Analysis Tools for Electron and X-ray diffraction

Textures Simulation – Crystal Plasticity

Benoît Beausir & Jean-Jacques Fundenberger

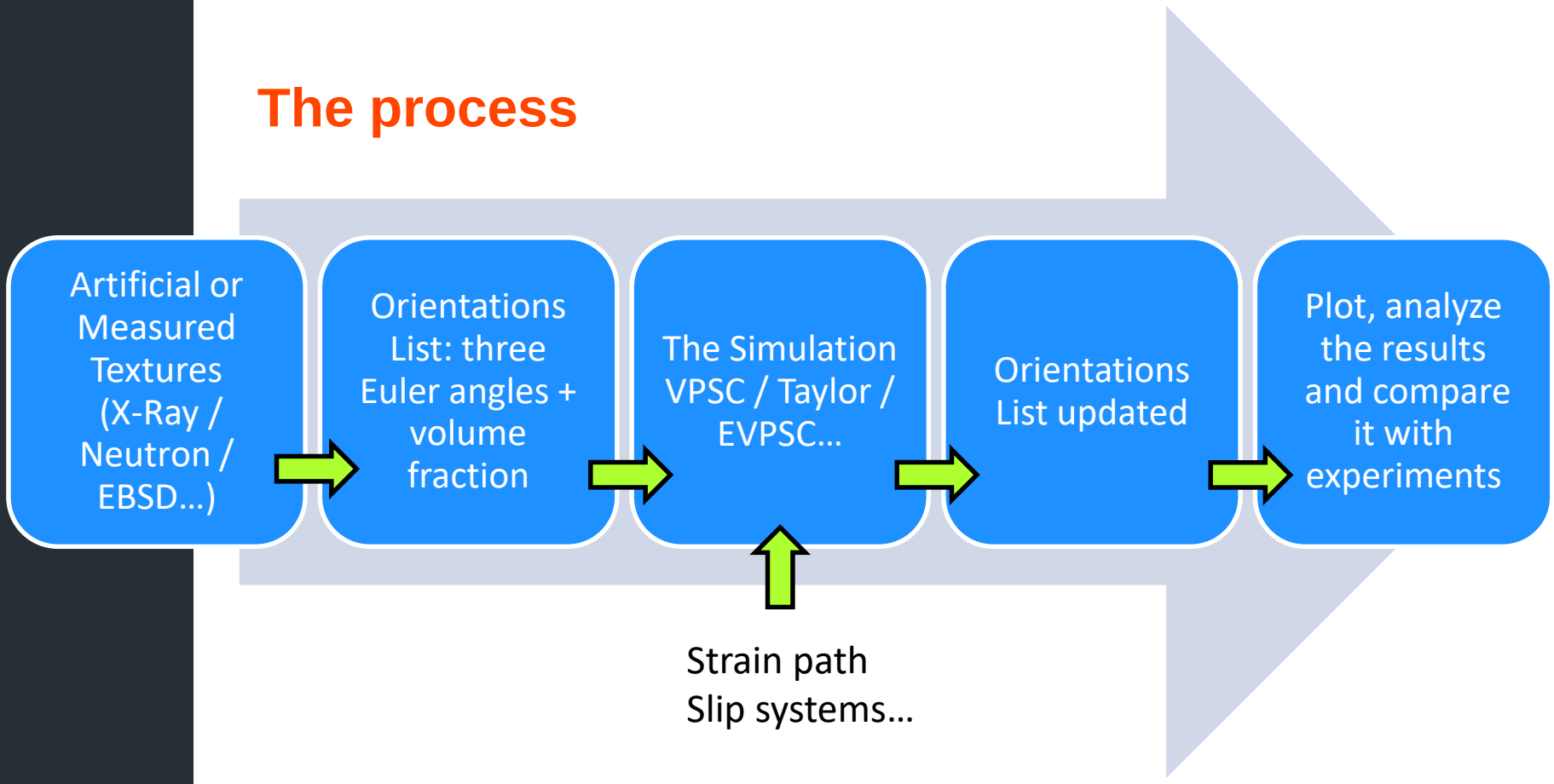
University of Lorraine, Metz, France

www.atex-software.eu
www.atex-software.eu/help.html
Youtube channel "atex software"

UNIVERSITÉ DE LORRAINE

ATEX is free for non-commercial use.

The process



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

Content

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

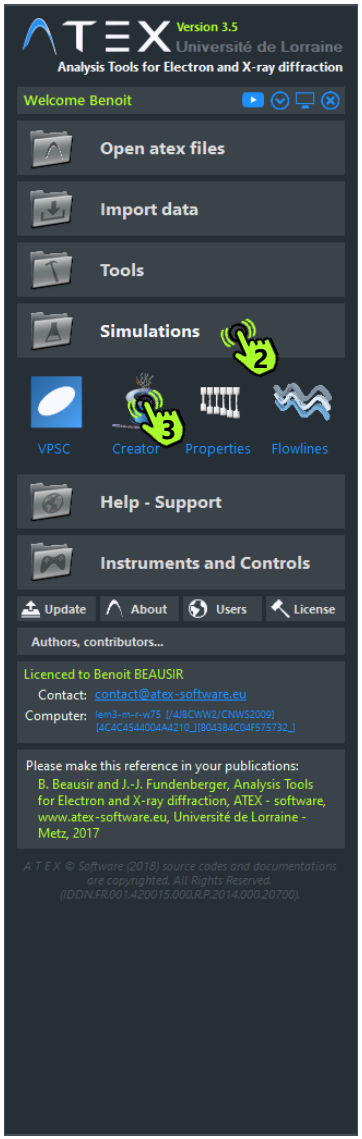
Content

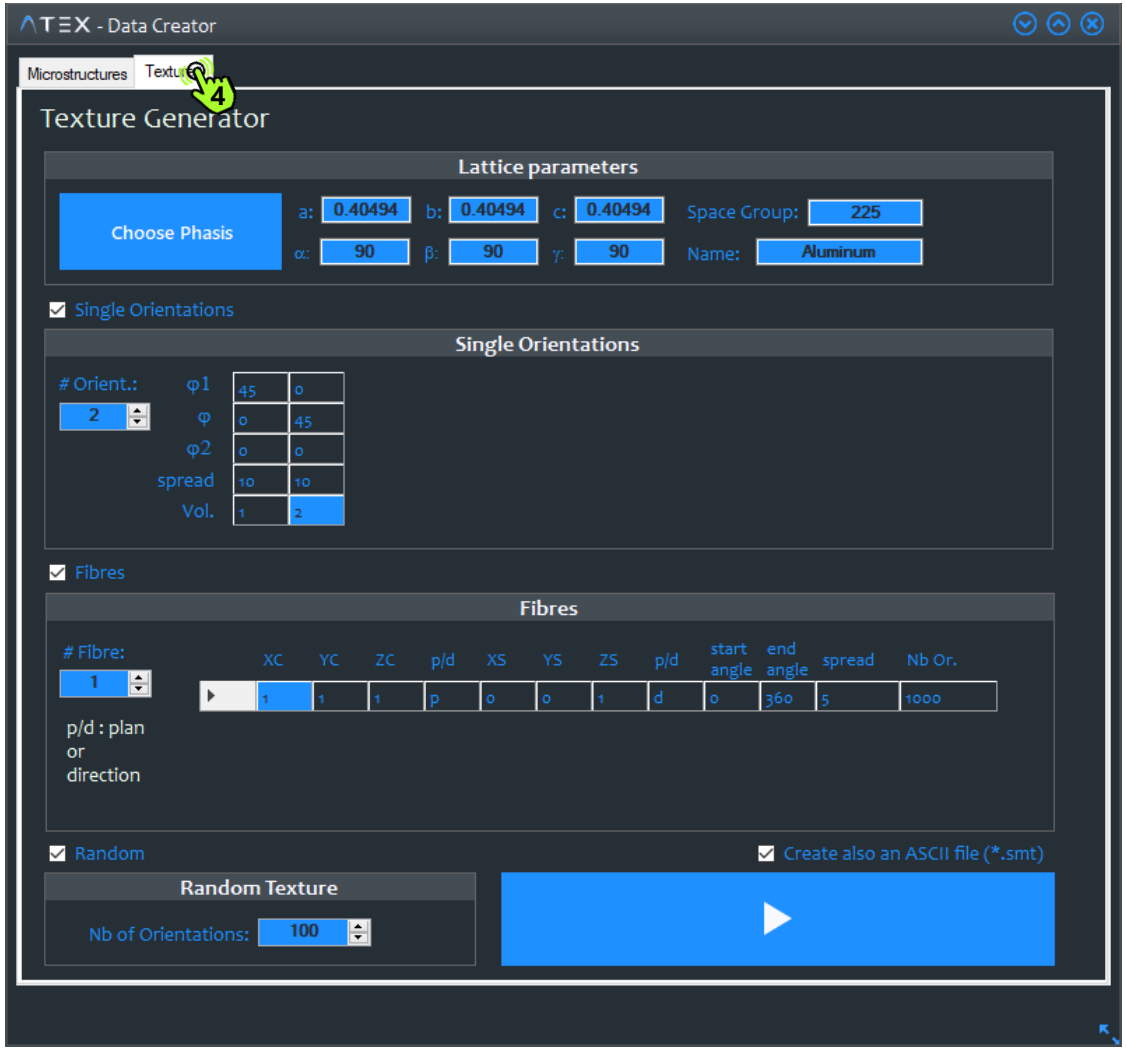
1. Input Data
   1. Generate textures
   2. X-Ray measurements
   3. Orientations Maps (EBSD)
2. Simulations (VPSC)
3. Simulations vs Experiments
   1. Ideal Orientations
   2. Correlation
4. Simulations On Orientations Maps

TUTORIAL Textures Simulation – Crystal Plasticity

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

→ Generate textures



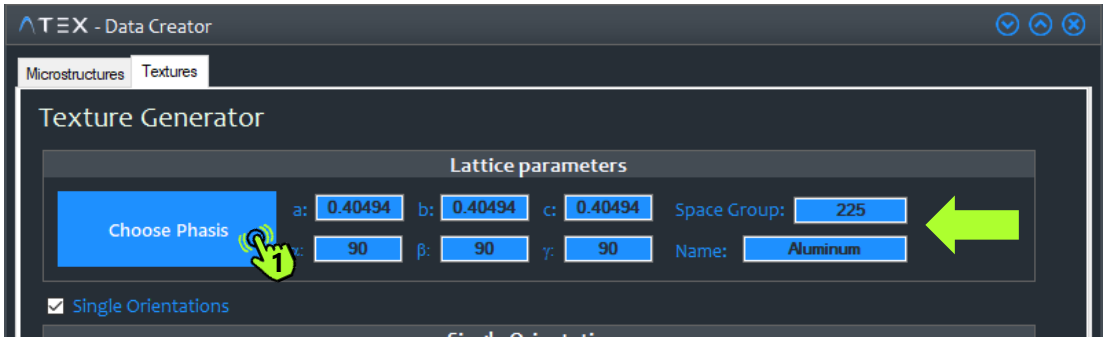


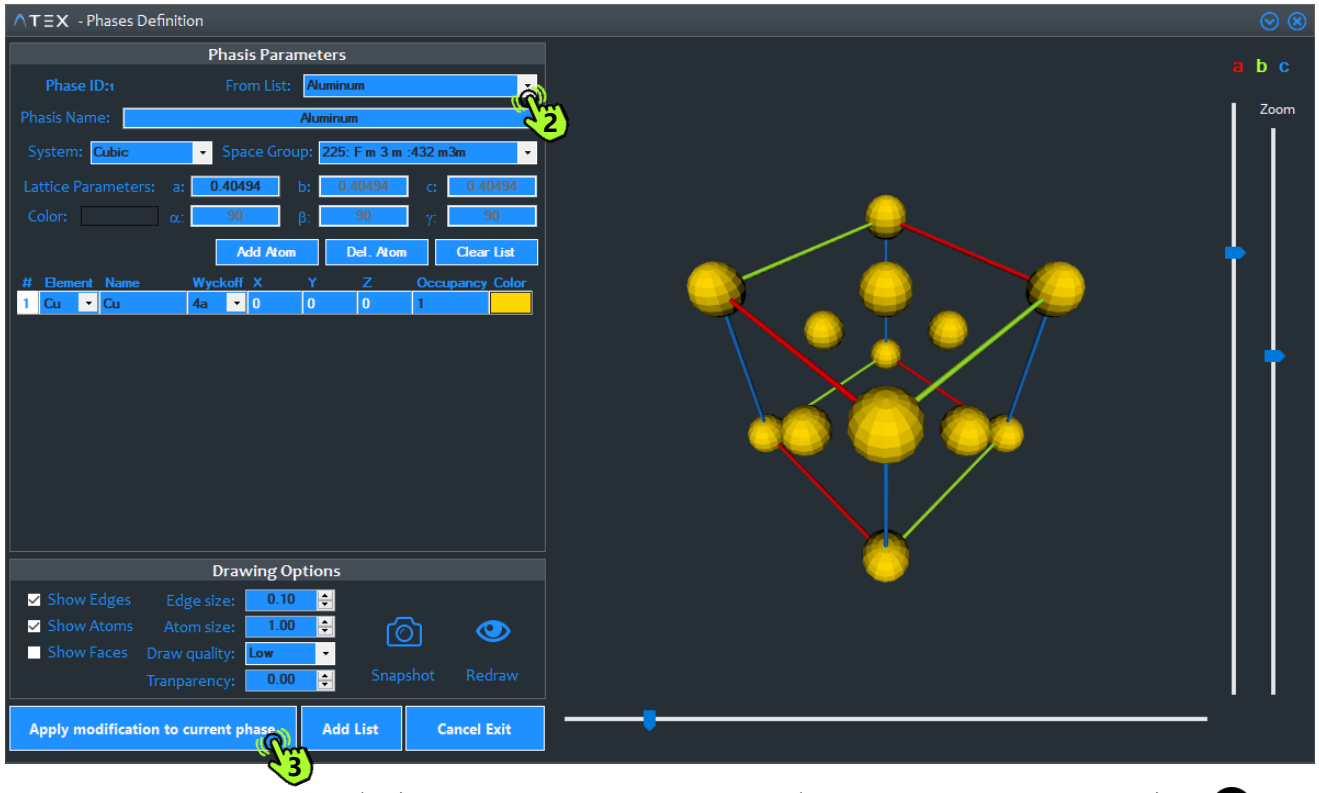
TUTORIAL Textures Simulation – Crystal Plasticity

→ 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





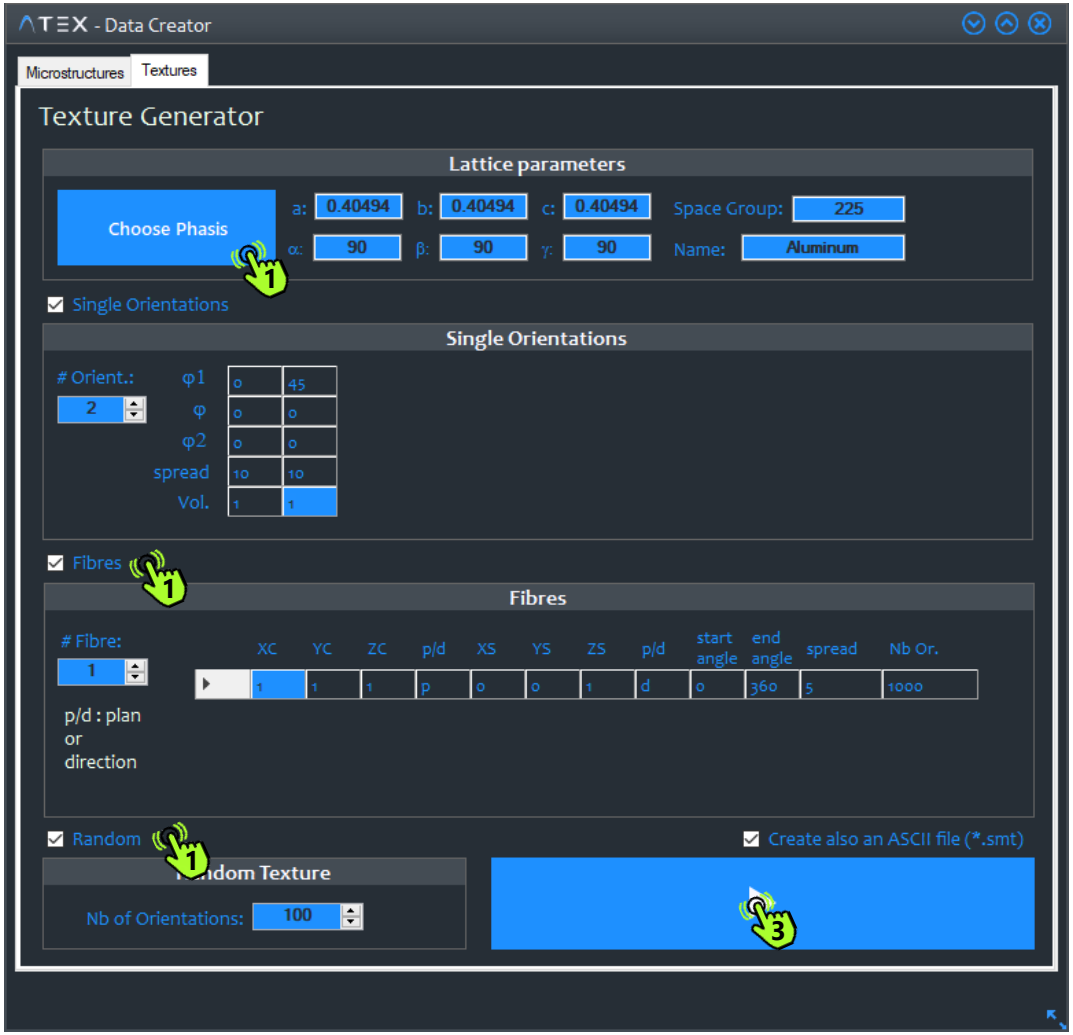
TUTORIAL Textures Simulation – Crystal Plasticity

→ Generate textures

1. Now choose the kind of orientations you want to add to your texture
   - Single Orient.
   - Fibre
   - Random
2. You can also mix them
3. 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
4. ATEX will ask you if you want to open your generated texture to plot it for instance, answer YES"



TUTORIAL Textures Simulation – Crystal Plasticity

→ Generate textures

1. 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 ←

2. 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

3. YOU NOW HAVE AN ORIENTATION LIST READY FOR THE SIMULATIONS

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

Content

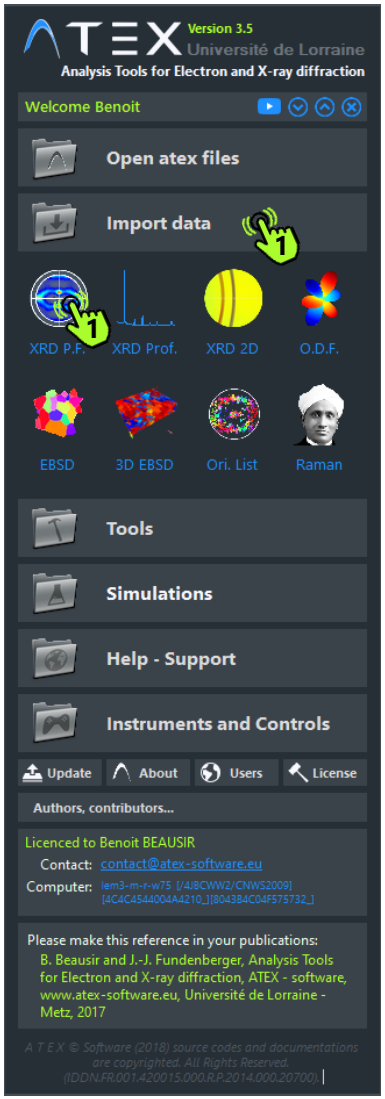
1. Input Data
    1. Generate textures
    2. X-Ray measurements
    3. Orientations Maps (EBSD)
2. Simulations (VPSC)
3. Simulations vs Experiments
    1. Ideal Orientations
    2. Correlation
4. Simulations On Orientations Maps

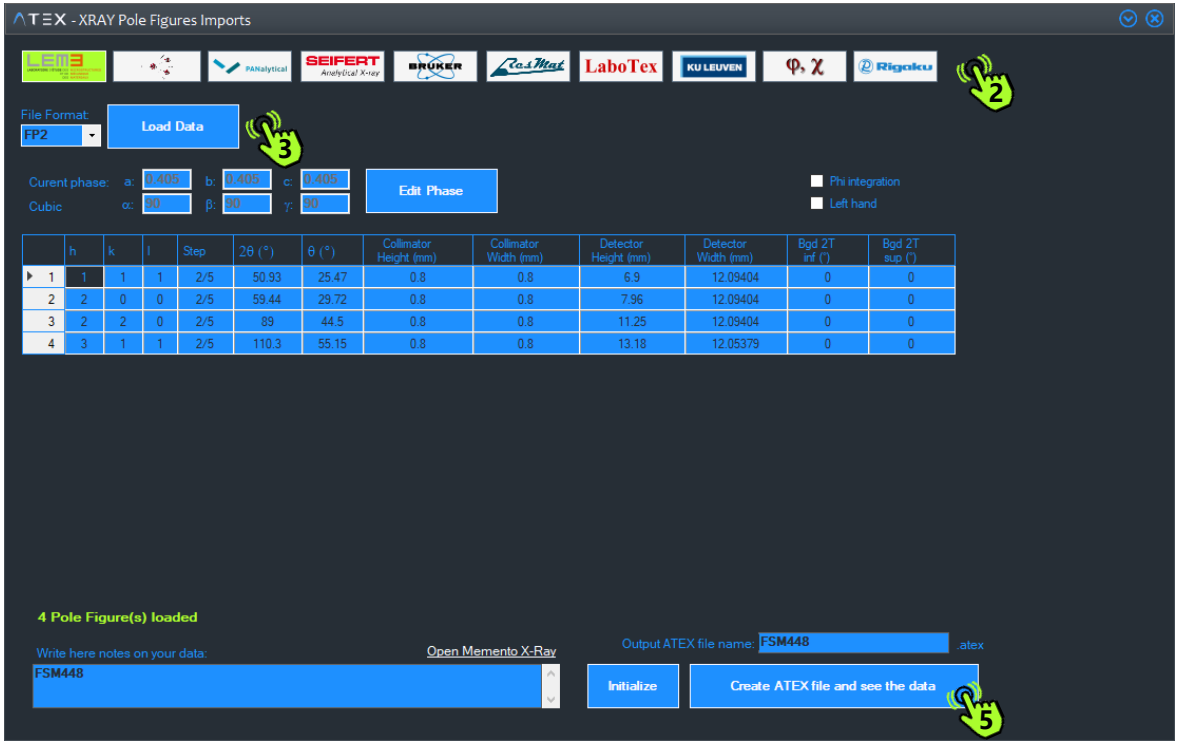
TUTORIAL Textures Simulation – Crystal Plasticity

→ 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





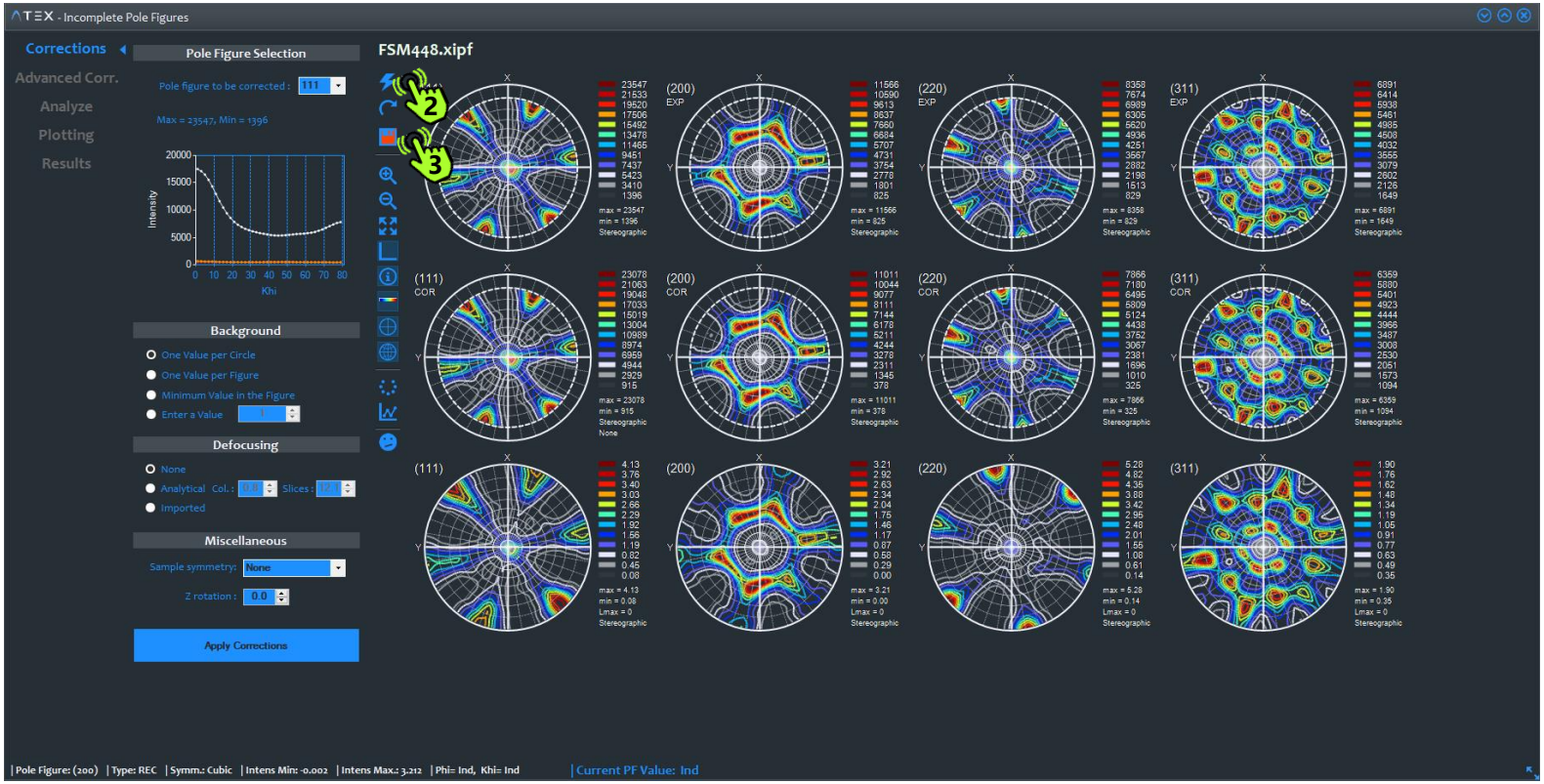
	h	k	l	Step	2θ (°)	θ (°)	Collimator Height (mm)	Collimator Width (mm)	Detector Height (mm)	Detector Width (mm)	Bgd 2T inf (°)	Bgd 2T sup (°)
1	1	1	1	2/5	50.93	25.47	0.8	0.8	6.9	12.09404	0	0
2	2	0	0	2/5	59.44	29.72	0.8	0.8	7.96	12.09404	0	0
3	2	2	0	2/5	89	44.5	0.8	0.8	11.25	12.09404	0	0
4	3	1	1	2/5	110.3	55.15	0.8	0.8	13.18	12.05379	0	0

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

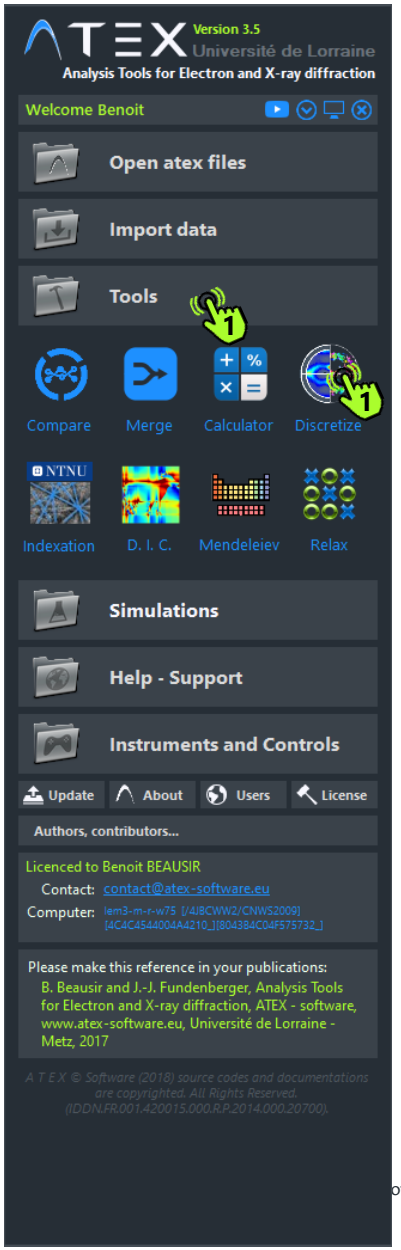


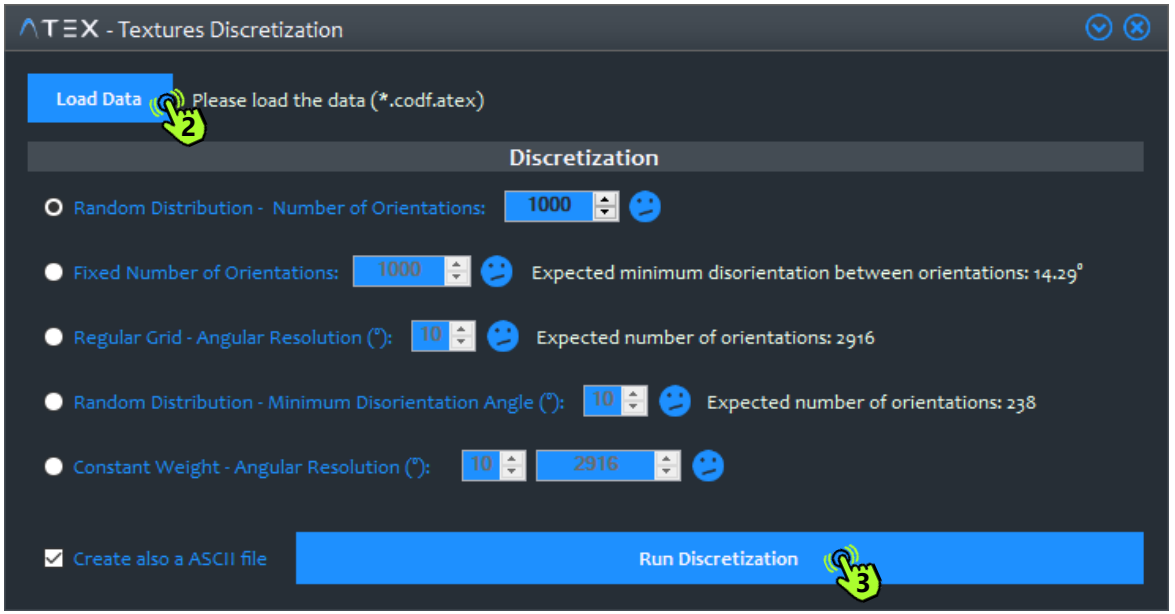
TUTORIAL Textures Simulation – Crystal Plasticity

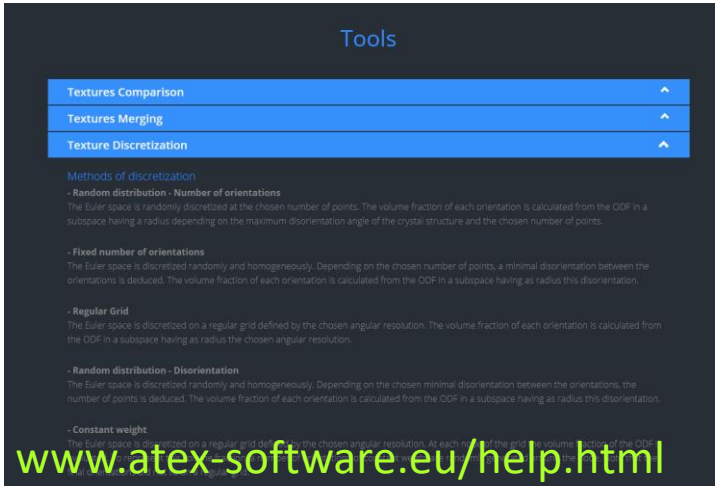
→ Discretize an ODF

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 "orli.atex" file containing the orientation list for the simulations





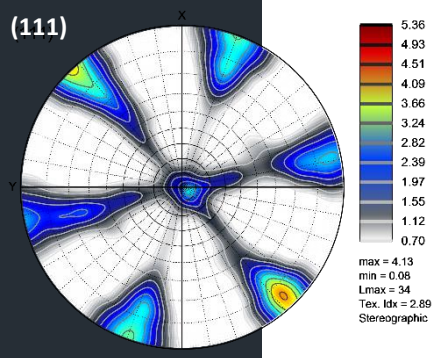
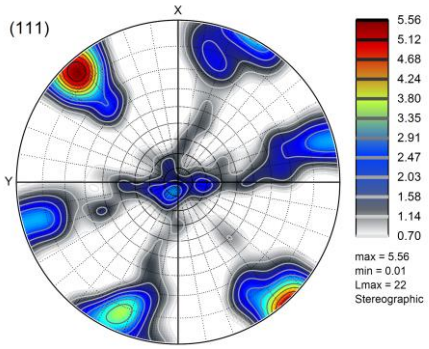
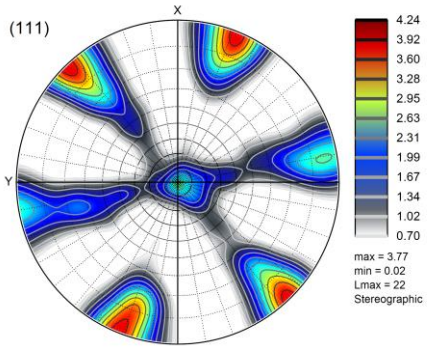
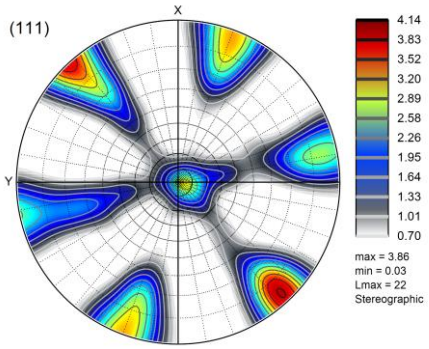
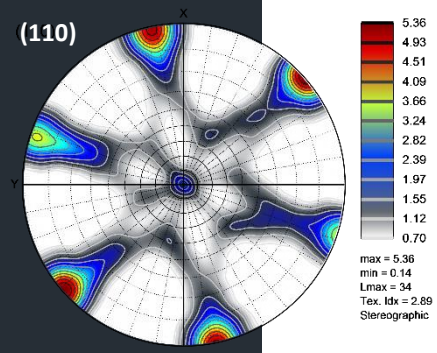
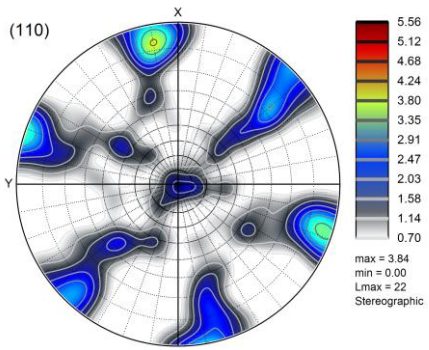
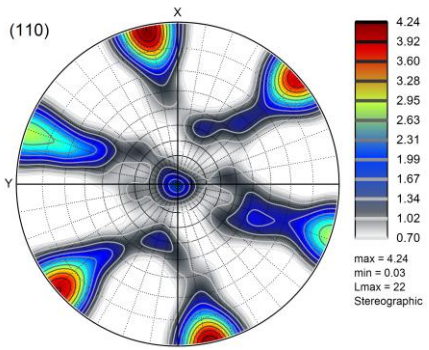
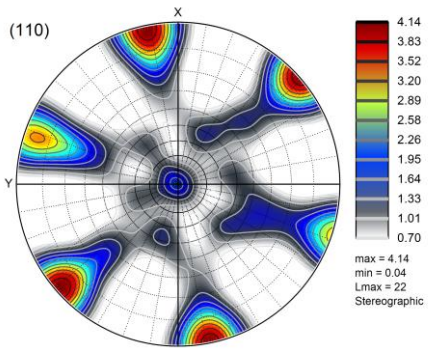


www.atex-software.eu/help.html

TUTORIAL Textures Simulation – Crystal Plasticity

→ Discretize an ODF

ODF discretized → ODF re-calculated

X-Ray measurements	100 Orientations	1000 Orientations	10000 Orientations
			
			

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

TUTORIAL Textures Simulation – Crystal Plasticity

→ 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:

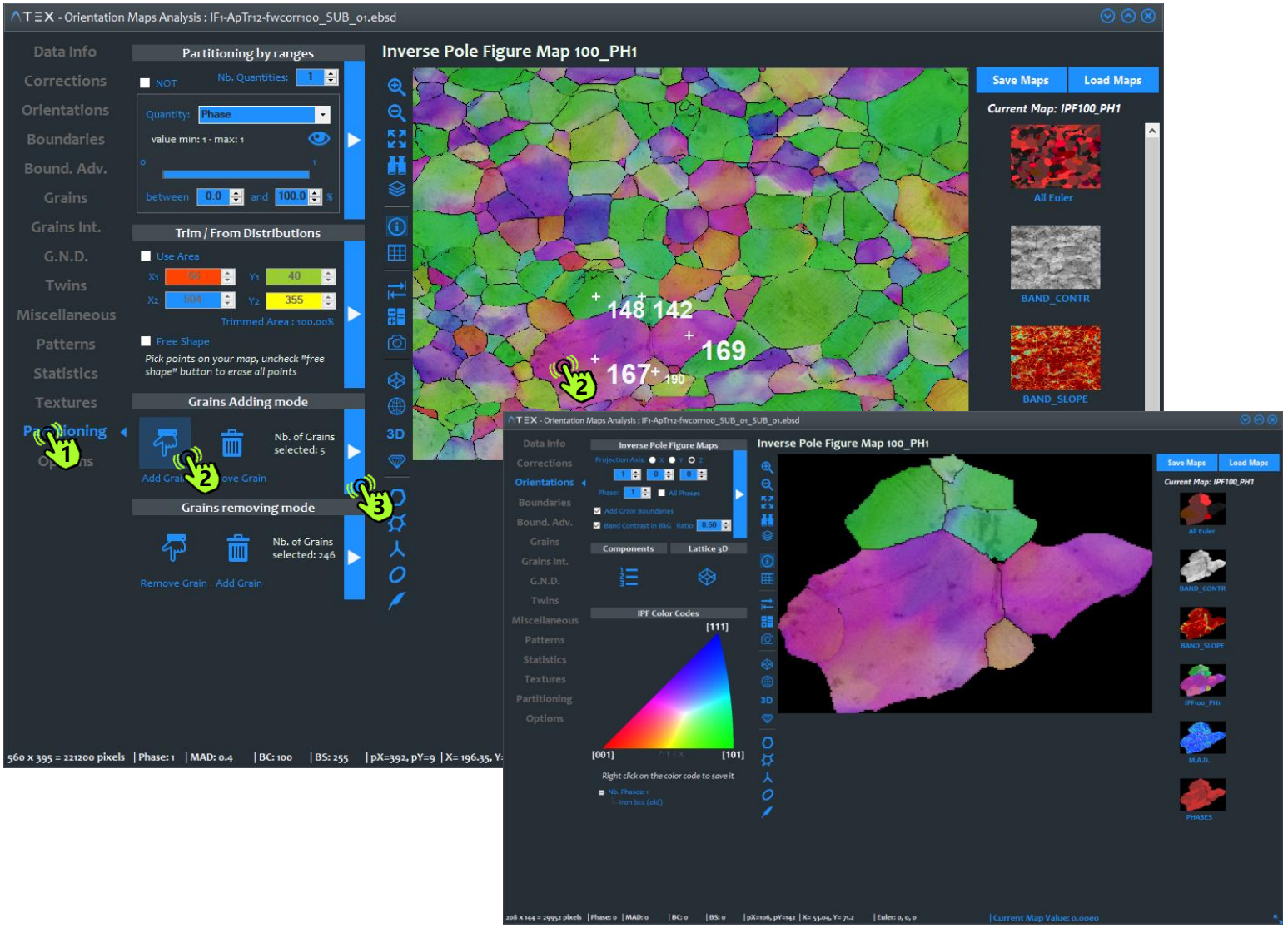
   1 – SMT and TXT
   2 – ORLI.ATEX
   3 – CTF
3. Question: From what my orientation list should be composed ?

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

TUTORIAL Textures Simulation – Crystal Plasticity

→ 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

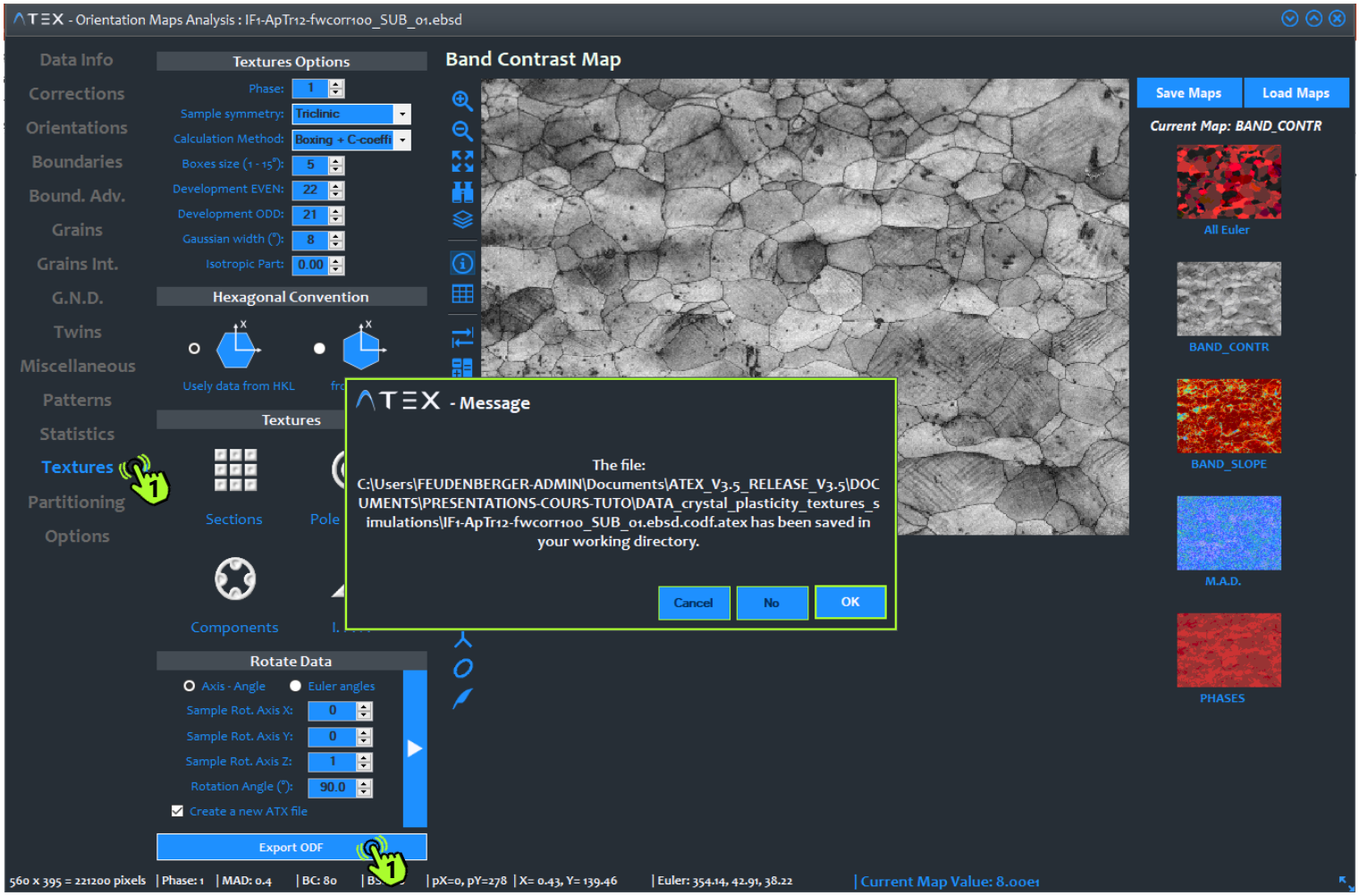


TUTORIAL Textures Simulation – Crystal Plasticity

→ EBSD -> ODF -> Discretization

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

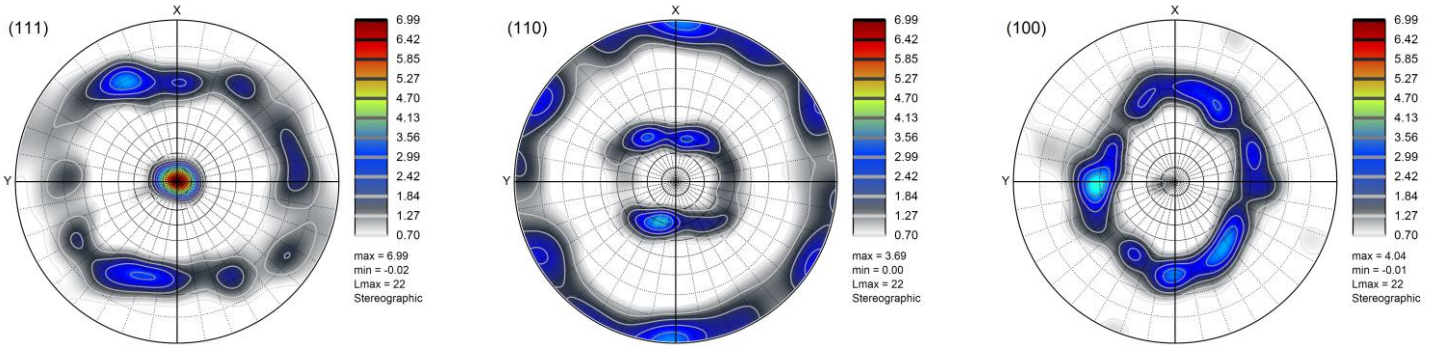
1. Go on tab “TEXTURES” and just export your ODF by clicking on the “Export ODF” button
2. See the slide “Discretization” to prepare your data for simulation



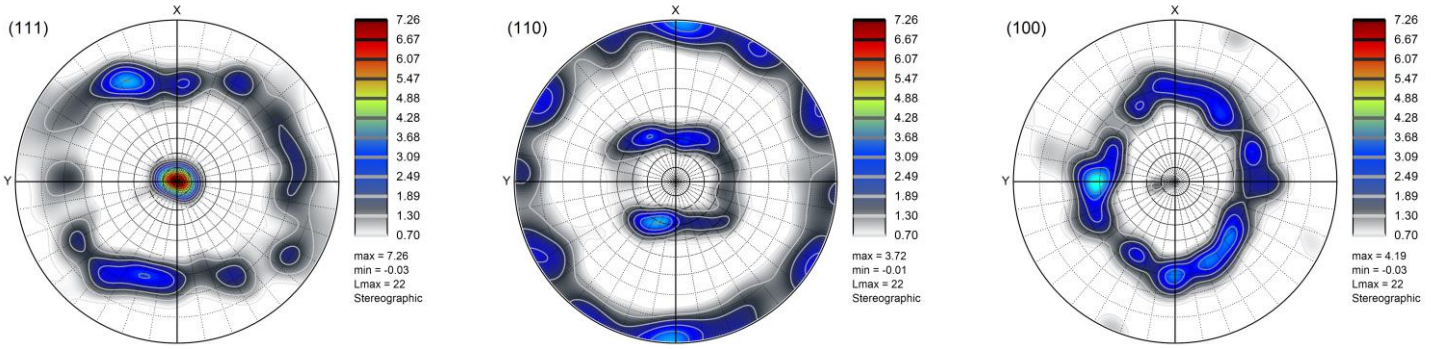
TUTORIAL Textures Simulation – Crystal Plasticity

→ Examples of orientation list with the different methods

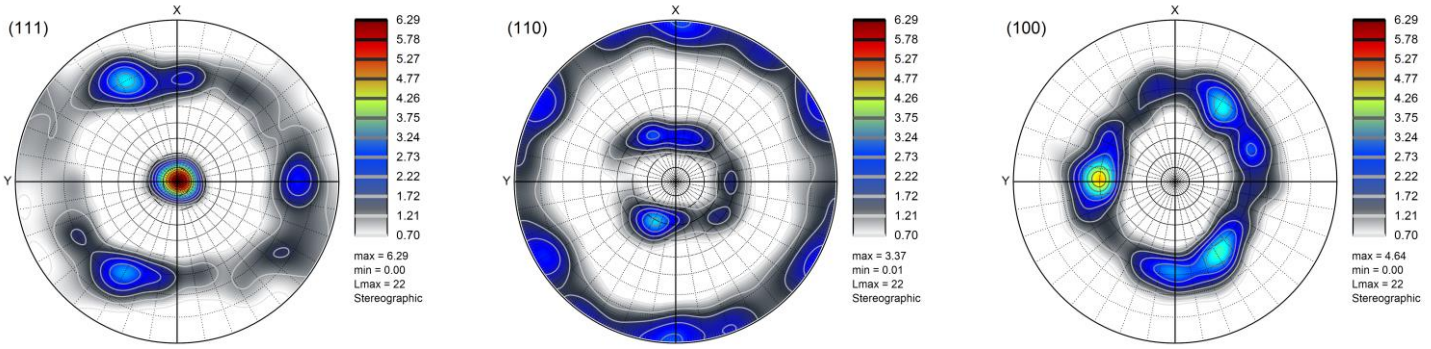
EBSD → full texture ODF calculated from all the 221000pixels



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



EBSD → ODF → Discretization 1000 orientations



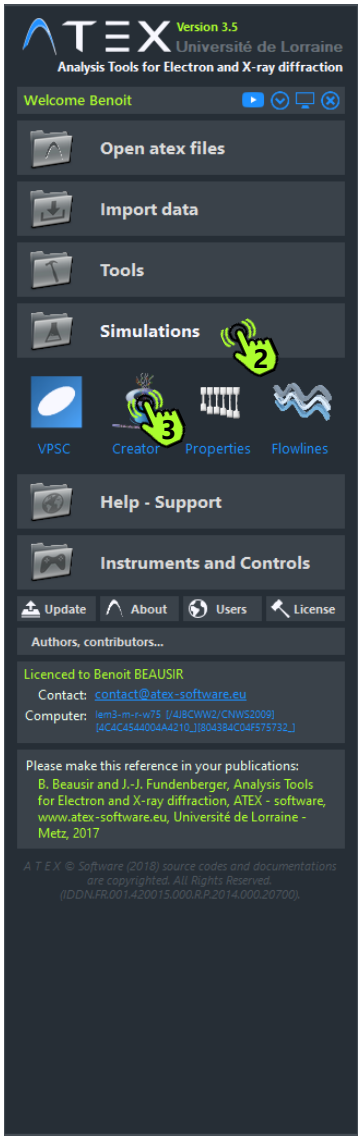
1. Here is written the list of what to do
2. This hand tells you where to click

Content

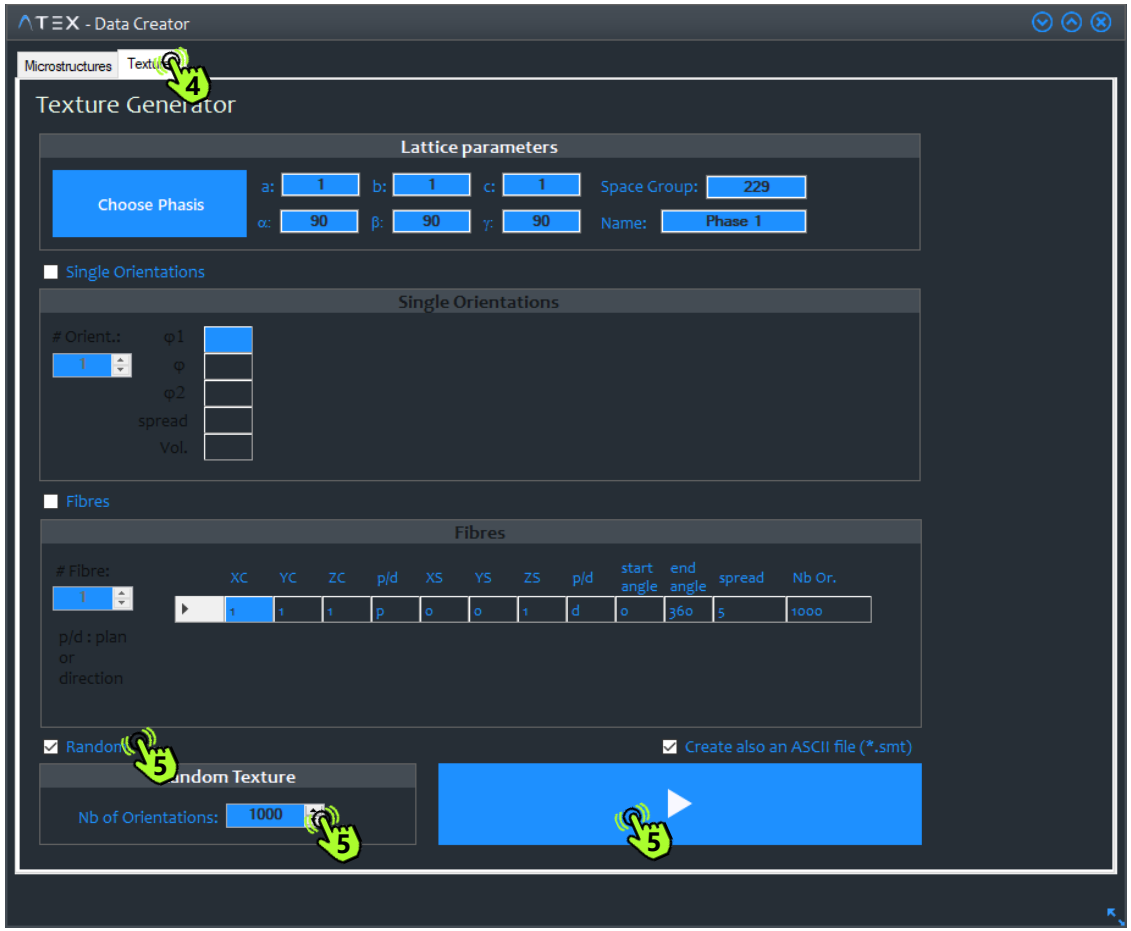
1. Input Data
   1. Generate textures
   2. X-Ray measurements
   3. Orientations Maps (EBSD)
2. Simulations (VPSC)
3. Simulations vs Experiments
   1. Ideal Orientations
   2. Correlation
4. Simulations On Orientations Maps

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

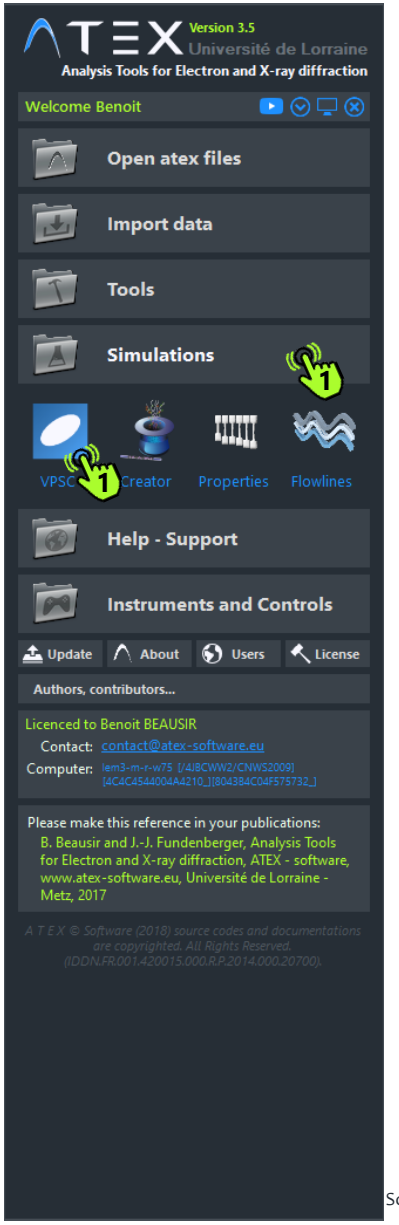
Check the generated texture

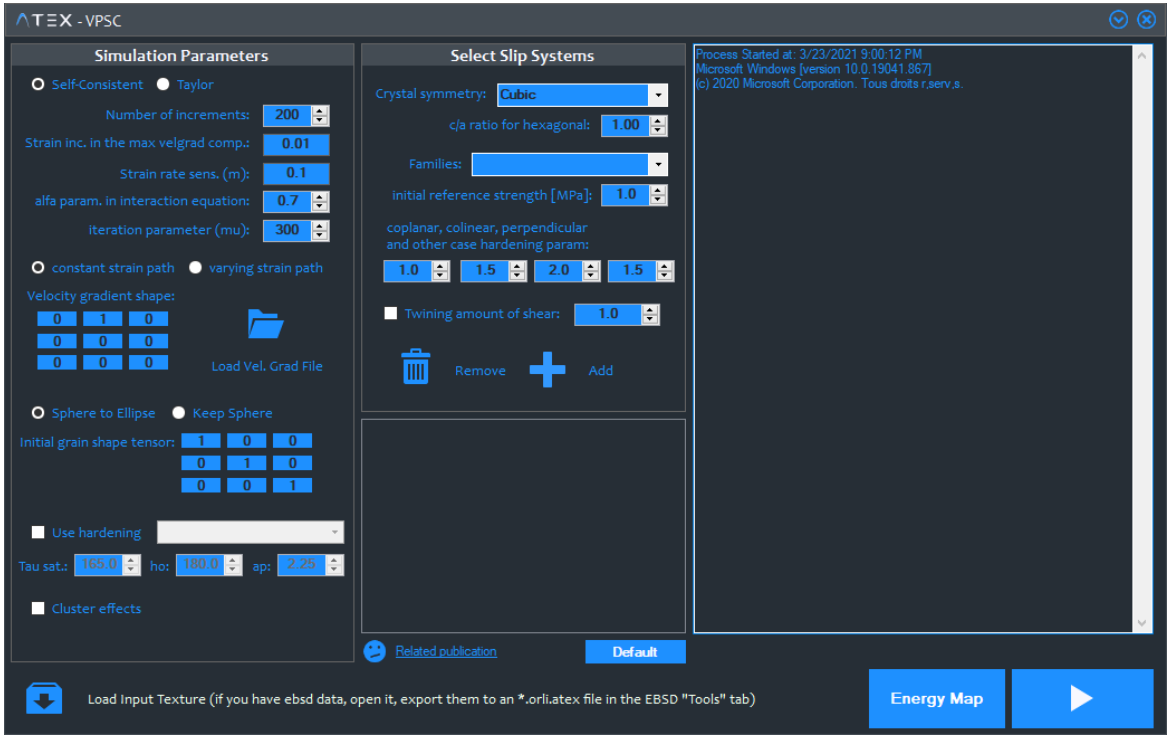
1000 random orientations

TUTORIAL Textures Simulation – Crystal Plasticity

→ Simulations (VPSC)

1. Select the "SIMULATIONS" tab and click on VPSC button to open the VPSC module

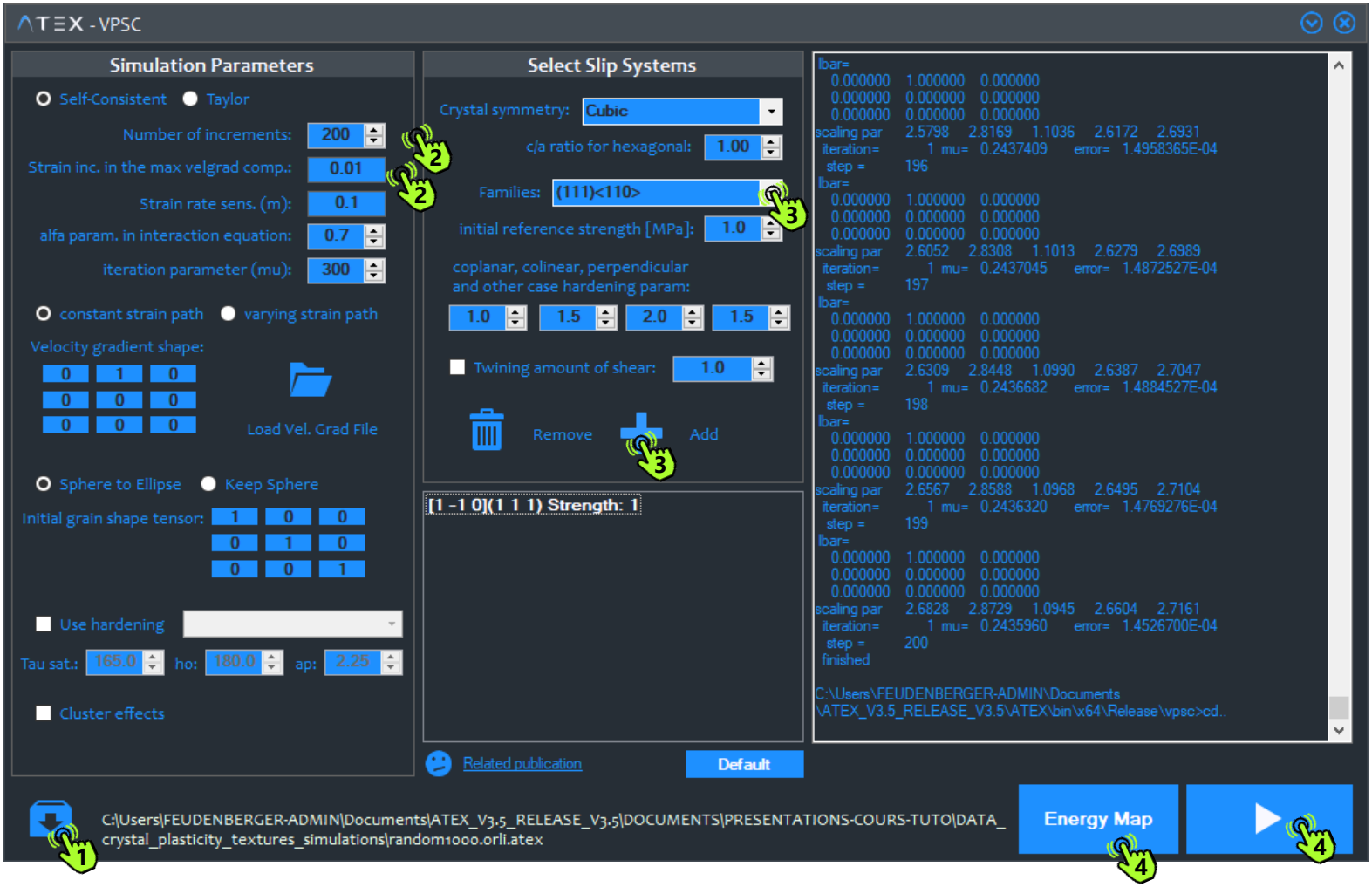




TUTORIAL Textures Simulation – Crystal Plasticity

→ 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,

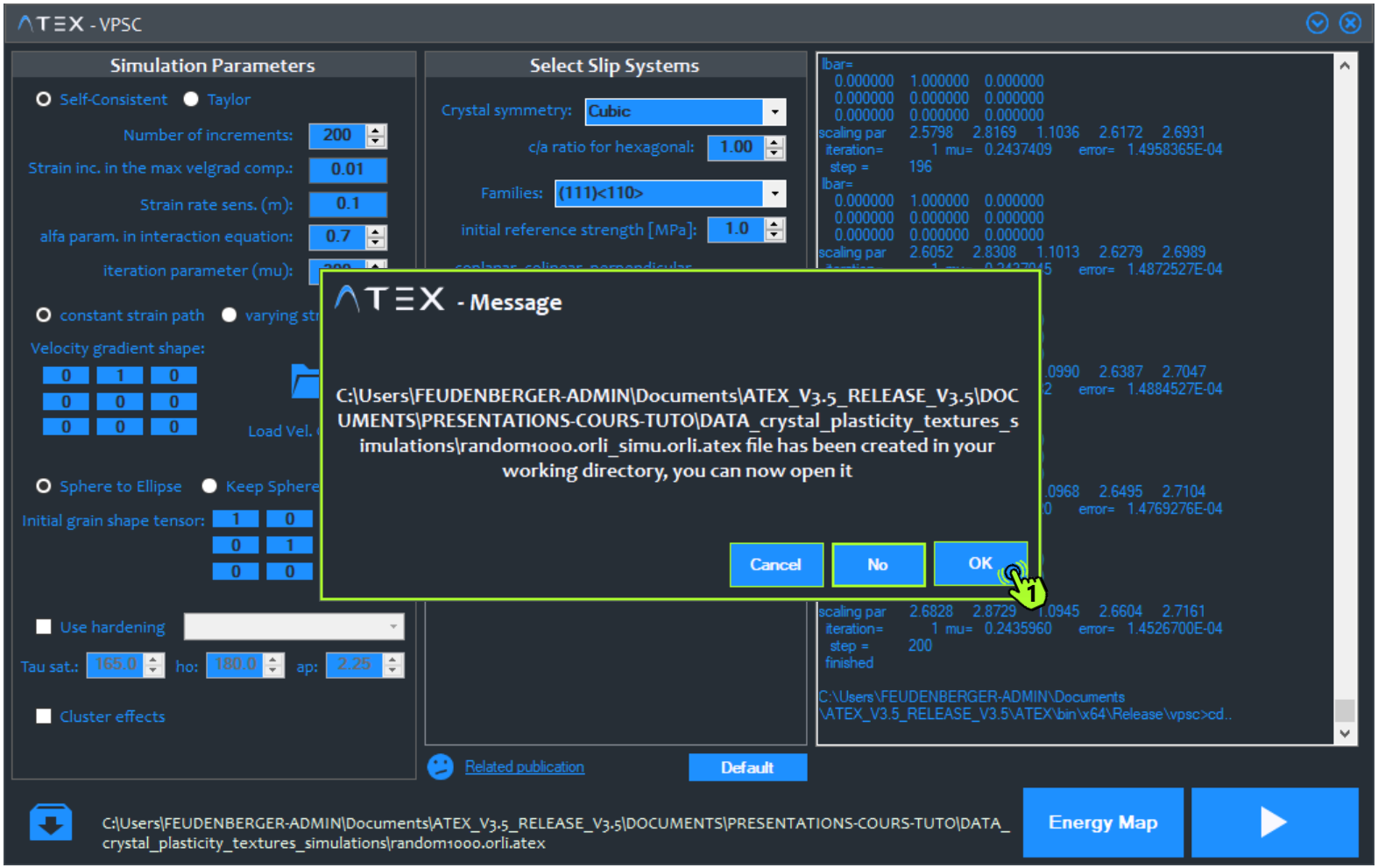


Shear = 2, Aluminium

TUTORIAL Textures Simulation – Crystal Plasticity

→ Simulations (VPSC)

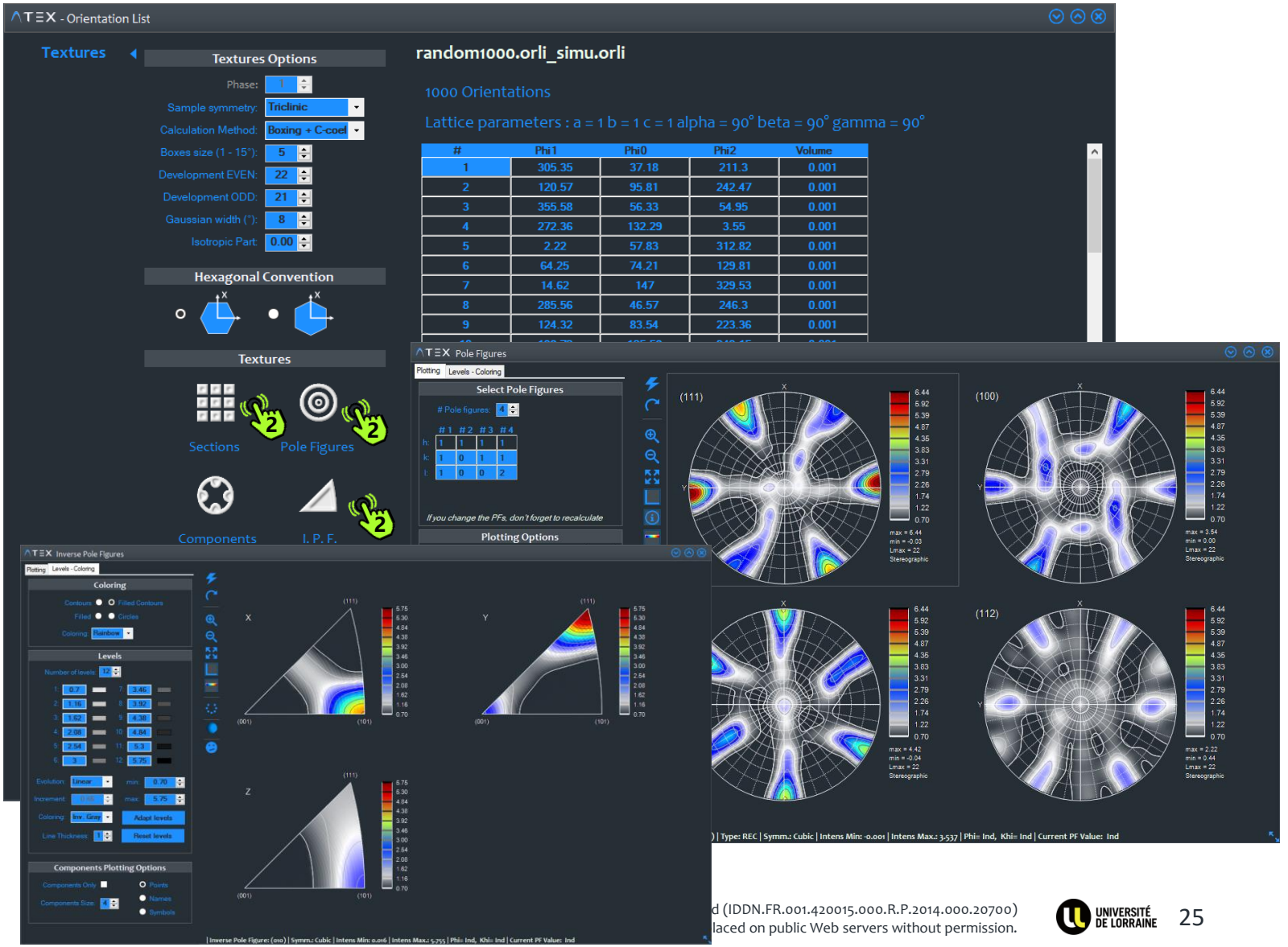
1. Once the simulations are finished an new file *_simu.orli.atex is created in your working directory, answer OK to open it



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

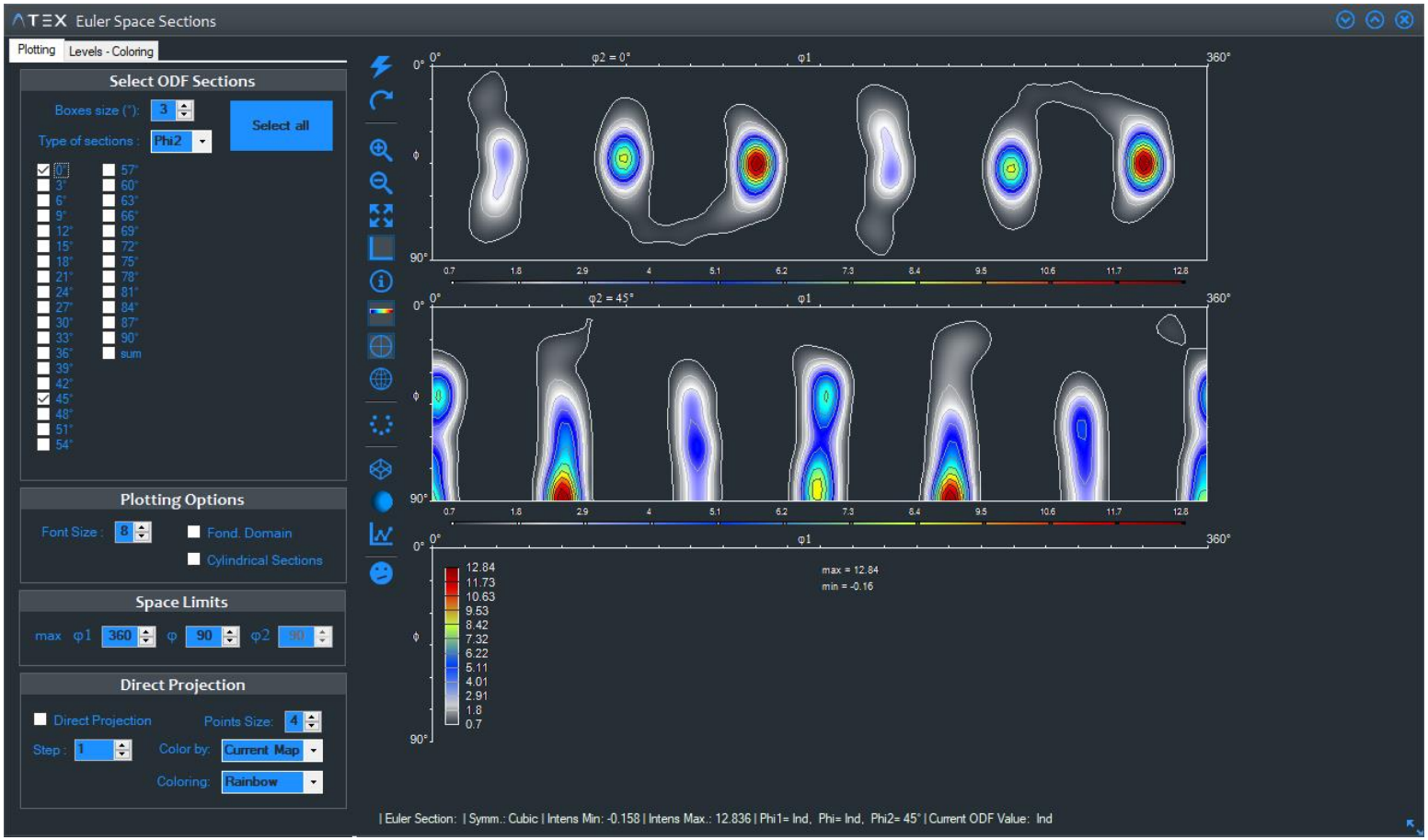


TUTORIAL Textures Simulation – Crystal Plasticity

→ Simulations (VPSC)

1. Euler space Sections of the simulated texture, here phi2=0° and 45°

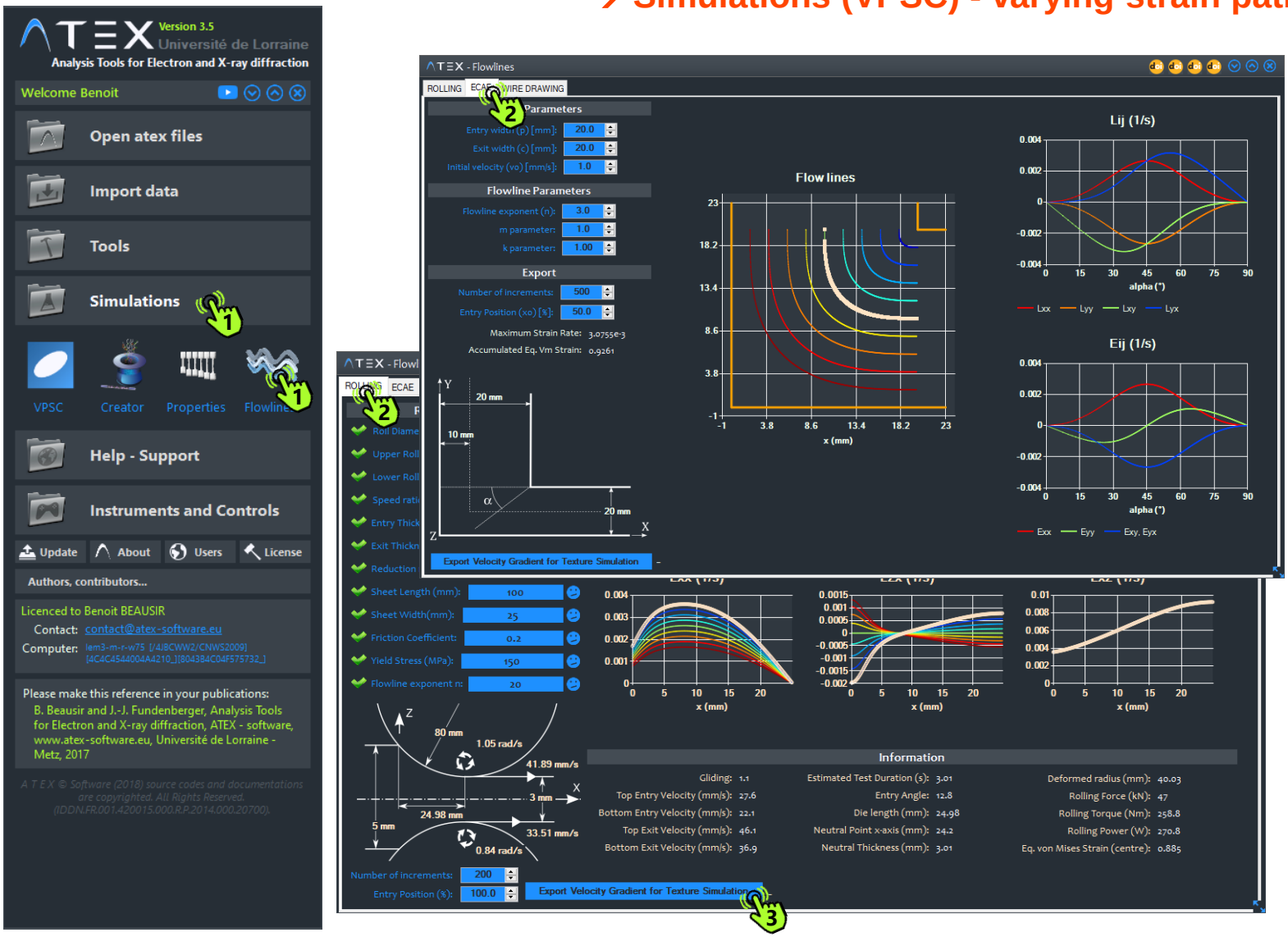
   Typical representative sections cubic materials under simple shear



TUTORIAL Textures Simulation – Crystal Plasticity

→ Simulations (VPSC) - varying strain path

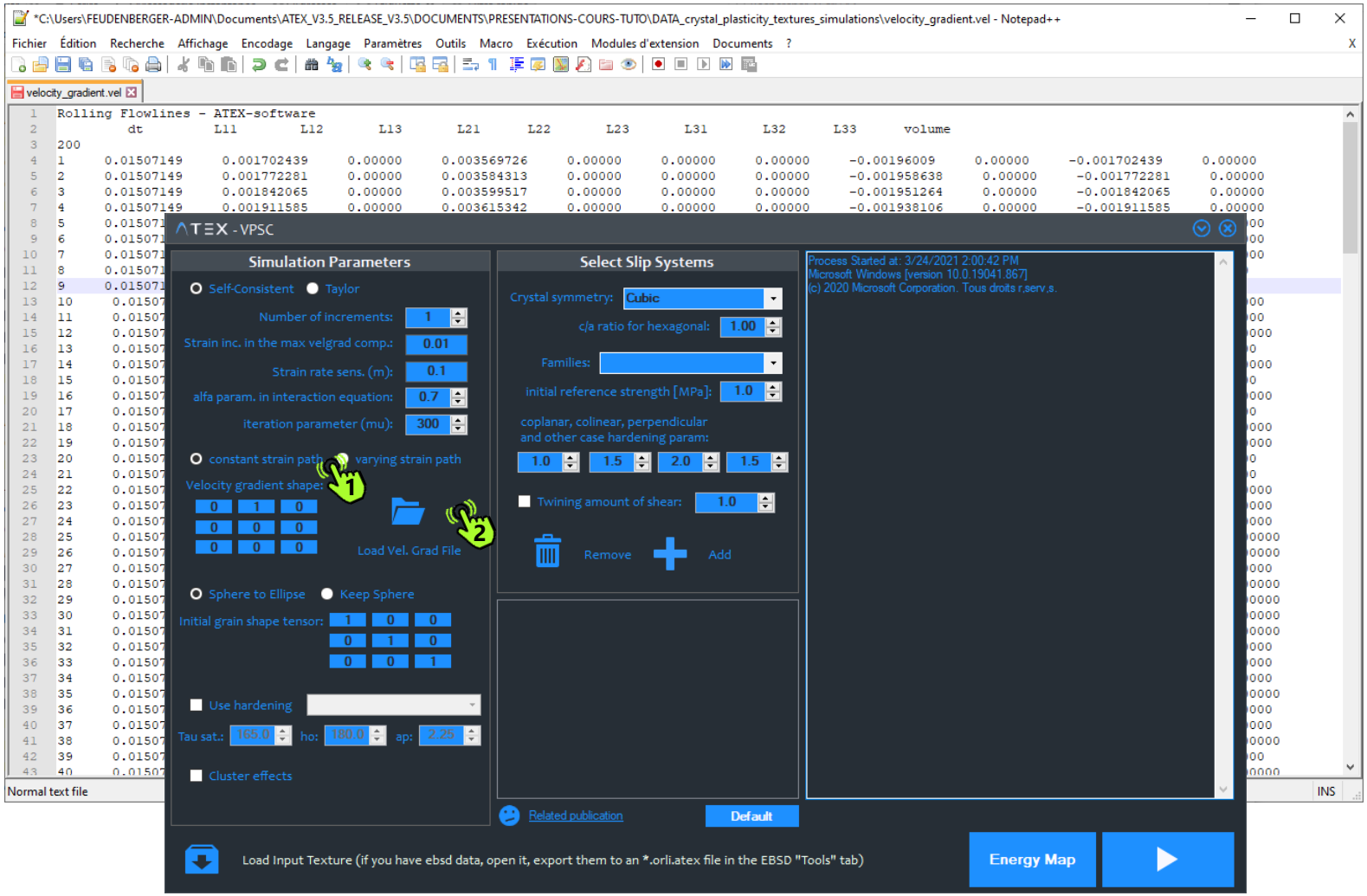
1. Select the "SIMULATIONS" tab and click on "Flowlines" button to open corresponding module
2. Select either ECAP or ROLLING tab
3. Set your parameters and click on "Export velocity gradient…" button



TUTORIAL Textures Simulation – Crystal Plasticity

→ Simulations (VPSC) - varying strain path

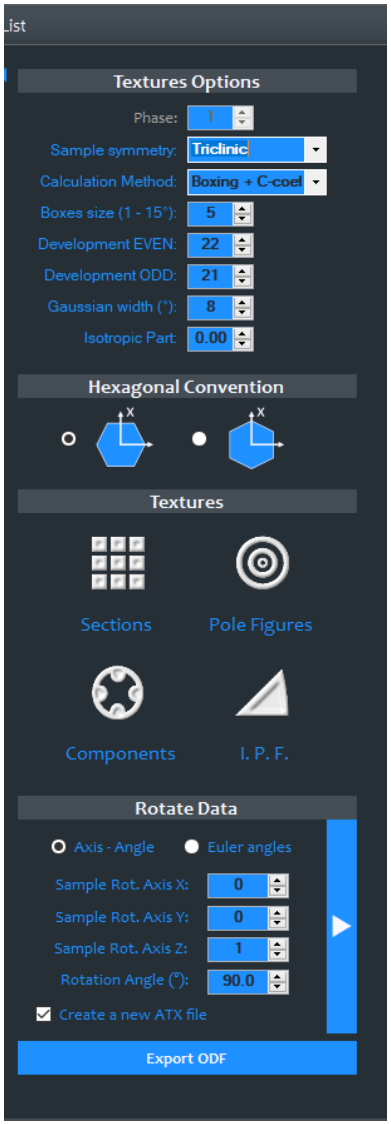
1. Select “varying strain path”
2. Choose your *.vel” file

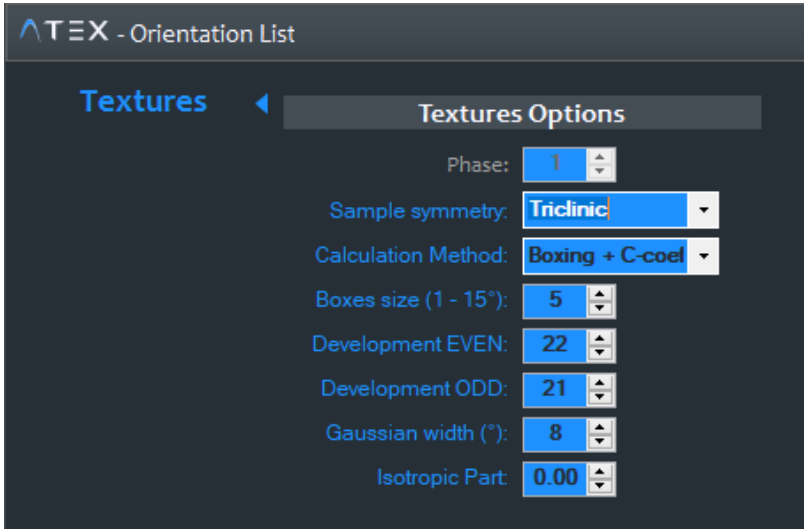


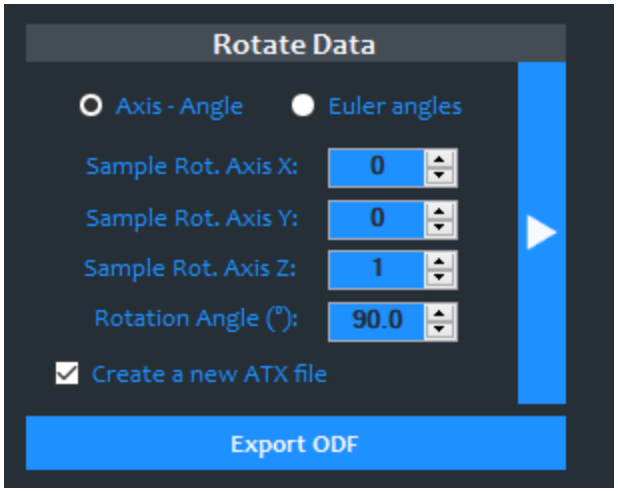
TUTORIAL Textures Simulation – Crystal Plasticity

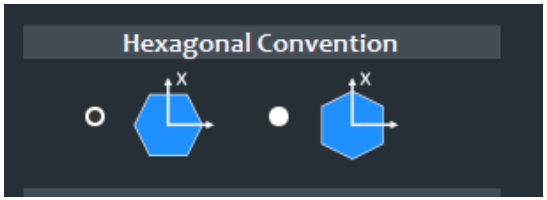
→ Texture calculation Options

1. Textures calculation options





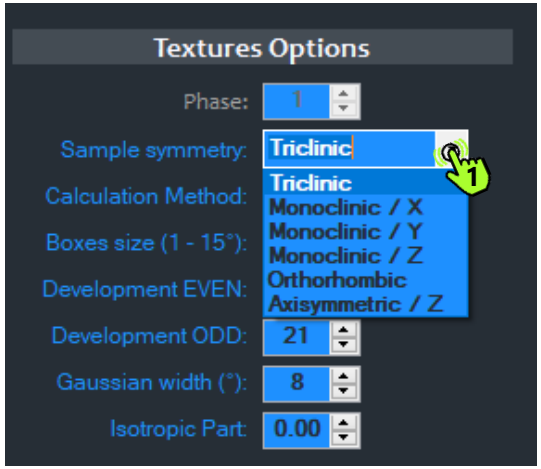


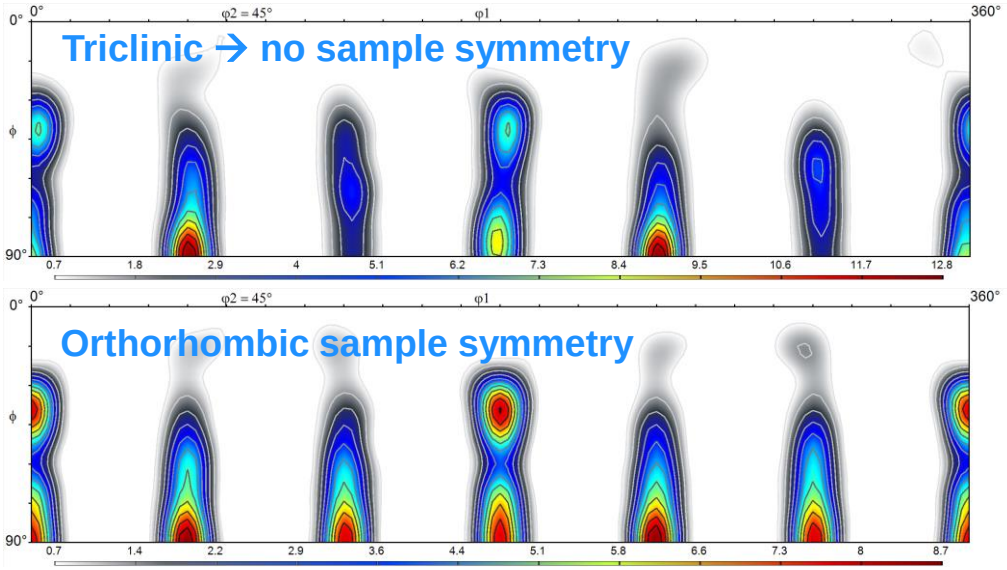


TUTORIAL Textures Simulation – Crystal Plasticity

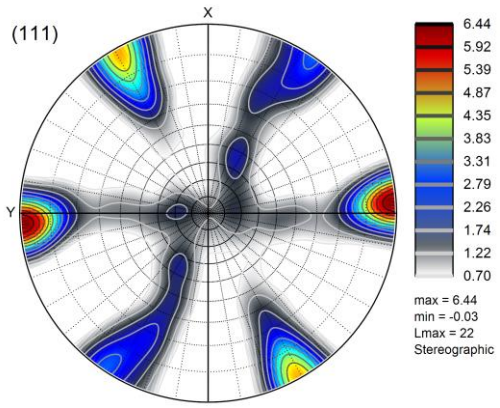
→ Texture calculation Options, Sample Symmetries

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

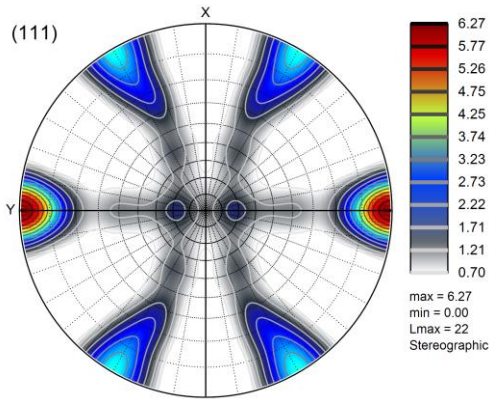




Triclinic → no sample symmetry



Orthorhombic sample symmetry



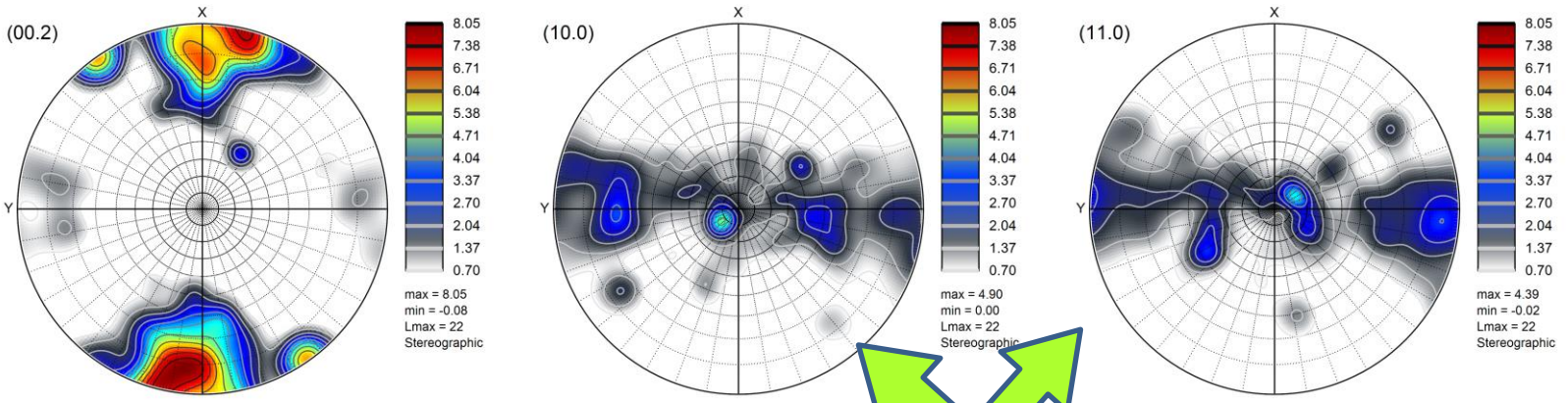
TUTORIAL Textures Simulation – Crystal Plasticity

→ Texture calculation Options, Sample Symmetries

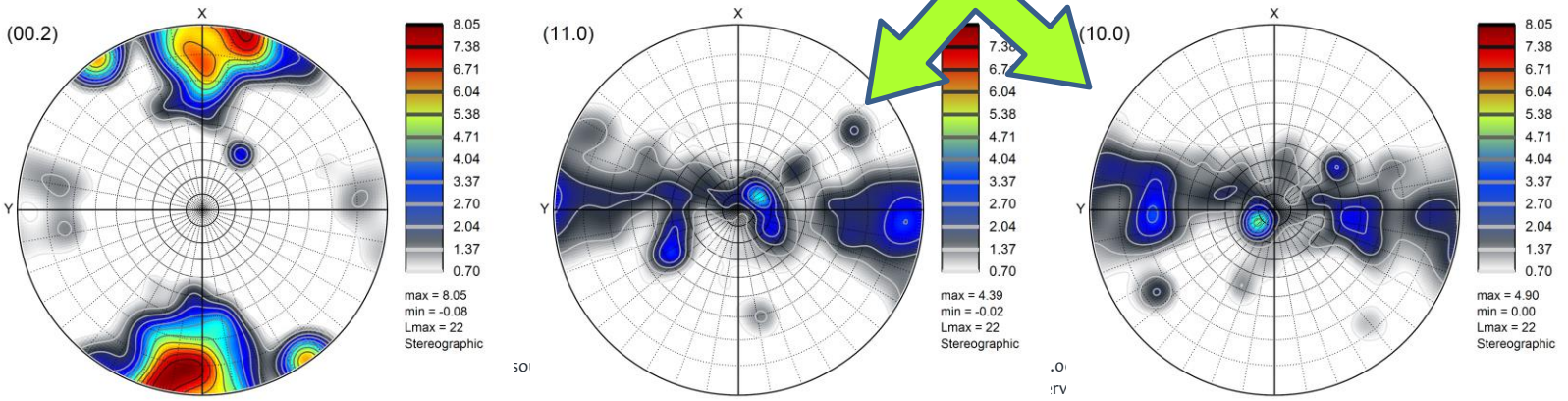
1. Be careful about the Hexagonal Convention

ROTATION by 30° around the c-axis (phi2=phi2+30°)

Convention x // a



Convention y // a



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

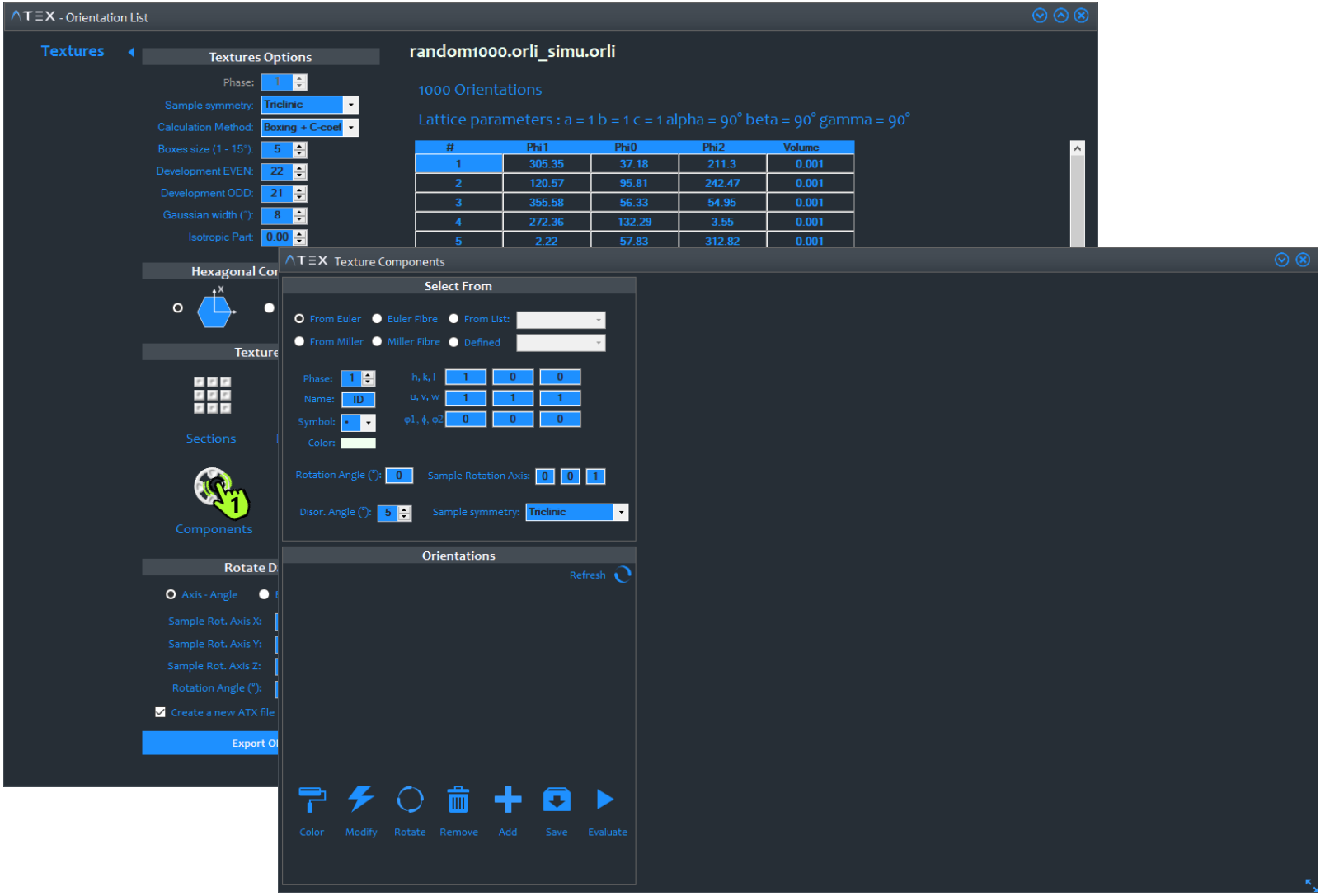
Content

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

TUTORIAL Textures Simulation – Crystal Plasticity

→ Ideal (stable) orientations

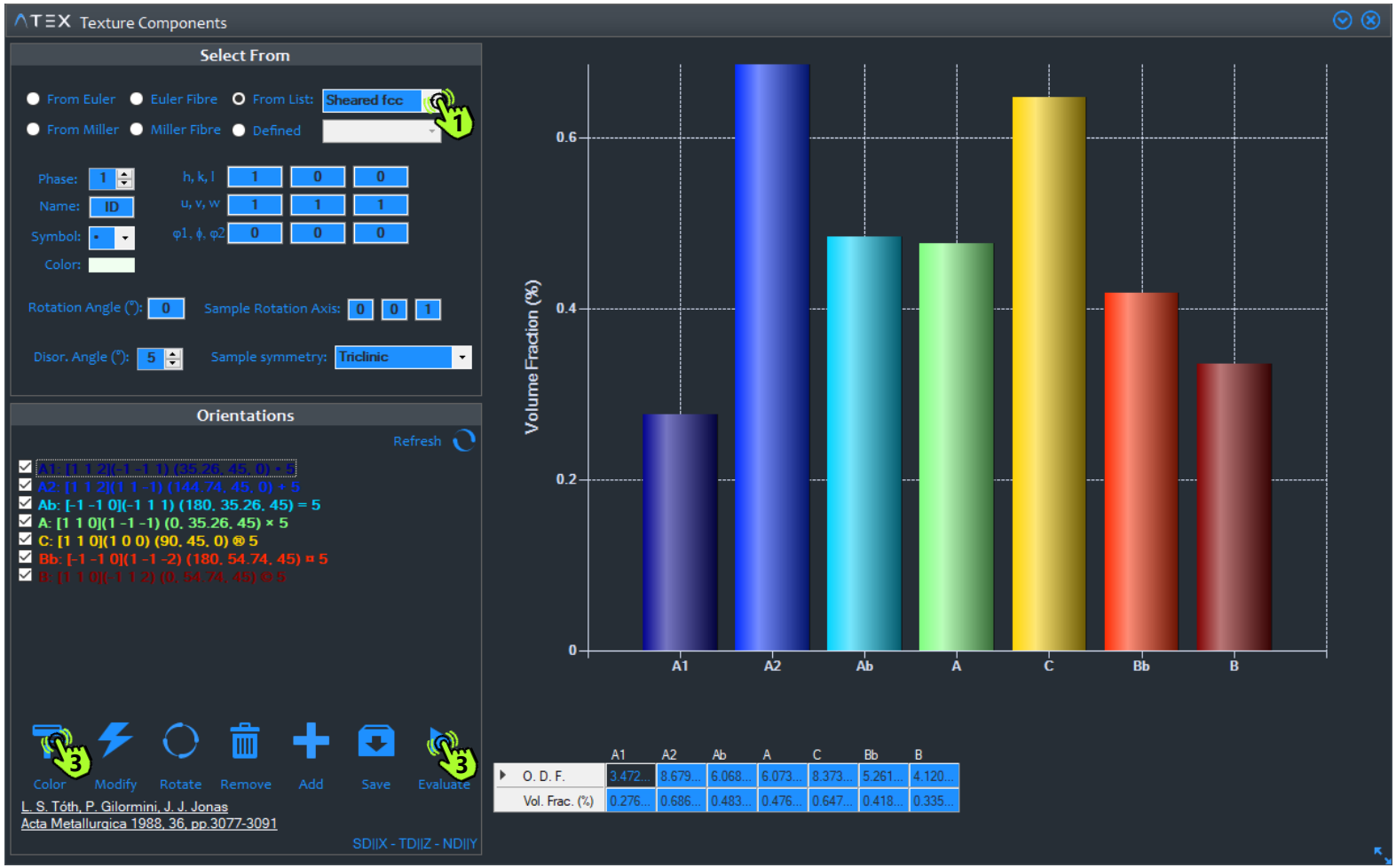
1. From the ORLI module, click the "COMPONENTS" button to open the TEXTURE COMPONENTS calculation module



TUTORIAL Textures Simulation – Crystal Plasticity

→ Ideal (stable) orientations

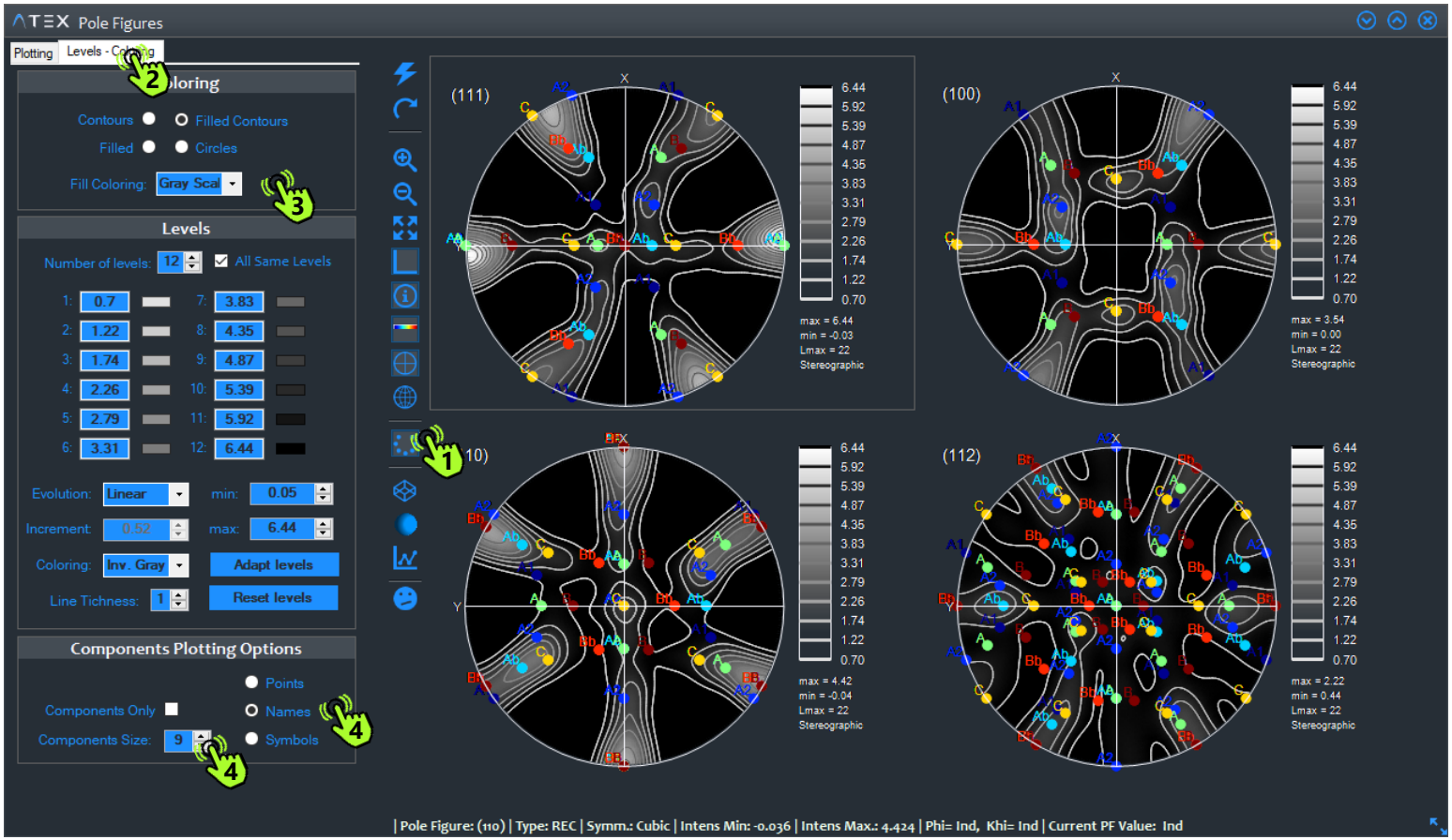
1. Select the components you want to know the volume fractions
2. Here the ideal orientations for fcc crystals under simple shear
3. Click on the "color" button and then on the "evaluate" button



TUTORIAL Textures Simulation – Crystal Plasticity

→ 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

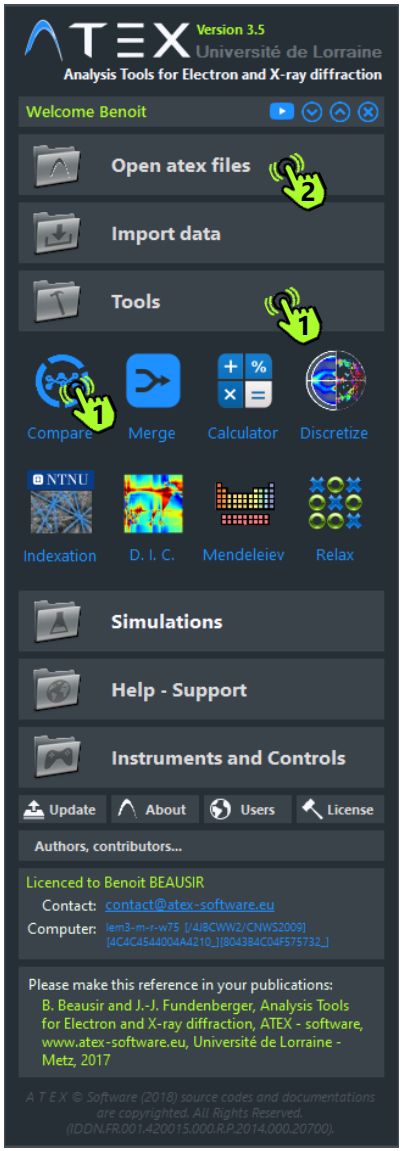
Content

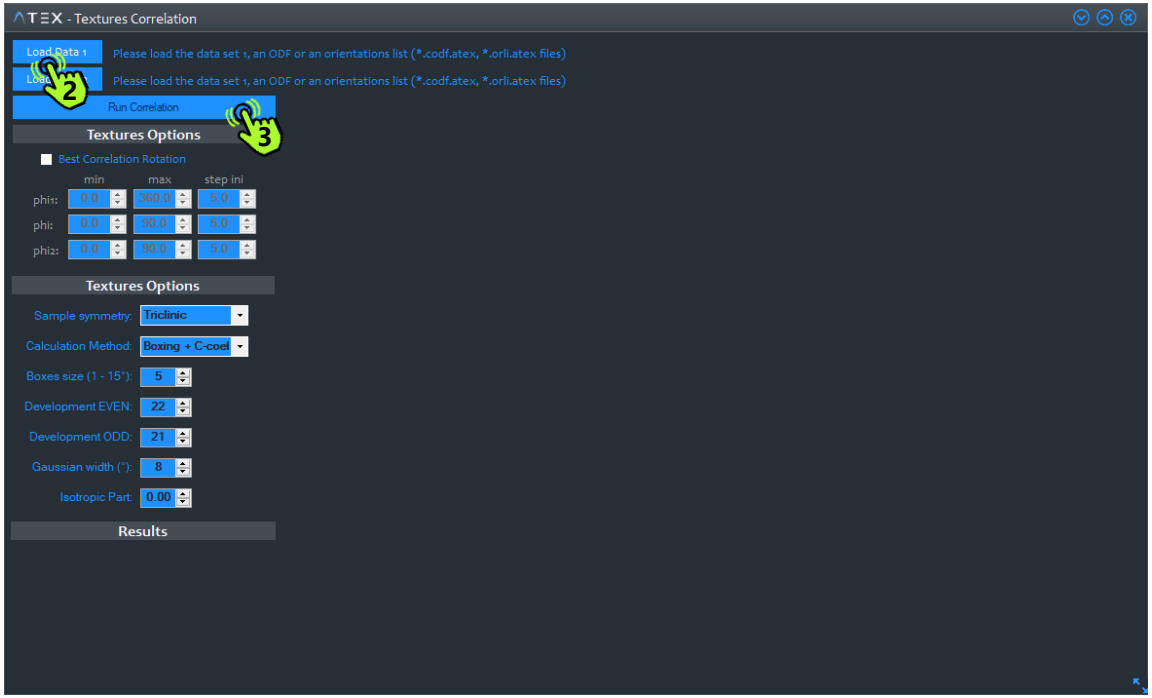
1. Input Data
   1. Generate textures
   2. X-Ray measurements
   3. Orientations Maps (EBSD)
2. Simulations (VPSC)
3. Simulations vs Experiments
   1. Ideal Orientations
   2. Correlation
4. Simulations On Orientations Maps

TUTORIAL Textures Simulation – Crystal Plasticity

→ 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

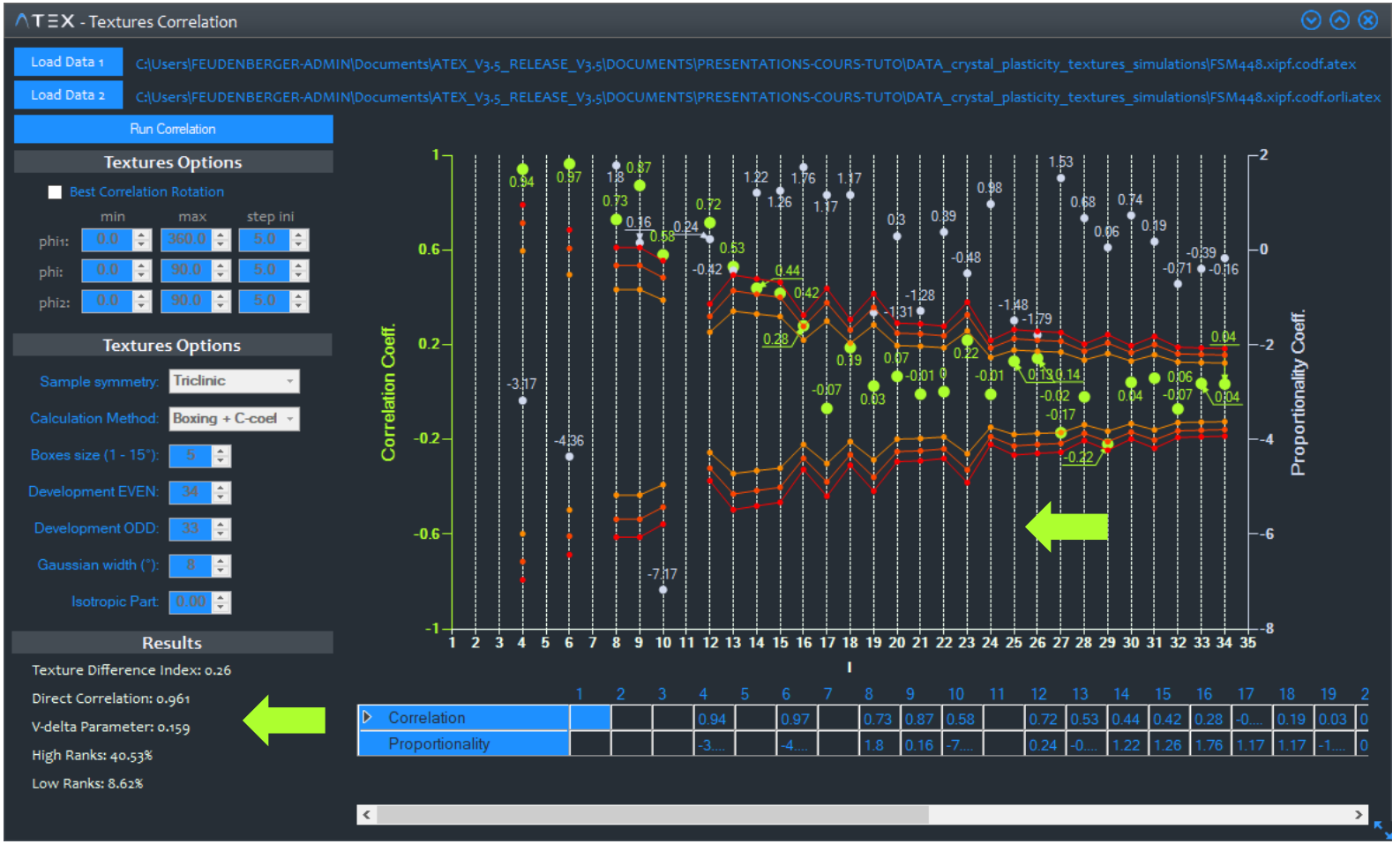




TUTORIAL Textures Simulation – Crystal Plasticity

→ Correlation

1. The results appears…



→ Correlation

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 t0 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
2. This hand tells you where to click

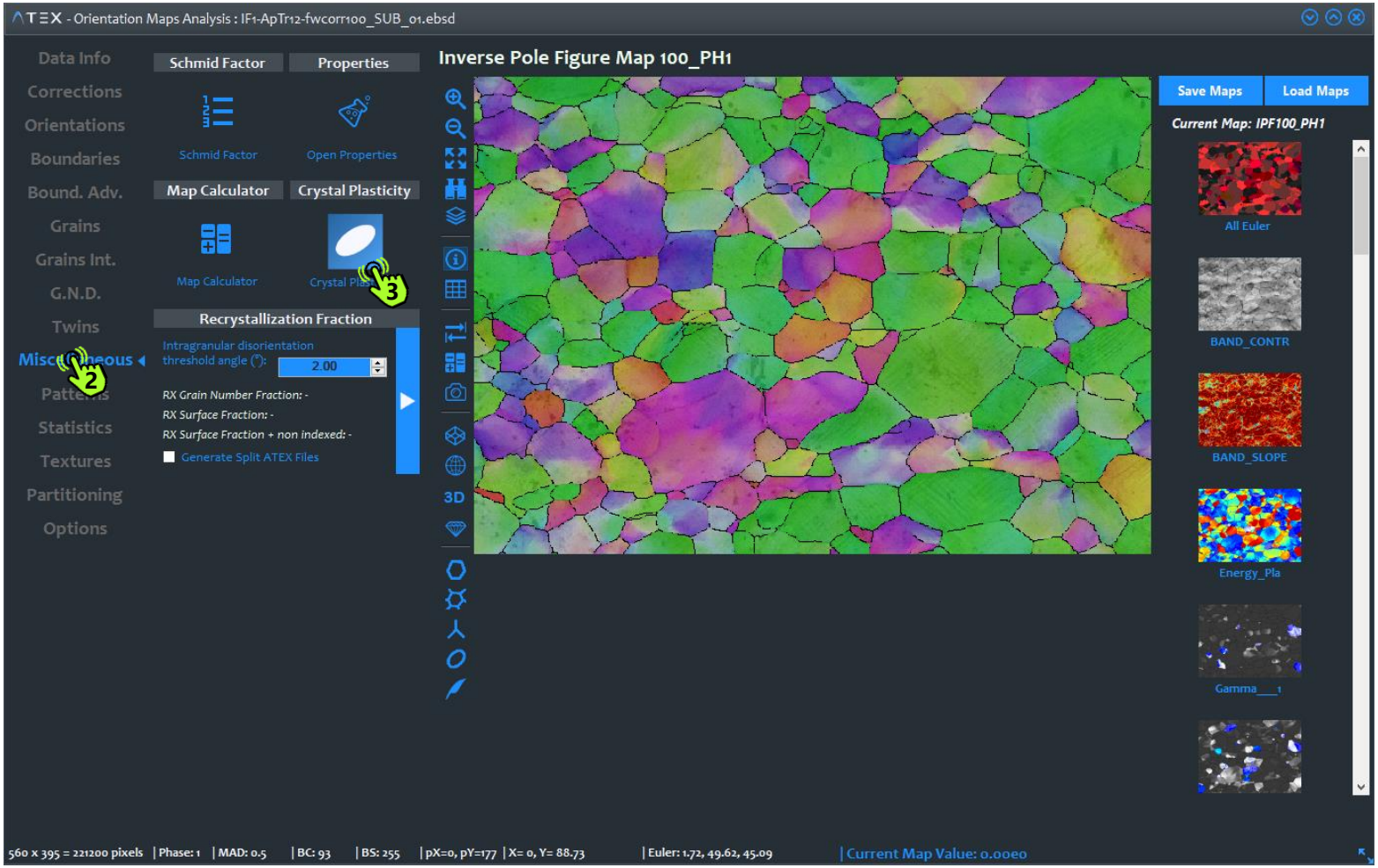
Content

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

TUTORIAL Textures Simulation – Crystal Plasticity

→ Simulations on Orientations Maps

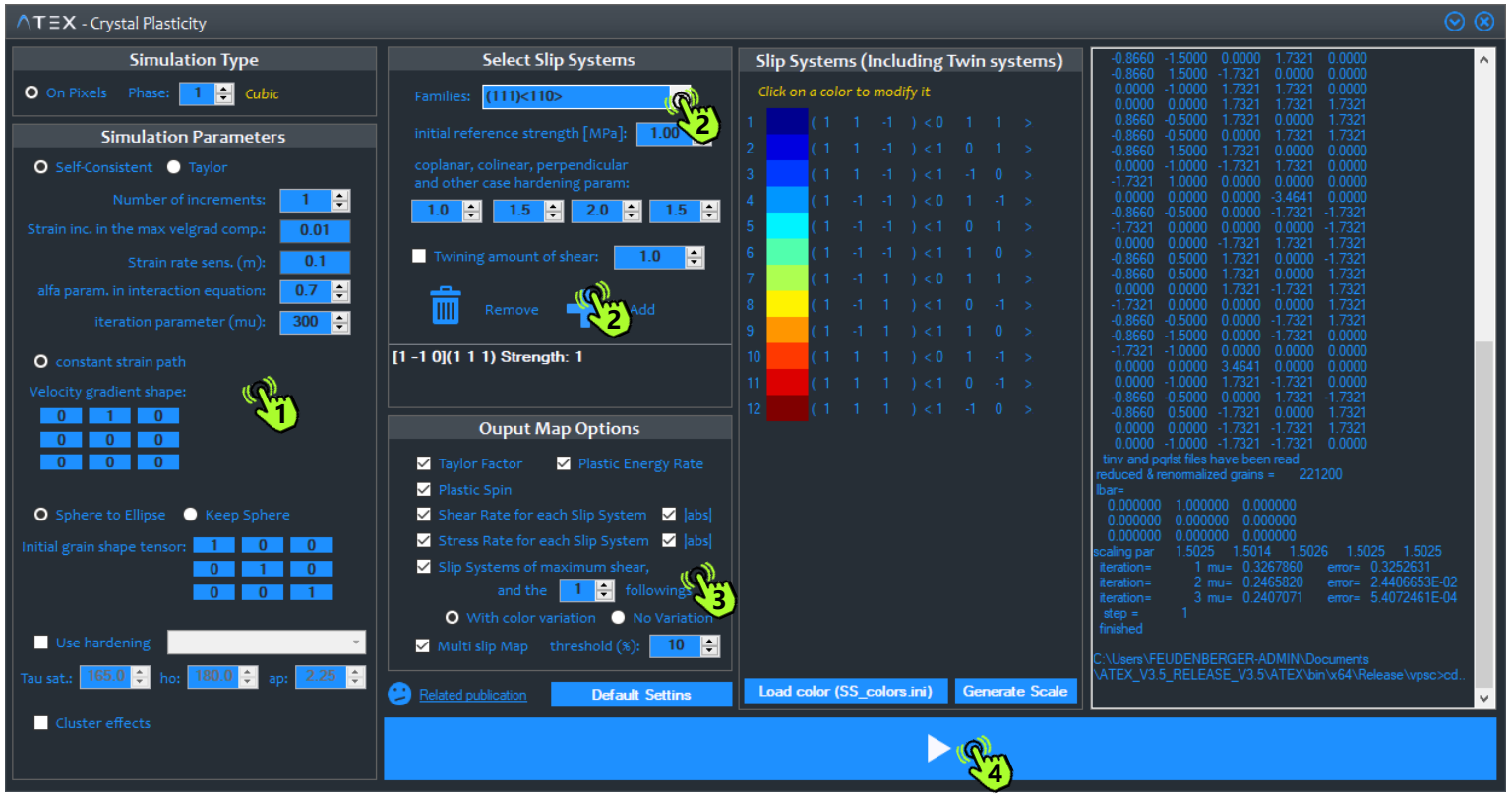
1. Open an EBSD maps
2. Go in tab “Miscellaneous”
3. Click on Crystal Plasticity button to open the corresponding module



TUTORIAL Textures Simulation – Crystal Plasticity

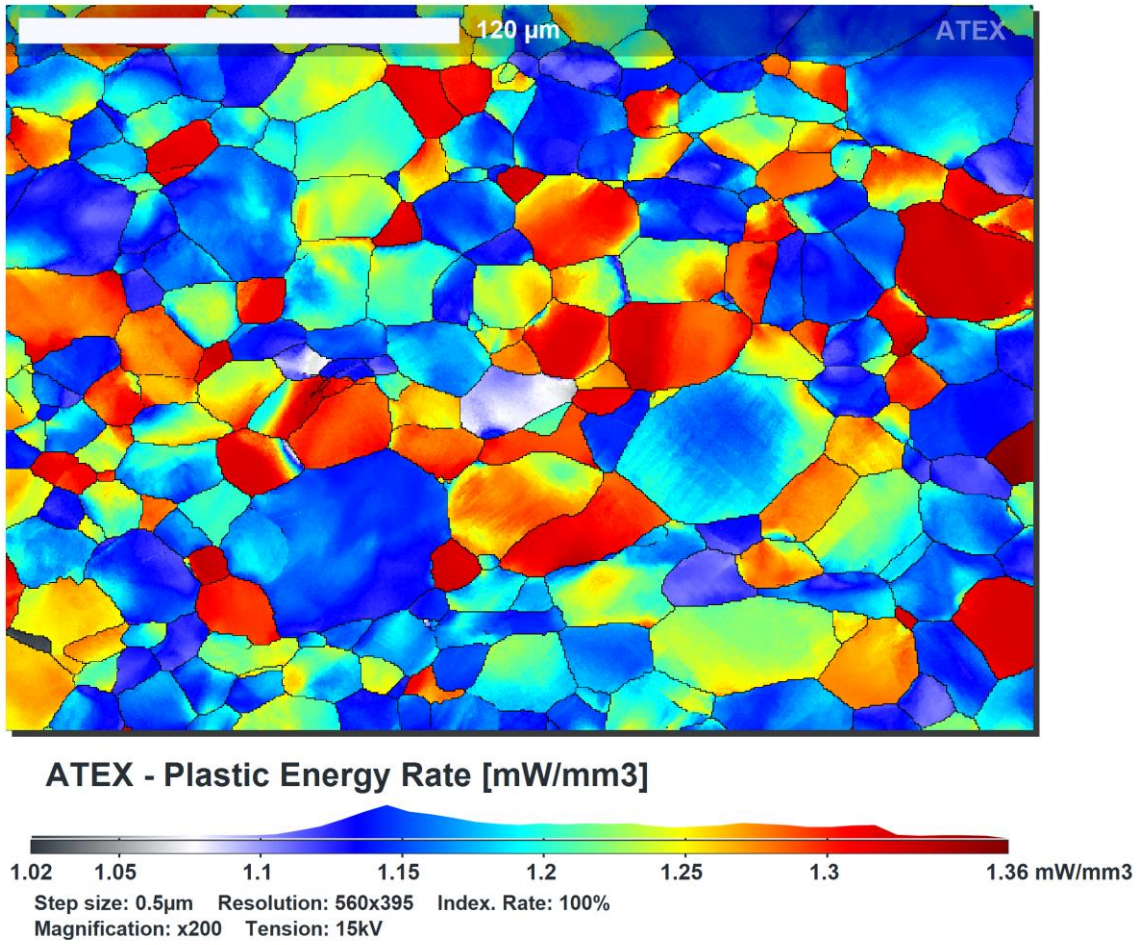
→ Simulations on Orientations Maps

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



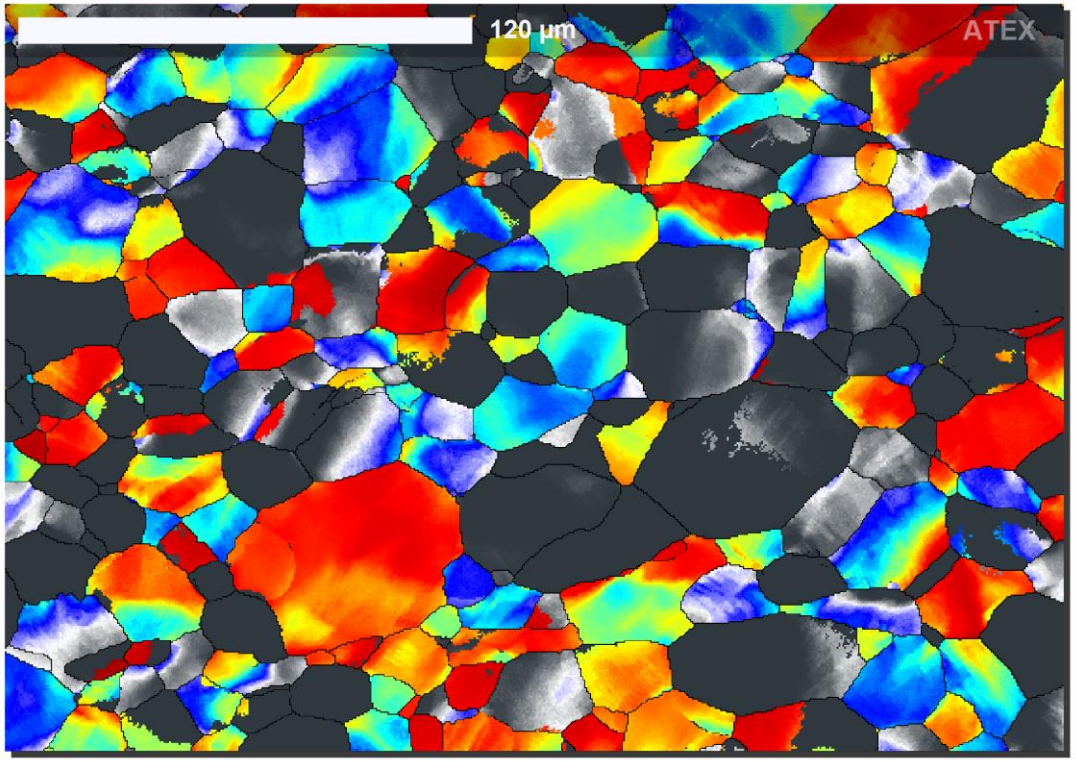
TUTORIAL Textures Simulation – Crystal Plasticity

→ Simulations on Orientations Maps



TUTORIAL Textures Simulation – Crystal Plasticity

→ Simulations on Orientations Maps

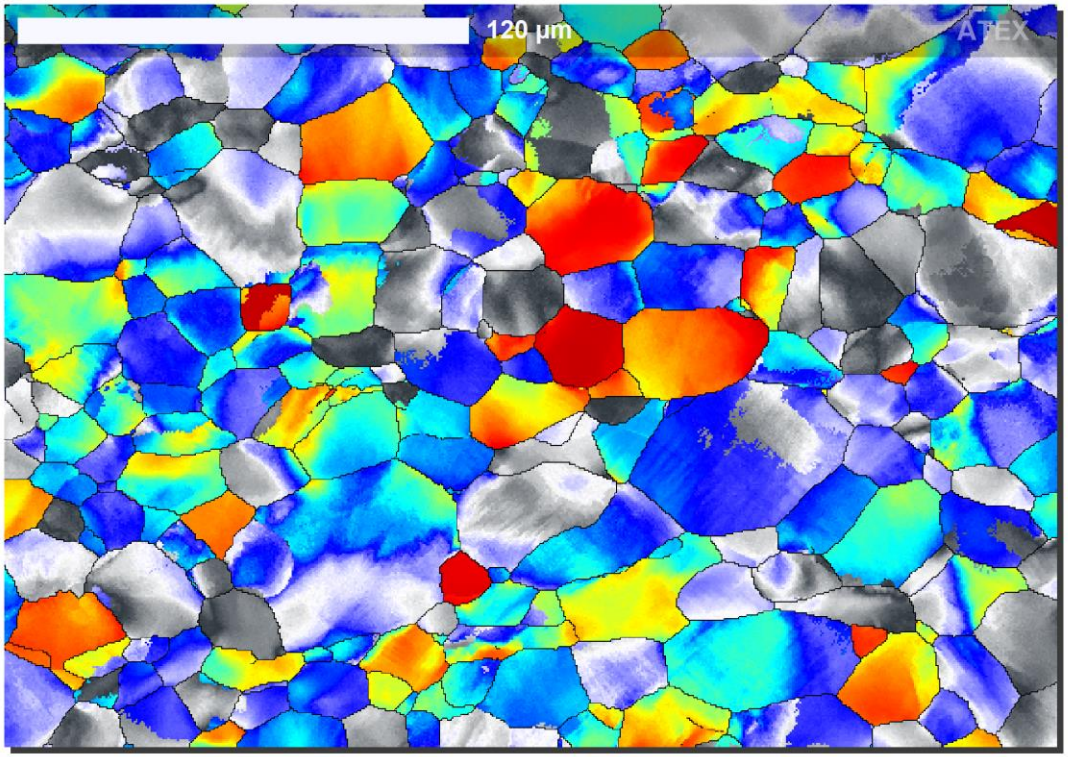


ATEX - Shear Rate in (1-1-1)<01-1> [s-1]

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

TUTORIAL Textures Simulation – Crystal Plasticity

→ Simulations on Orientations Maps



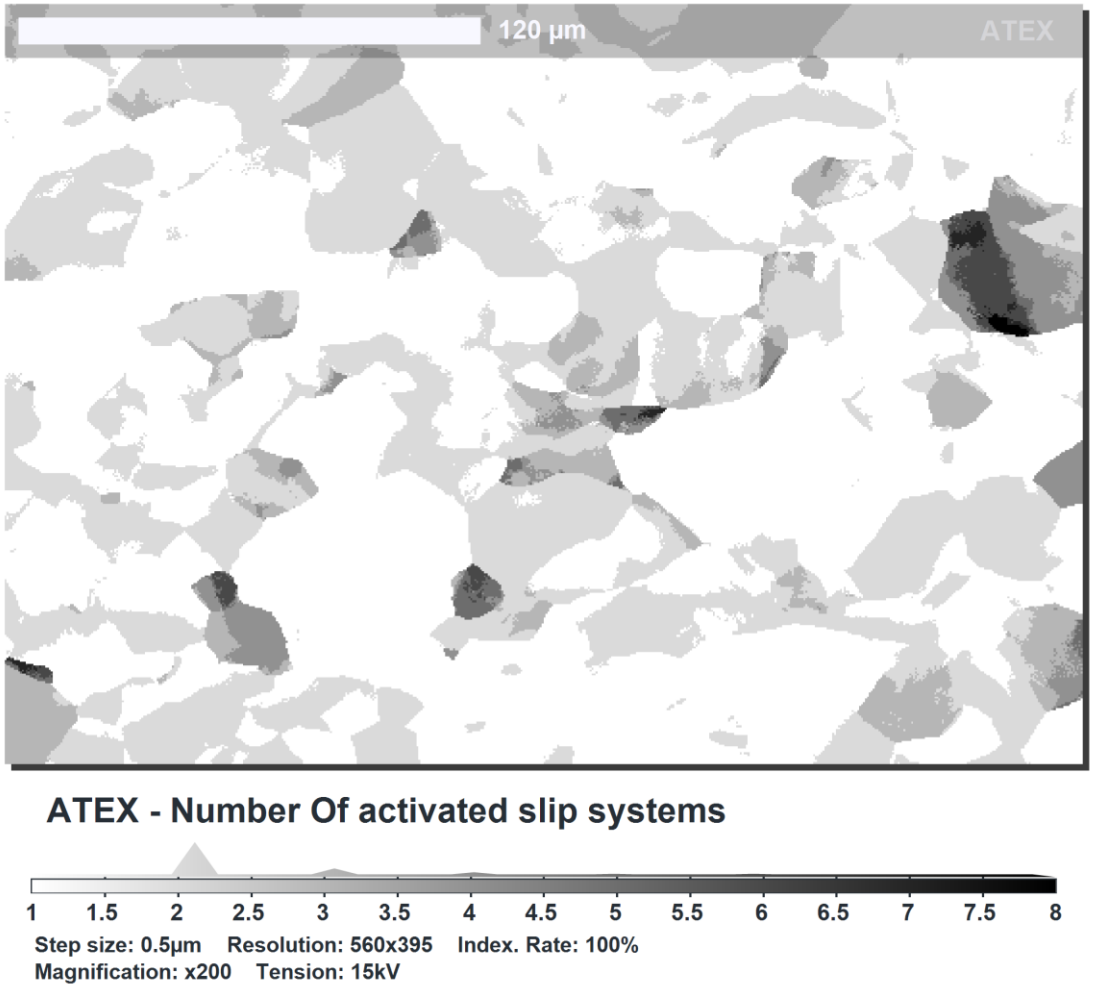
ATEX - Shear Stress in (11-1)<101> [Mpa]

0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.02 Mpa

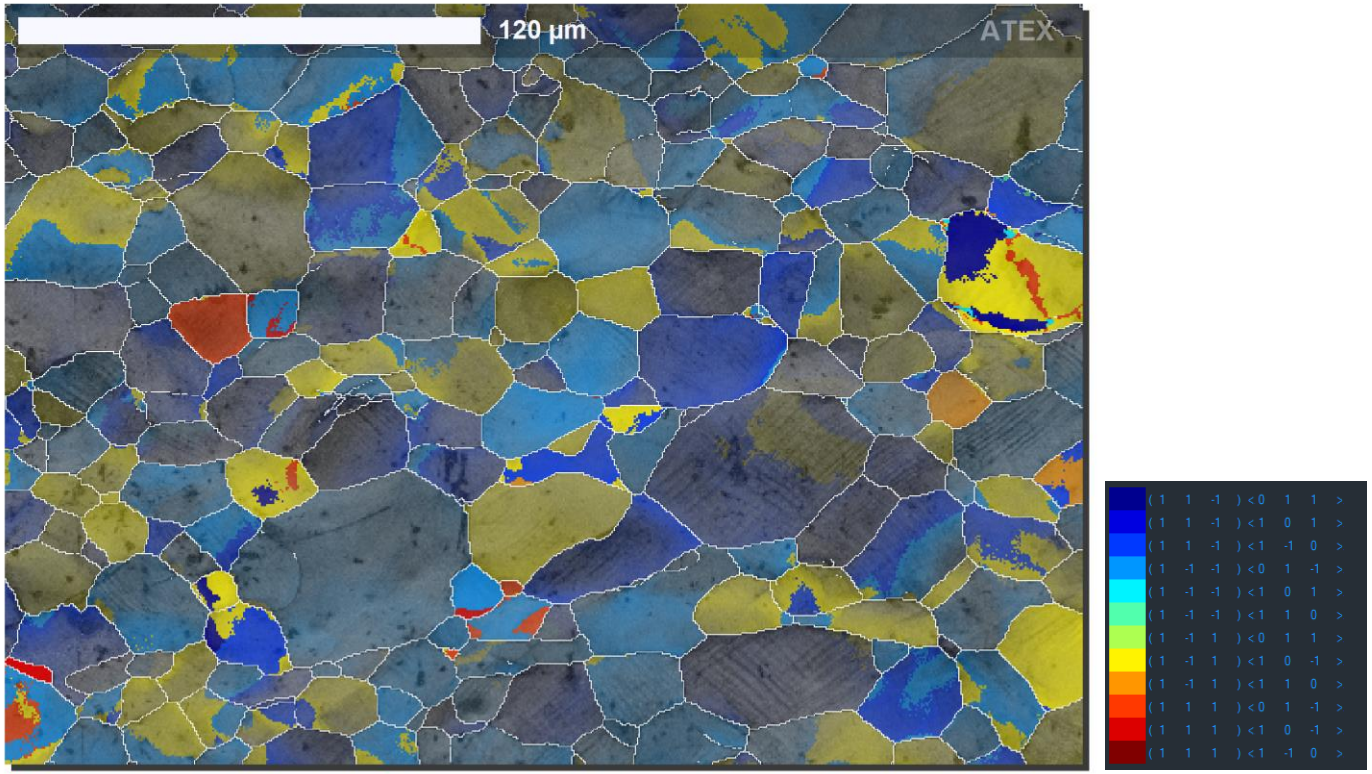
Step size: 0.5µm Resolution: 560x395 Index. Rate: 100%
Magnification: x200 Tension: 15kV

TUTORIAL Textures Simulation – Crystal Plasticity

→ Simulations on Orientations Maps



→ Simulations on Orientations Maps



ATEX - Slip Systems of maximum shear stress

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

Analysis Tools for Electron and X-ray diffraction

Textures Simulation – Crystal Plasticity

Benoît Beausir & Jean-Jacques Fundenberger

University of Lorraine, Metz, France

www.atex-software.eu
www.atex-software.eu/help.html
www.youtube.com/channel/UCQcAjUova-pa9bGYWVtizGA

UNIVERSITÉ DE LORRAINE

ATEX is free for non-commercial use.