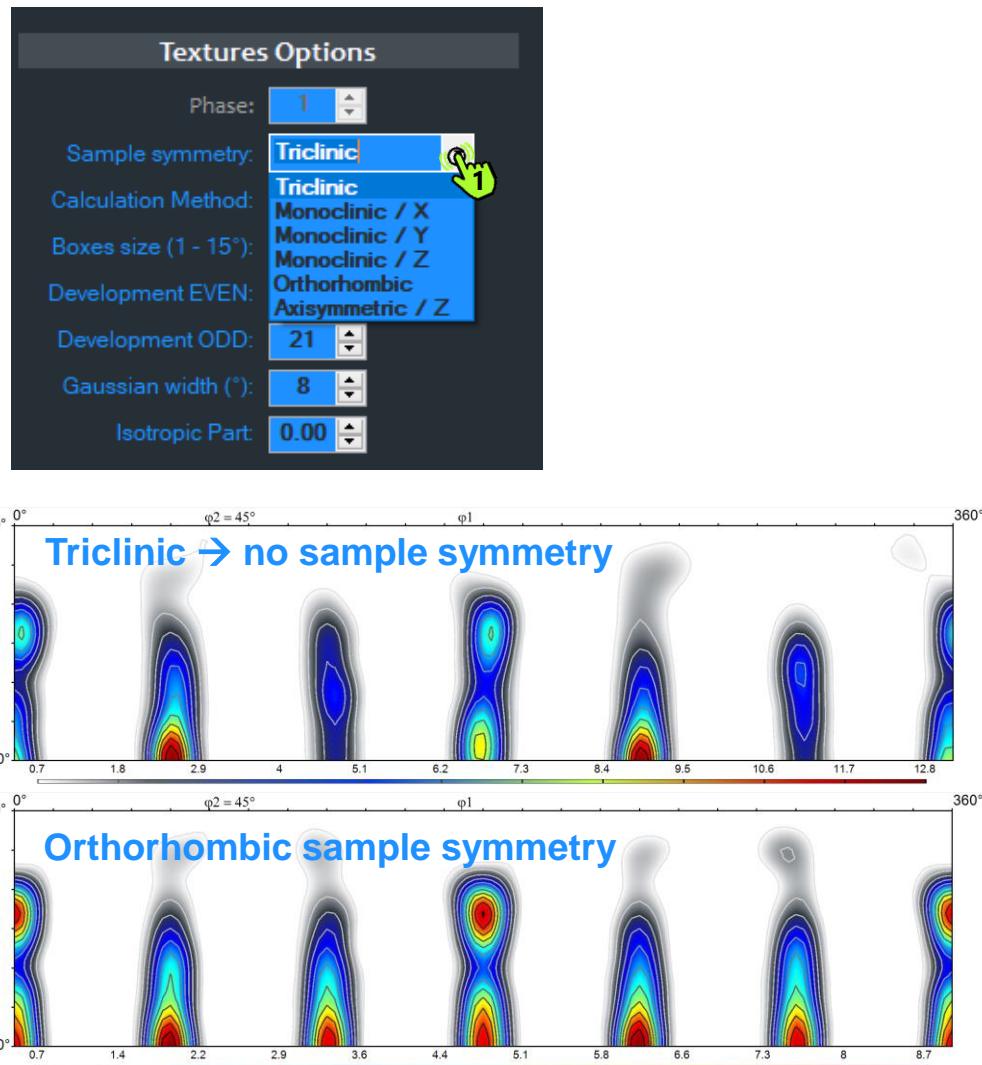
→ Texture calculation Options

1. Textures calculation options

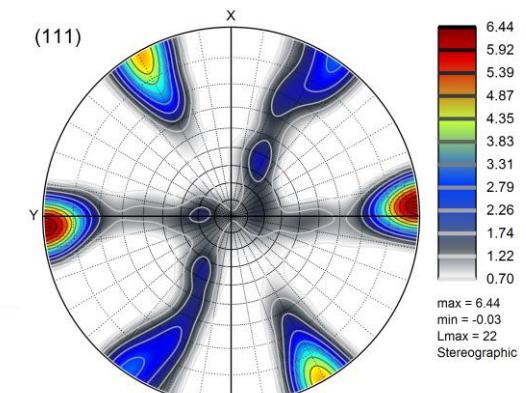


→ Texture calculation Options, Sample Symmetries

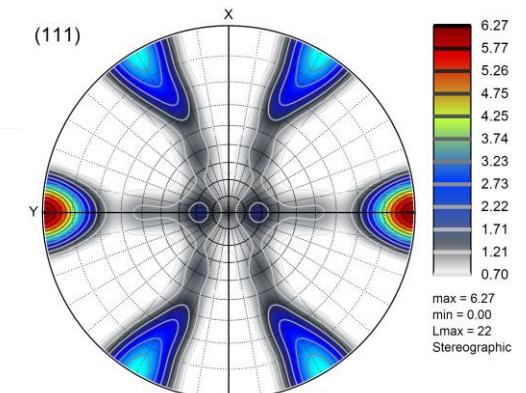
1. Plot the texture with no sample symmetry (triclinic)
2. Change the symmetry and plot the new texture



Triclinic → no sample symmetry



Orthorhombic sample symmetry



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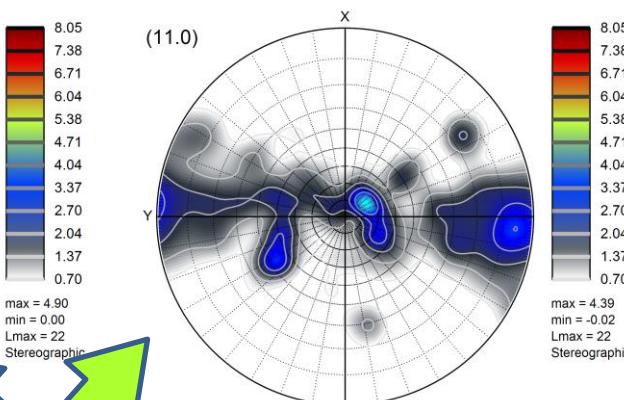
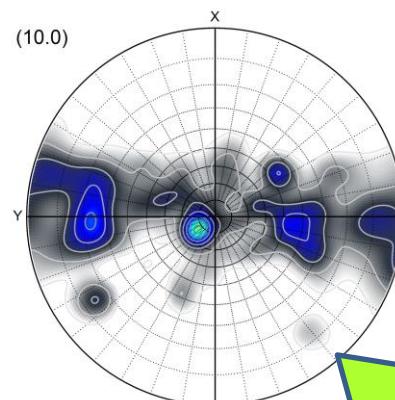
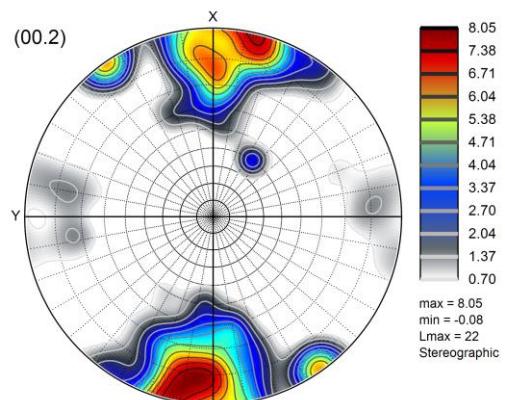
→ Texture calculation Options, Sample Symmetries

1. Be careful about the Hexagonal Convention

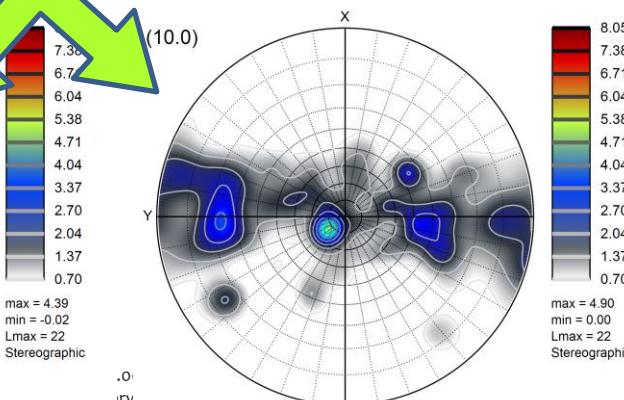
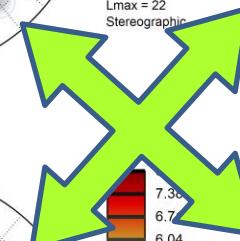
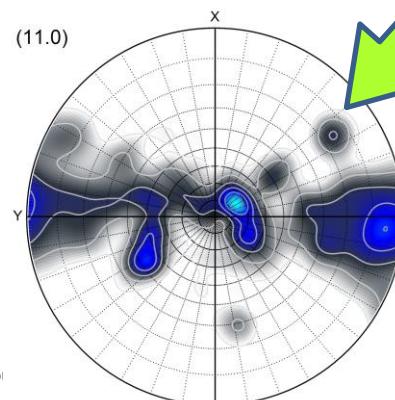
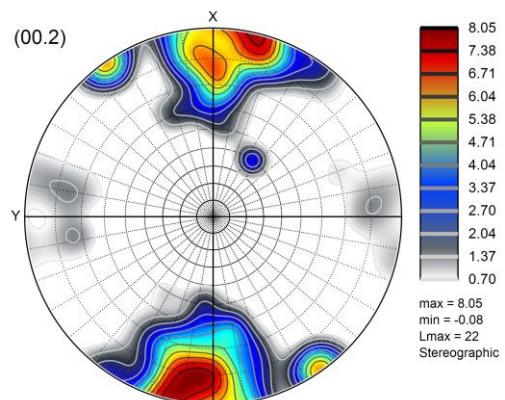


ROTATION by 30° around the c-axis ($\phi_2 = \phi_2 + 30^\circ$)

Convention $x // a$



Convention $y // a$



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→ Ideal (stable) orientations

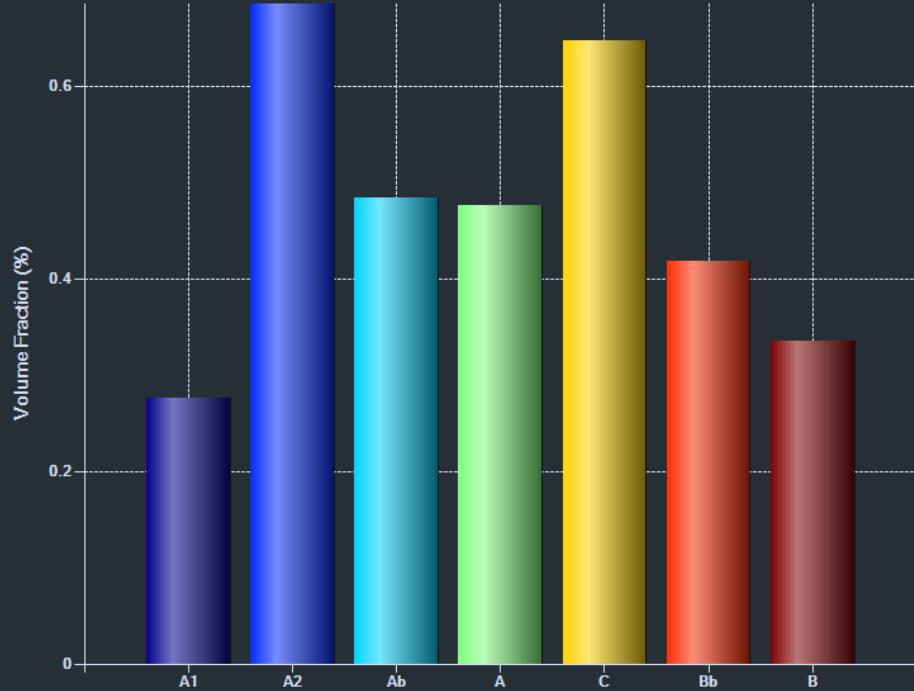
- From the ORLI module, click the “COMPONENTS” button to open the TEXTURE COMPONENTS calculation module

The screenshot shows the ATEX software interface with the following components:

- Textures Options:** Phase: 1, Sample symmetry: Triclinic, Calculation Method: Boxing + C-coef.
- random1000.orli_simu.orli:** 1000 Orientations. Lattice parameters: $a = 1$, $b = 1$, $c = 1$, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 90^\circ$. A table lists orientation parameters for 5 orientations.
- Texture Components:** Select From: From Miller, Phase: 1, Name: ID, Symbol: $\langle 111 \rangle$, Color: blue. Rotation Angle: 0, Disor. Angle: 5, Sample symmetry: Triclinic.
- Components:** Shows a hand icon over a circular component.
- Rotate Data:** Axis - Angle, Sample Rot. Axis X: 1, Sample Rot. Axis Y: 0, Sample Rot. Axis Z: 0, Rotation Angle: 0, Create a new ATX file checked.
- Export Options:** Buttons for Color, Modify, Rotate, Remove, Add, Save, Evaluate.

→ Ideal (stable) orientations

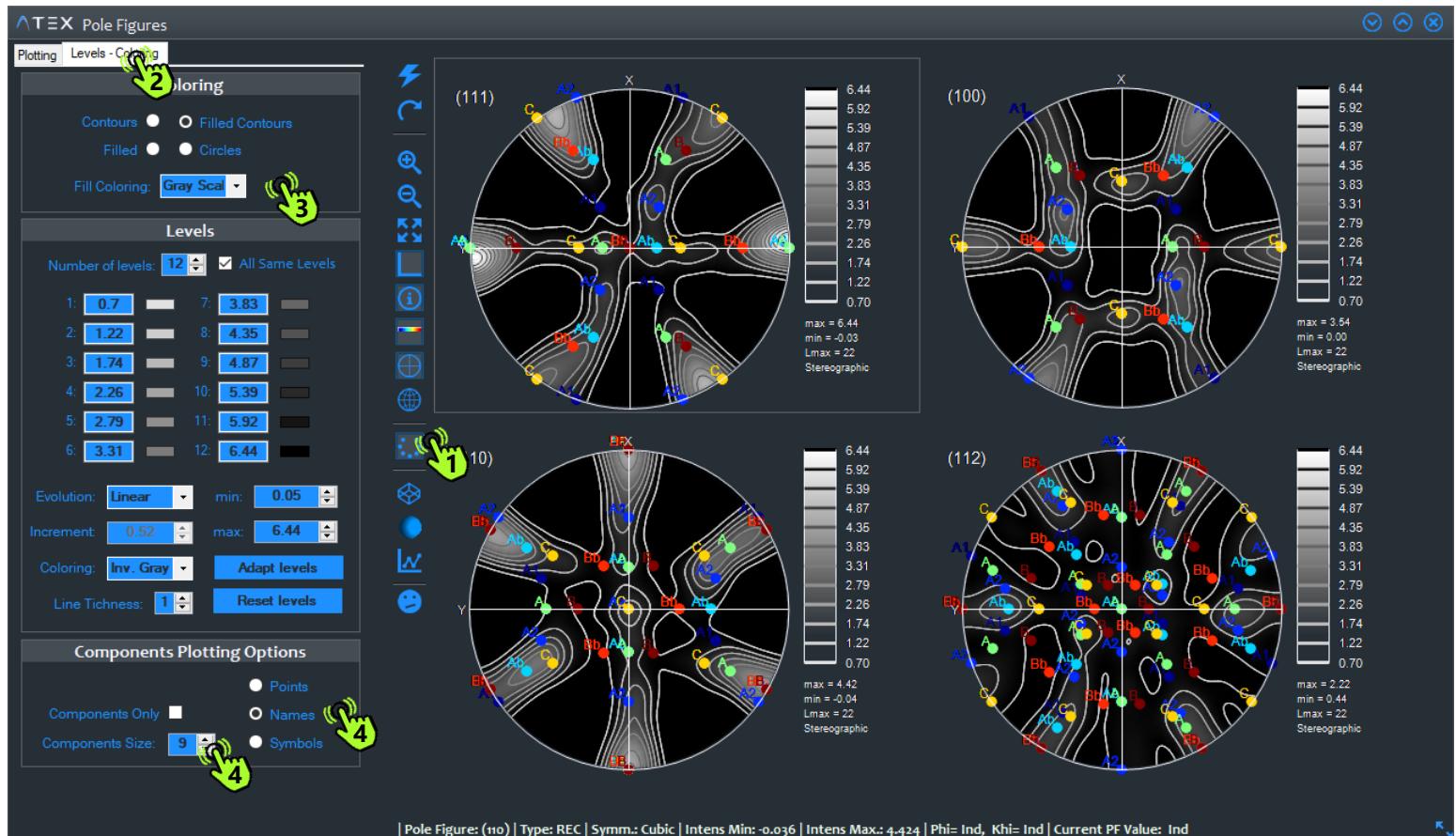
1. Select the components you want to know the volume fractions
2. Here the ideal orientations for fcc crystals under simple shear
3. Click on the “color” button and then on the “evaluate” button



	A1	A2	Ab	A	C	Bb	B
O. D. F.	3.472...	8.679...	6.068...	6.073...	8.373...	5.261...	4.120...
Vol. Frac. (%)	0.276...	0.686...	0.483...	0.476...	0.647...	0.418...	0.335...

→ Ideal (stable) orientations

1. Click on the “show components” button in the vertical tool bar next to the pole figure plots
2. Select “Levels – coloring’ tab
3. Fill coloring -> “Gray scale”
4. In Components Plotting Options - increase the size of the components - select “Names”



1. Here is written the list of what to do
2. This hand tells you where to click



Content

1. Input Data
 1. Generate textures
 2. X-Ray measurements
 3. Orientations Maps (EBSD)
2. Simulations (VPSC)
3. Simulations vs Experiments
 1. Ideal Orientations
 2. Correlation
4. Simulations On Orientations Maps

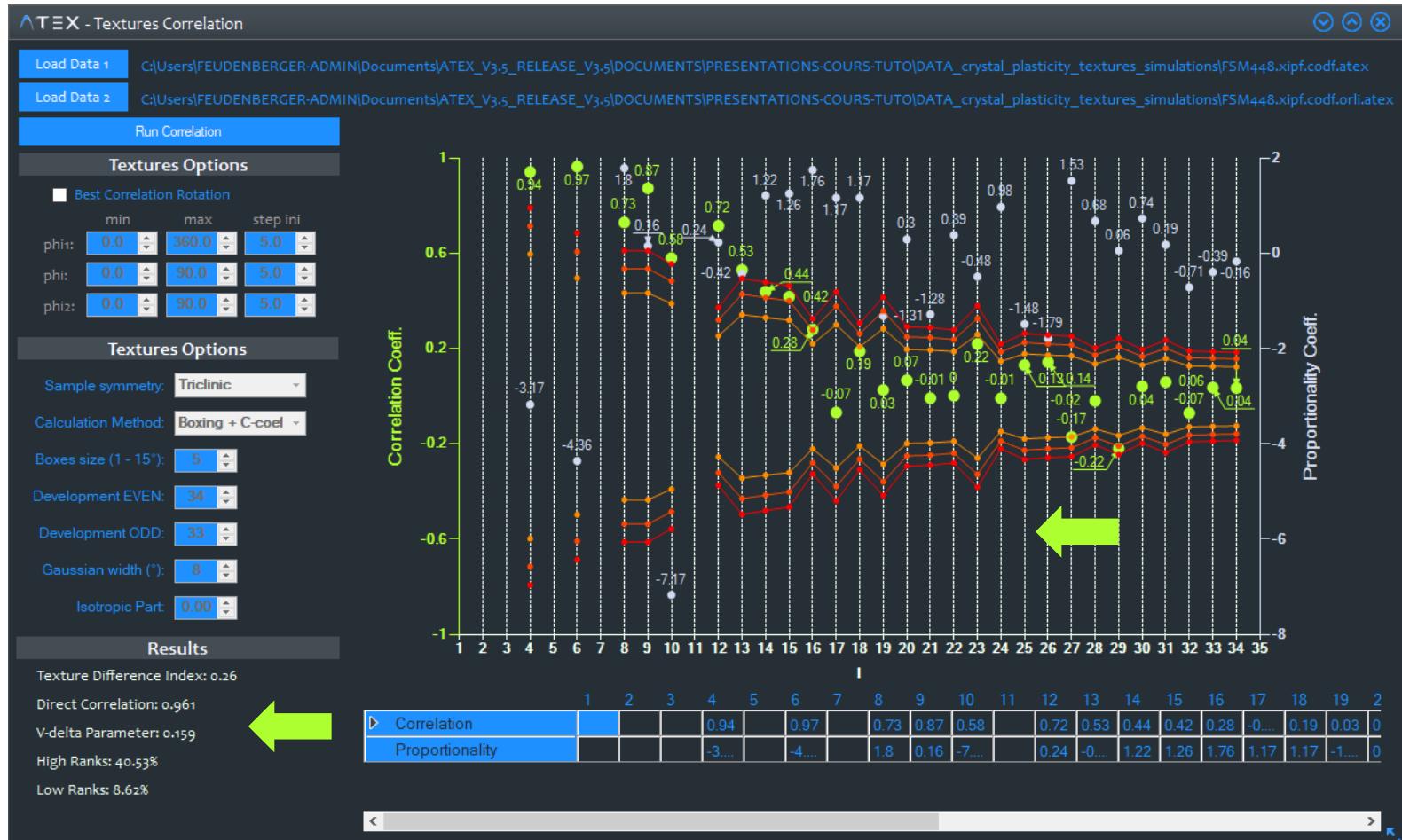
→ Correlation

1. Click on the “TOOLS” tab then select the “Compare” module.
2. Select the two textures to be compared, It can be either an ODF or an ORientation List
3. Run the computation

The screenshot shows the ATEX software interface. On the left, the 'Tools' tab is selected, and the 'Compare' module is open. The main window displays the 'Textures Correlation' dialog. The dialog has three tabs: 'Textures Options', 'Sample symmetry' (set to Triclinic), 'Calculation Method' (set to Boxing + C-coel), 'Boxes size (1 - 15°)' (set to 5), 'Development EVEN:' (set to 22), 'Development ODD:' (set to 21), 'Gaussian width (°)' (set to 8), and 'Isotropic Part' (set to 0.00). Below the dialog is a large, mostly empty 'Results' section.

→ Correlation

1. The results appears...



Correlation indicators

Texture Index:

$$J_{index} = \int_g f(g)^2 dg$$

Texture Difference Index:

$$J_{diff} = \int_g (f_A(g) - f_B(g))^2 dg$$

V-delta Parameter:

$$V_{delta} = \frac{1}{2} \int_g |f_A(g) - f_B(g)| dg$$

Direct Correlation:

$$D = \frac{\int_g f_A(g)f_B(g)dg^2}{\sqrt{\int_g f_A^2(g)dg^2 \cdot \int_g f_B^2(g)dg^2}}$$

High Ranks:

$$H = \frac{1}{\sum l} \sum_{l=l_{min}}^{l_{max}} l \cdot C(l)$$

Low Ranks:

$$L = \frac{1}{\sum l} \sum_{l=l_{min}}^{l_{max}} (l_{max} - l) \cdot C(l)$$

Textures Comparison



Theory

Let A and B two textures expressed on the basis of spherical harmonics,

$$A_i^{m,n}$$

and

$$B_i^{m,n}$$

the corresponding series of complex numbers.

The correlation coefficient between the two textures is then given by:

$$C(l) = \frac{\sum_m \sum_n A_l^{m,n} B_l^{m,n} + \sum_m \sum_n A_l^{m,n*} B_l^{m,n*}}{\sqrt{(\sum_m \sum_n A_l^{m,n} A_l^{m,n} + \sum_m \sum_n A_l^{m,n*} A_l^{m,n*})(\sum_m \sum_n B_l^{m,n} B_l^{m,n} + \sum_m \sum_n B_l^{m,n*} B_l^{m,n*})}}$$

If $C(l)=1$ then A and B are proportional at rank l

A and B will be identical if both all $C(l)=1$ and all $P(l)=1$

$$P(l) = \frac{\sum_m \sum_n A_l^{m,n}}{\sum_m \sum_n B_l^{m,n}}$$

In n-degrees of freedom problem, the probability that the

$$t = \sqrt{n/(1 - r^2)}$$

variable be less than a certain value t_0 is the student's t-distribution $Q(t,n)$. Thus the value $1-Q(t,n)$ is the confidence level at which the hypothesis of a correlation due to chance is invalidated.

1. Here is written the list of what to do
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Content

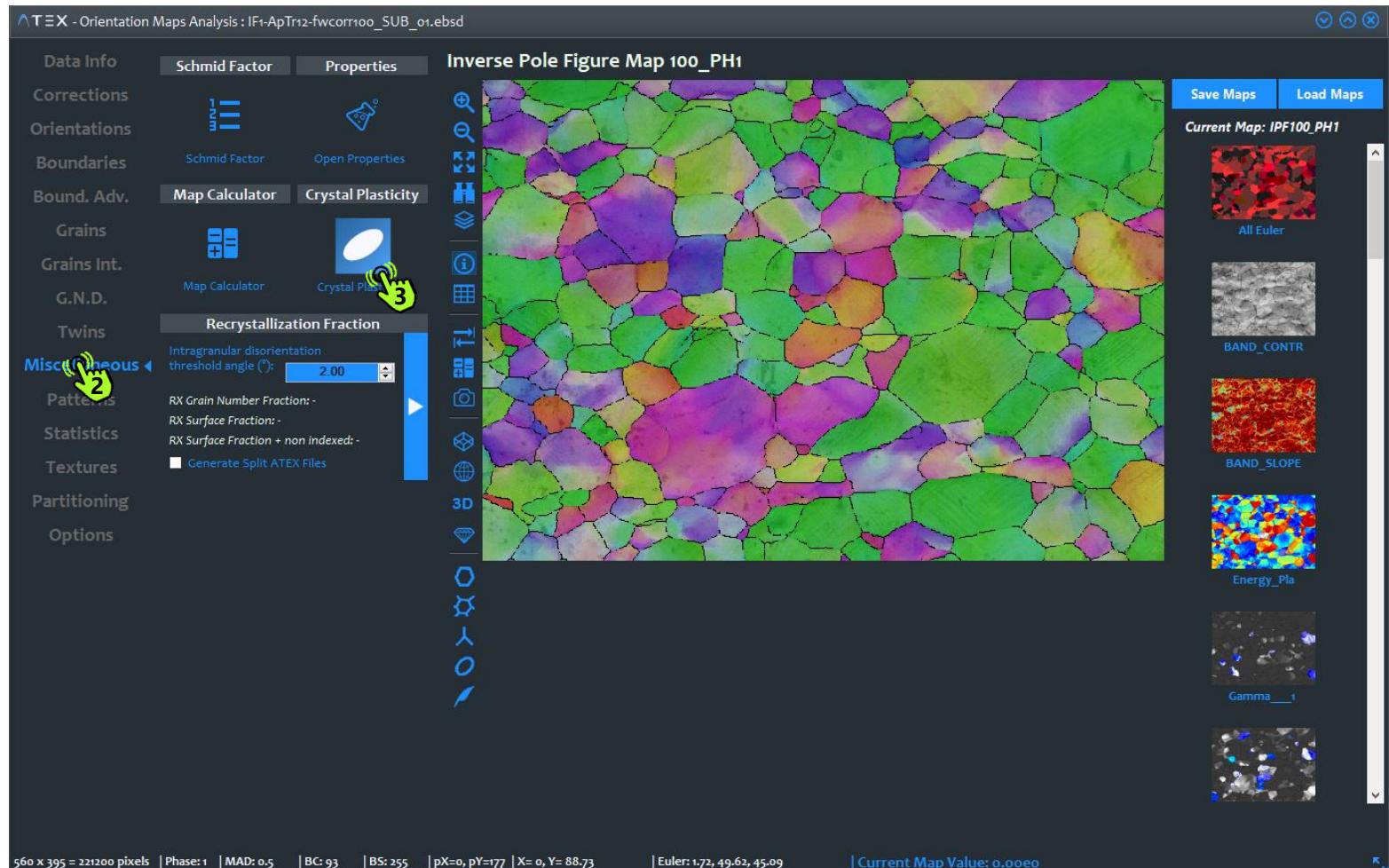
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TUTORIAL Textures Simulation – Crystal Plasticity

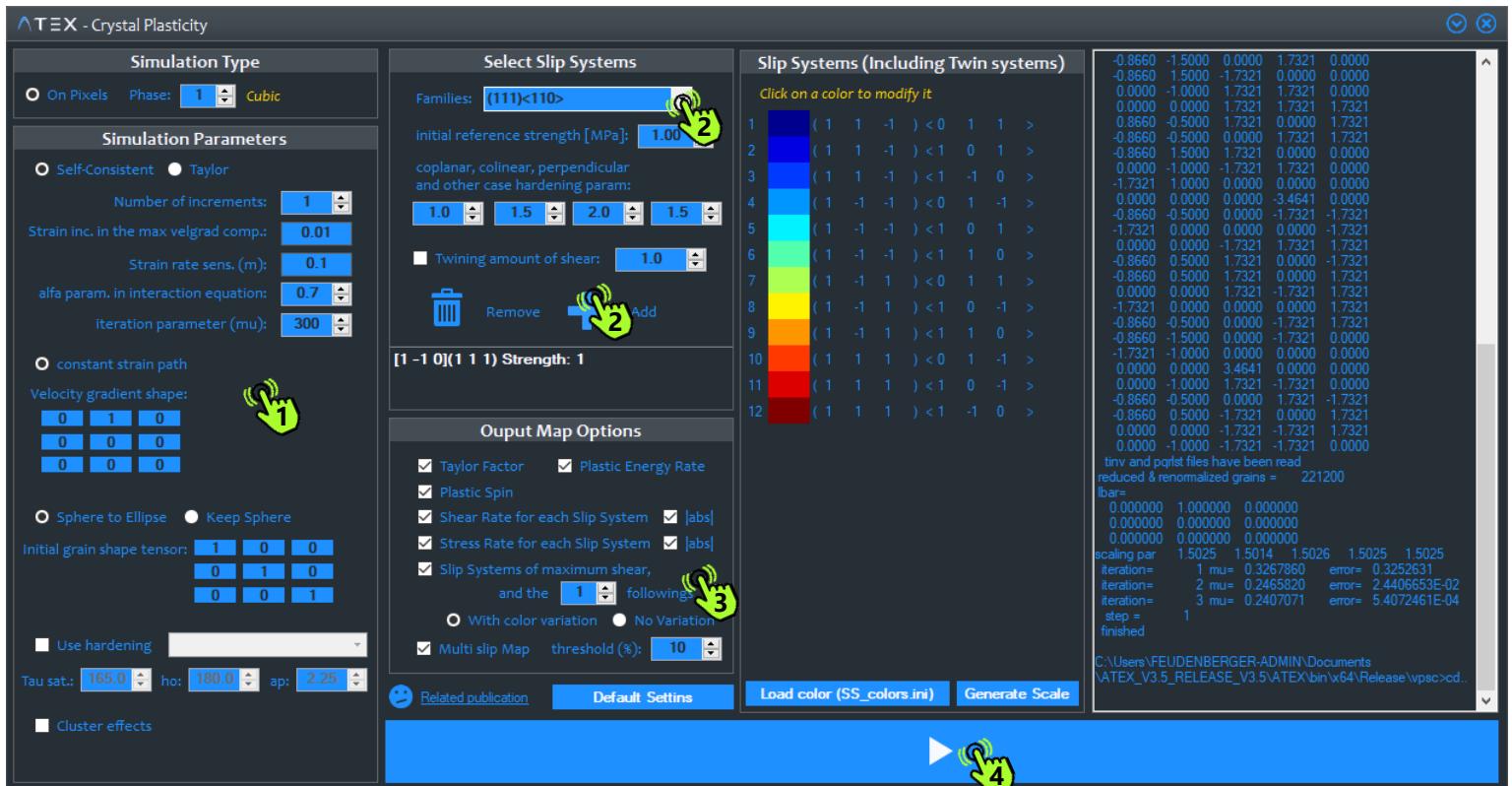
→ Simulations on Orientations Maps

1. Open an EBSD maps
2. Go in tab “Miscellaneous”
3. Click on Crystal Plasticity button to open the corresponding module

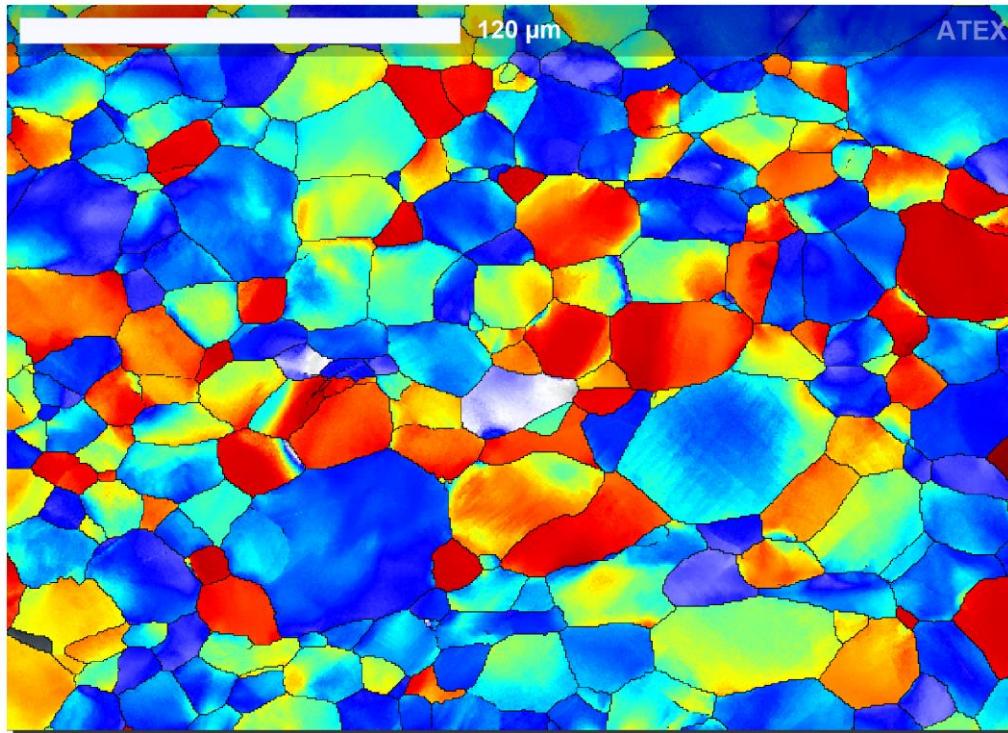


→ Simulations on Orientations Maps

1. Fill all the parameters, it is the same than previously in the VPSC module
2. Choose your slip systems
3. Choose the output maps you would like to obtain
4. Run the simulation



→ Simulations on Orientations Maps

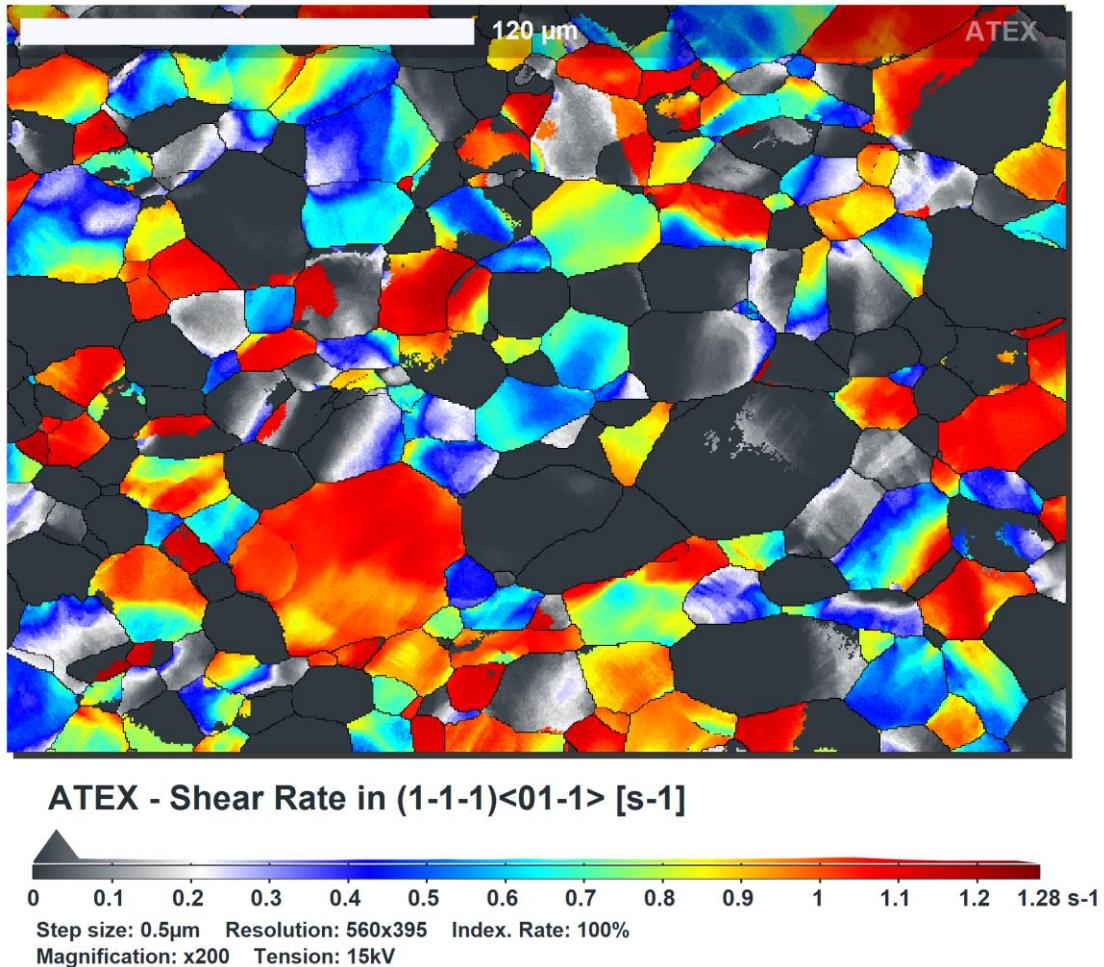


ATEX - Plastic Energy Rate [mW/mm³]

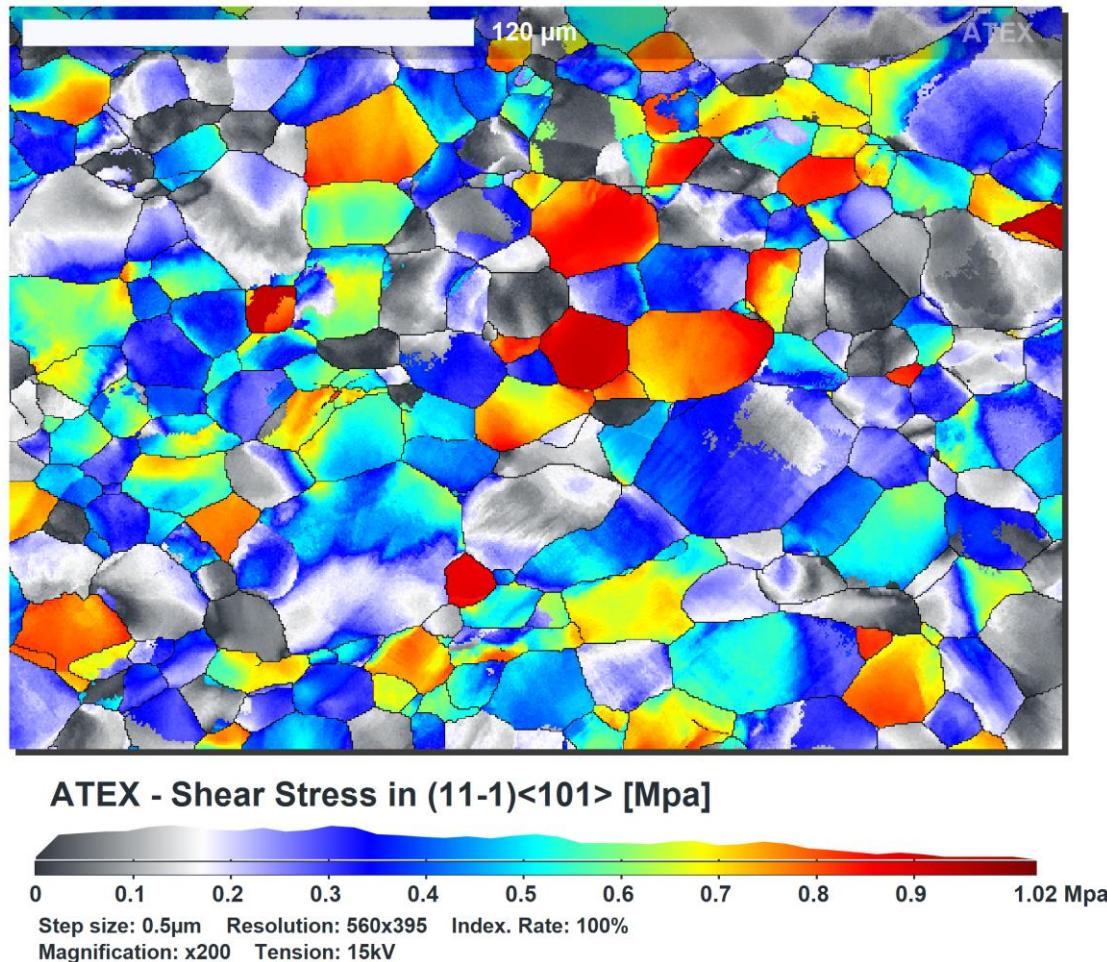


Step size: 0.5μm Resolution: 560x395 Index. Rate: 100%
Magnification: x200 Tension: 15kV

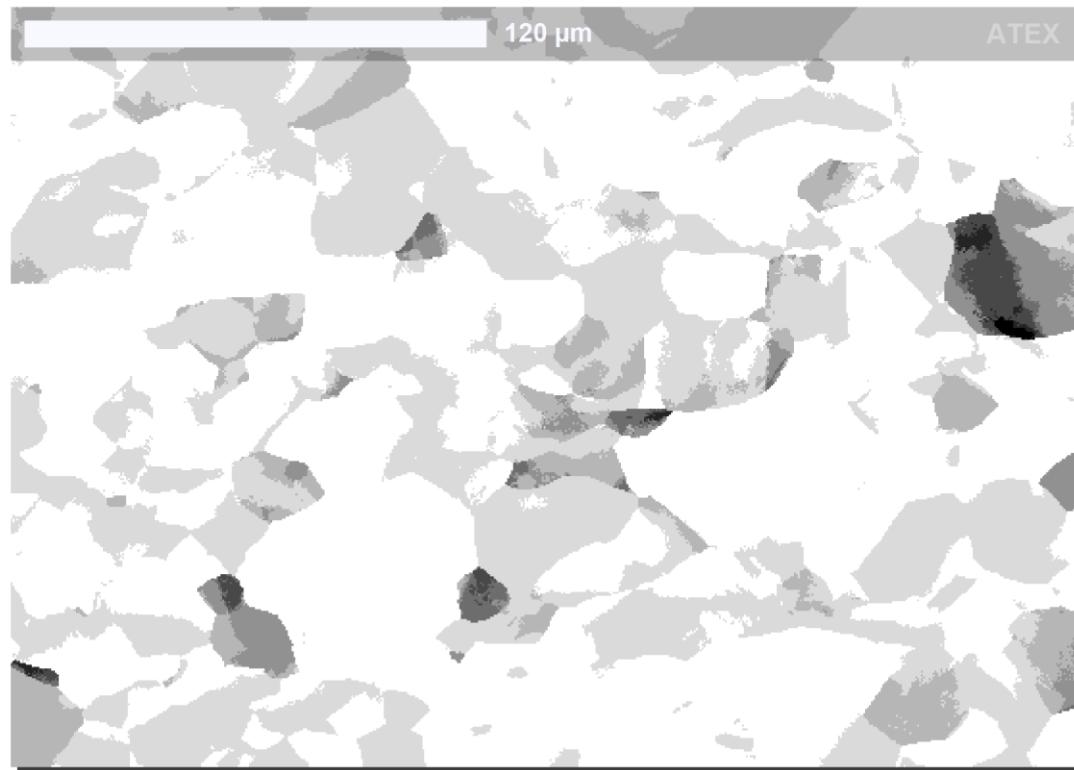
→ Simulations on Orientations Maps



→ Simulations on Orientations Maps



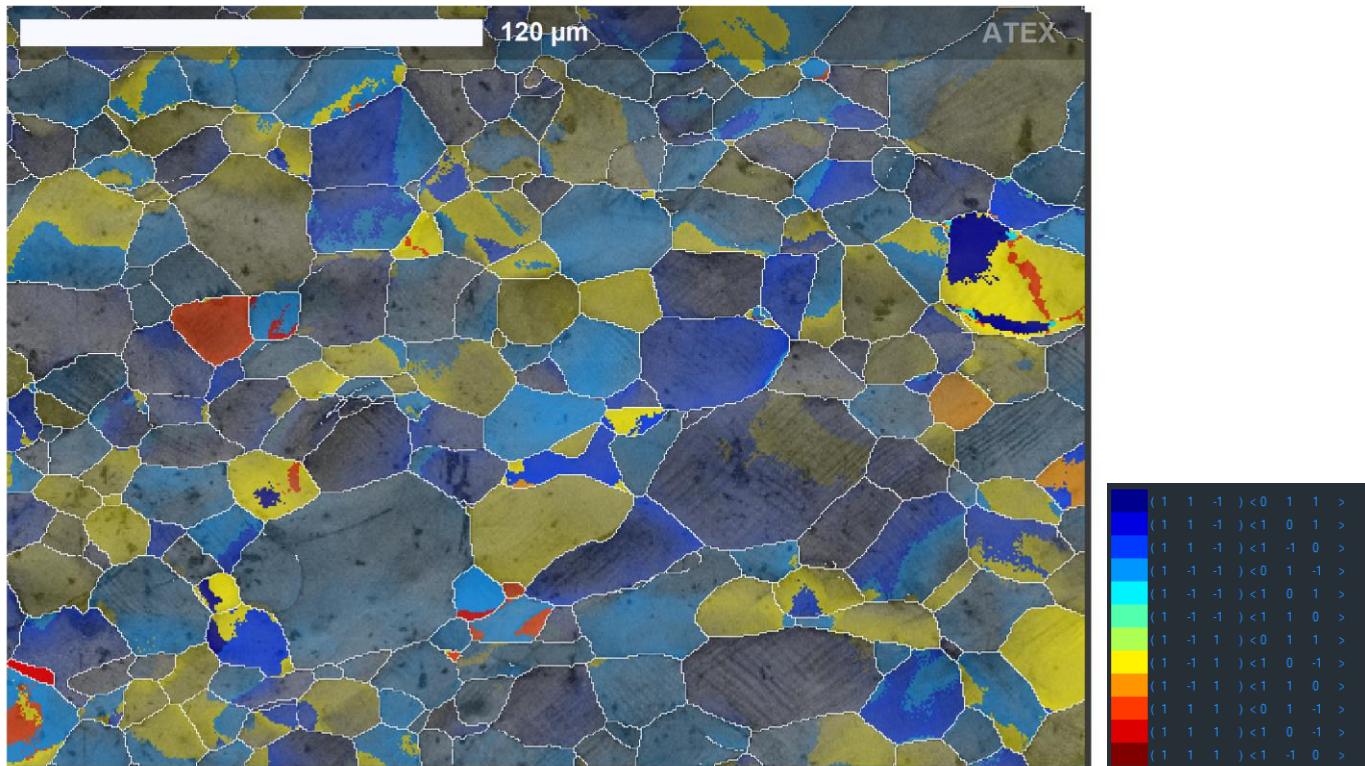
→ Simulations on Orientations Maps



ATEX - Number Of activated slip systems



→ Simulations on Orientations Maps



ATEX - Slip Systems of maximum shear stress

Step size: 0.5μm Resolution: 560x395 Index. Rate: 100%
Magnification: x200 Tension: 15kV



Textures Simulation – Crystal Plasticity

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University of Lorraine, Metz, France

www.atex-software.eu

www.atex-software.eu/help.html

www.youtube.com/channel/UCQcAjUova-pa9bGYWVtizGA

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