

Analysis Tools for Electron and X-ray diffraction



Orientation List

Benoît Beausir & Jean-Jacques Fundenberger

University of Lorraine, Metz, France

www.atex-software.eu

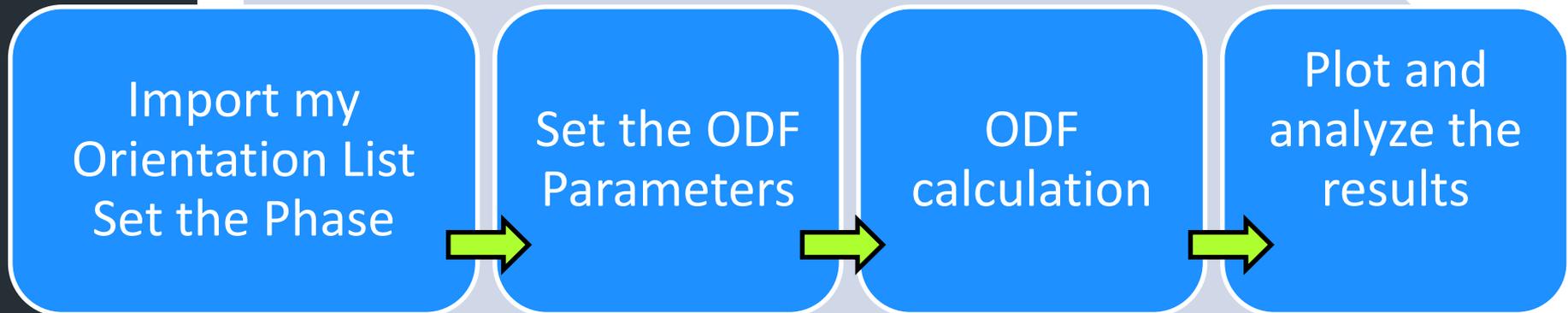
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Youtube channel “atex software”

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The process



1. Here is written the list of what to do

2. This hand tells you where to click



ODF as
Orientation
Density
Function

OrLi as
Orientaion List

Content



1. Import the Orientation List
 1. Select the data file (*.txt, *.csv, *.smt)
 2. Set the import parameters
 3. Set the Phase

2. Texture calculation
 1. Set the parameters
 2. Launch the ODF calculation

3. Plot the Texture (Pole Figures, inverse Pole Figures, ODF)

Definition

Orientation List means a list of orientations defined by three angles and a volume fraction associated to this orientation. The three Euler angles are those used by Bunge.

→ Import an Orientation List

1. Open ATEX
2. Click on the "Import data" button
3. Select "Ori. List" module
4. Select the file type you want to import

ATEX Version 3.30
- Academic Edition -
Analysis Tools for Electron and X-ray diffraction

Welcome My Creator

Open atex files

Import data

XRD P.F. XRD Prof. XRD 2D O.D.F.

EBSD 3D EBSD Ori. List Raman

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Licensed to Jean-Jacques Fundenberger
Affiliation: Atex-Software
Address: Metz, France
Email: jean-jacques.fundenberger@univ-lorraine.fr
Dongle: 15849817H422V66640

Activated EBSD Advanced HR-EBSD/TKD
Modules: X-Ray Advanced Devices Control

Please copy/past this reference in your publications:
B. Beausir and J.-J. Fundenberger, Analysis Tools for Electron and X-ray diffraction, ATEX-software, www.atex-software.eu, Université de Lorraine - Metz, 2017

Contact: contact@atex-software.eu

Ouvrir

Ce PC > DATA (D:) > DATA_TEST > RIGAKU > Leo_Monier

Rechercher dans : Leo_Monier

Organiser Nouveau dossier

Nom	Modifié le	Type	Taille
SLM.TXT	06/08/2022 19:57	Document texte	15 335 Ko

Nom du fichier: openFileDialog

*.txt, *.csv, *.smt

Ouvrir Annuler

*.txt
*.csv
*.smt

→ Import an Orientation List

- Fill in the number of lines of the header (here: 1)
- Check the character used as separator (usually Space or Tab)
- Set the column numbers corresponding to the Euler angles
- Set the column number of the volume fraction
- Select the phase
- Finalize the importation by clicking on the "Create ATEX file..." button. A "*.orli.atex" file will be created

File Info

Nb Lines in Header: 1

Columns Separator: Space

○ Degrees ● Radians

Column Selection

Phase: 0 Channel 1: 0

Euler1: 0 Channel 2: 0

Euler2: 0 Channel 3: 0

Euler3: 0 Channel 4: 0

Volume: 0 Channel 5: 0

"o" for equal volume fractions

Phases

Selected phase: 1

Crystal Structure: [dropdown]

Create ATEX file

Output File: D:\DATA_TEST\RIGAKU\Leo_Monier\SLMorli.atex

so first lines:

```

001: PH1 PH2 PHI ODF
002: 0.00 0.00 0.00 0.469002E+00
003: 2.00 0.00 0.00 0.485128E+00
004: 4.00 0.00 0.00 0.408737E+00
005: 6.00 0.00 0.00 0.431322E+00
006: 8.00 0.00 0.00 0.497378E+00
007: 10.00 0.00 0.00 0.663501E+00
008: 12.00 0.00 0.00 0.569730E+00
009: 14.00 0.00 0.00 0.484018E+00
010: 16.00 0.00 0.00 0.597434E+00
011: 18.00 0.00 0.00 0.643571E+00
012: 20.00 0.00 0.00 0.645868E+00
013: 22.00 0.00 0.00 0.285141E+00
014: 24.00 0.00 0.00 0.276258E+00
015: 26.00 0.00 0.00 0.286147E+00
016: 28.00 0.00 0.00 0.304676E+00
017: 30.00 0.00 0.00 0.354271E+00
018: 32.00 0.00 0.00 0.415165E+00
019: 34.00 0.00 0.00 0.435519E+00
020: 36.00 0.00 0.00 0.441600E+00
021: 38.00 0.00 0.00 0.423162E+00
022: 40.00 0.00 0.00 0.423748E+00
023: 42.00 0.00 0.00 0.469207E+00
024: 44.00 0.00 0.00 0.505409E+00
025: 46.00 0.00 0.00 0.522513E+00
026: 48.00 0.00 0.00 0.547240E+00
027: 50.00 0.00 0.00 0.541355E+00
028: 52.00 0.00 0.00 0.500243E+00
029: 54.00 0.00 0.00 0.469323E+00
030: 56.00 0.00 0.00 0.482740E+00
031: 58.00 0.00 0.00 0.510240E+00
032: 60.00 0.00 0.00 0.538965E+00
033: 62.00 0.00 0.00 0.587115E+00
034: 64.00 0.00 0.00 0.591495E+00
035: 66.00 0.00 0.00 0.585179E+00
036: 68.00 0.00 0.00 0.528710E+00
037: 70.00 0.00 0.00 0.460225E+00
038: 72.00 0.00 0.00 0.407402E+00
039: 74.00 0.00 0.00 0.492949E+00
040: 76.00 0.00 0.00 0.548772E+00
041: 78.00 0.00 0.00 0.548959E+00
042: 80.00 0.00 0.00 0.317045E+00
043: 82.00 0.00 0.00 0.645469E+00
044: 84.00 0.00 0.00 0.563658E+00

```

First 50 lines of the *.txt file

Complement to step 3: Euler1 corresponds to Phi1 according to Bunge's notation
 Euler2 corresponds to Phi
 Euler3 corresponds to Phi2

Complement to step 4:

If no volume fraction is present or if you do not want to take it into account, enter « 0 » and all orientations will have the same volume fraction.

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The Orientation List is imported, now you can calculate the ODF

1. Set the texture calculation parameters (if you have no idea what to enter, let the default values.

2. Click on the output you want to see

3. If a sample reference system has to be changed, enter the rotation parameter and click on the button

4. You may want to save the ODF

I.P.F. stands for Inverse Pole Figure

The screenshot shows the 'Orientation List' window with the following sections:

- Textures Options:**
 - Phase: 1
 - Sample symmetry: Triclinic
 - Calculation Method: Boxing + C-coef
 - Boxes size (1 - 15°): 5
 - Development EVEN: 22
 - Development ODD: 21
 - Gaussian width (*): 8.0
 - Isotropic Part: 0.00
- Hexagonal Convention:** Two diagrams showing different crystallographic conventions.
- Textures:**
 - Sections: A 3x3 grid icon.
 - Pole Figure: A target icon with a hand cursor (labeled 2).
 - Components: A circular icon with four quadrants.
 - I. P. F.: A triangle icon.
- Rotate Data:**
 - Axis - Angle (selected) / Euler angles
 - Sample Rot. Axis X: 0
 - Sample Rot. Axis Y: 0
 - Sample Rot. Axis Z: 1
 - Rotation Angle (°): 90.0
 - Create a new ATX file:
 - Export ODF: A button with a hand cursor (labeled 4).
- SLM.orli:**
 - 382996 Orientations (only the first 200 orientations are displayed in the table below)
 - Lattice parameters : a = 1 b = 1 c = 1 alpha = 90° beta = 90° gamma = 90°

#	Phi1	Phi0	Phi2	Volume
1	0	0	90	1.5708
2	2	0	90	1.5708
3	4	0	90	1.5708
4	6	0	0	1.5708
5	8	0	0	1.5708
6	10	0	0	1.5708
7	12	0	0	0
8	14	0	0	0
9	16	0	0	0
10	18	0	0	0.469002
11	20	0	0	0.485128
12	22	0	0	0.408757
13	24	0	0	0.431392
14	26	0	0	0.497378
15	28	0	0	0.663501
16	30	0	0	0.56973
17	32	0	0	0.484018
18	34	0	0	0.597434
19	36	0	0	0.643571
20	38	0	0	0.645868
21	40	0	0	0.285141
22	42	0	0	0.275258
23	44	0	0	0.286147
24	46	0	0	0.304676
25	48	0	0	0.354271
26	50	0	0	0.415165
27	52	0	0	0.435519
28	54	0	0	0.4416
29	56	0	0	0.423162
30	58	0	0	0.423748
31	60	0	0	0.469207

Hover over the buttons to get a short description of what they do

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