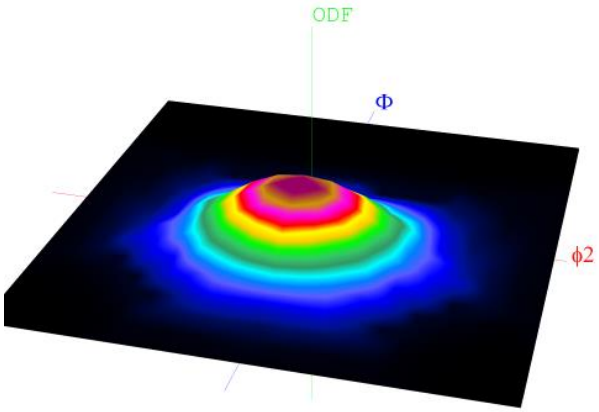
LABSOFT

LaboTex

Version 3.0

The Texture Analysis Software for Windows



LaboTex: Modelling of ODF, Pole Figures and Inverse Pole Figure

Release 3.

© LaboSoft s.c.
Telephone: +48 502311838
Telefax: +48 12 3953891
E-mail: office@labosoft.com.pl

Contents

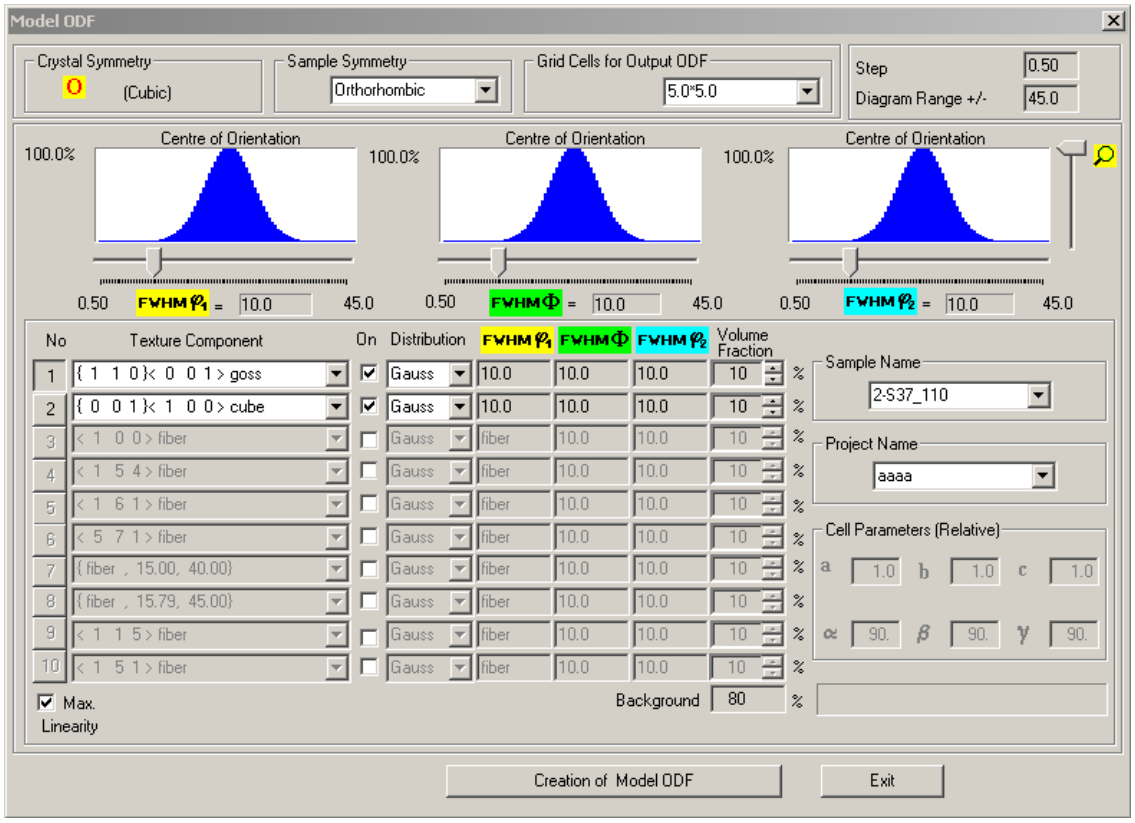
1. Models of Orientation Distribution Function

1.1 Opening of dialog window for ODF modelling

User can open dialog for ODF modelling from menu 'Modelling' :

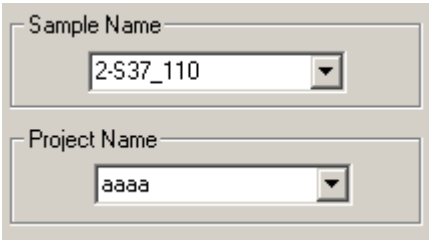
or he can use icon which is marked on the image below:

Dialog window for ODF modelling ('Model ODF') contains many options:

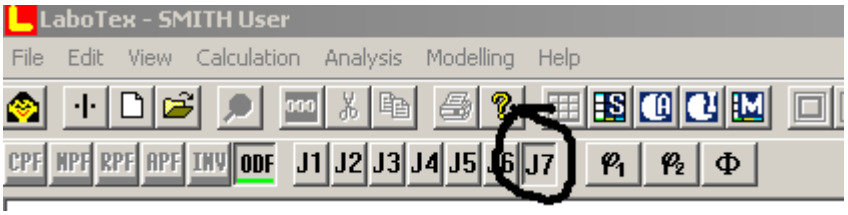


1.2 Project name, sample name and job name of model ODF

In first step user should choose project name from the 'Project Name' combo box and sample name from the 'Sample Name' combo box.



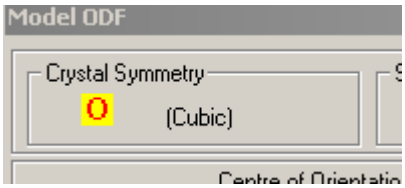
When LaboTex creates model ODF it place new ODF in the next free job for sample. For example if user had 6 jobs (for J1 to J6) then LaboTex creates new - job number 7 (J7) and in this job is placed new ODF.



User can also defines new project name and new sample name by change of name in combo box. In this case model ODF will be placed in first job of new sample.

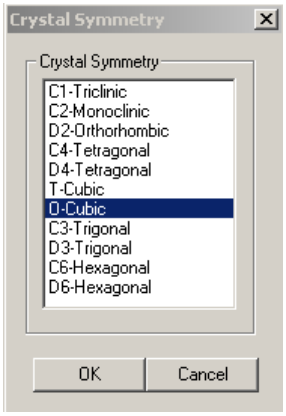
1.3 Crystal Symmetry

The crystal symmetry of model ODF is current LaboTex crystal symmetry.



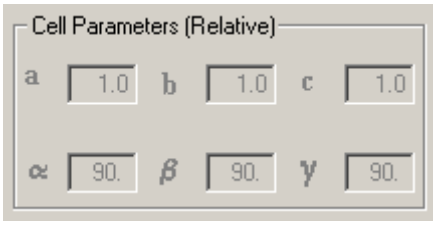
User can change current LaboTex crystal symmetry in menu file (item 'Crystal Symmetry ...') or by click on the crystal symmetry icon :

Next user can choose crystal symmetry for your model ODF from the list:

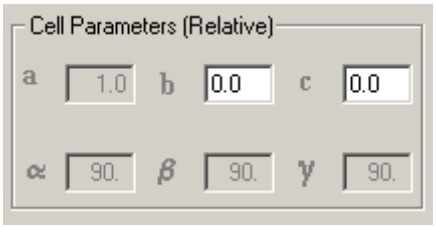


1.4 Cell parameters

LaboTex use relative cell parameters for ODF creations. All parameters are given by LaboTex in case of cubic system (all fields are grayed):

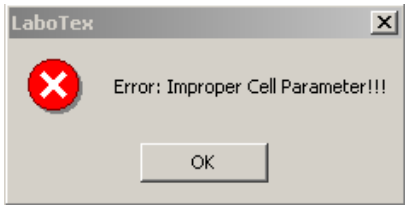


In case of crystal symmetry lower than cubic user has to complete appropriates cell parameters. For example, in case of orthorhombic crystal symmetry user has to complete two parameters: b and c:



Notice: *For details about convention for cell parameters which is used in LaboTex see to report: 'Pole figures: registration and plot conventions'*

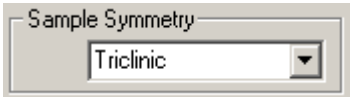
LaboTex completes 'free' cell parameters by 0.0 value. If user doesn't change these values on the proper one then LaboTex will give a message of the form:



1.5 Sample symmetry

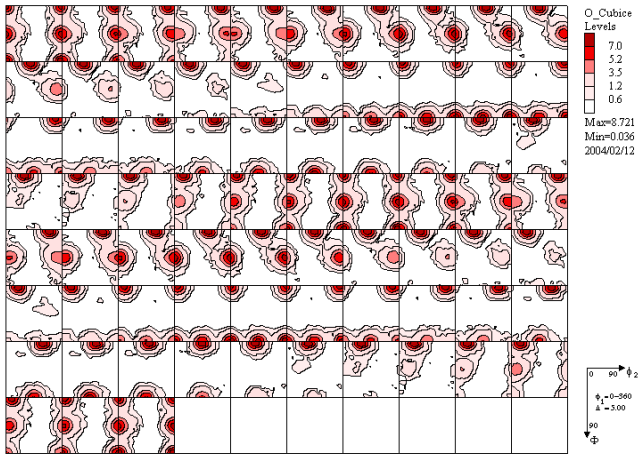
Choice of sample symmetry is very easy. User choose suitable sample symmetry from options:

- Triclinic
- Monoclinic
- Orthorhombic
- Axial

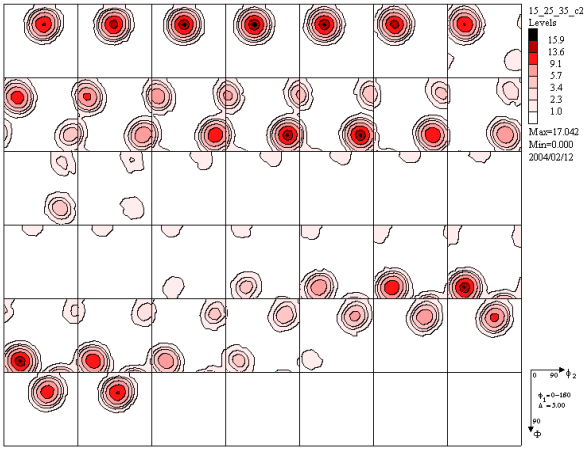


The figures below show examples of ODF for different sample symmetry (cubic c.s., φ_1=const. projection):

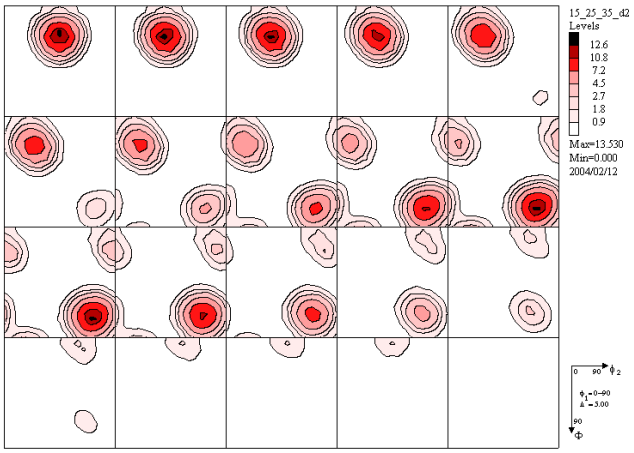
Triclinic sample symmetry



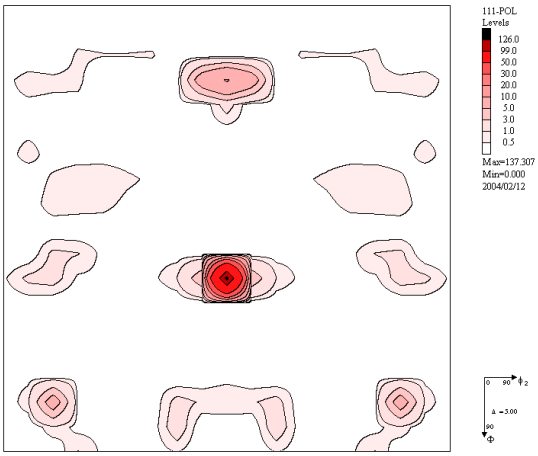
Monclinic sample symmetry



Orthorhombic sample symmetry



Axial sample symmetry



Examples of ODF for different sample symmetry (cubic crystal symmetry, projections : φ_1=const.)

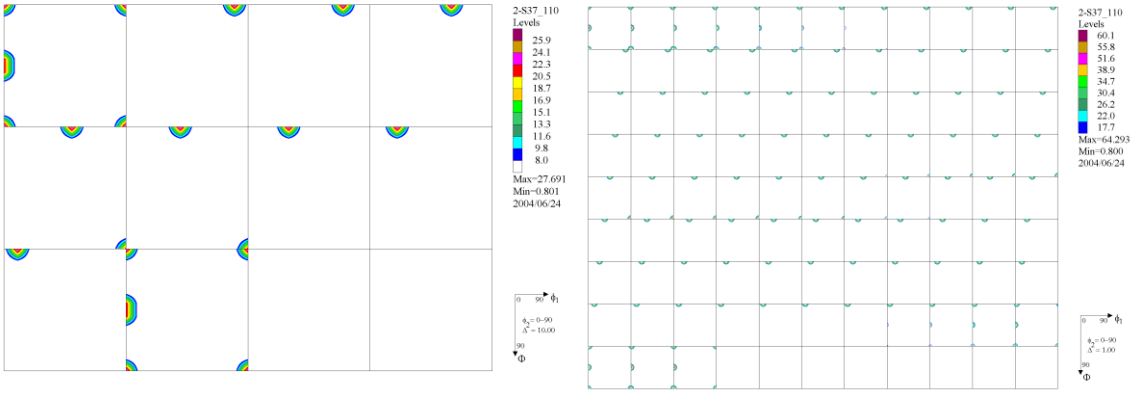
1.6 Grid cells for output ODF

The LaboTex allows on the creation of ODF in many different grids:

- 1.0º x 1.0º
- 1.2º x 1.2º
- 1.25º x 1.25º
- 1.5º x 1.5º
- 1.8º x 1.8º
- 2.0º x 2.0º
- 2.25º x 2.25º
- 2.5º x 2.5º
- 3.0º x 3.0º
- 3.6º x 3.6 º
- 3.75º x 3.75º
- 4.5º x 4.5º
- 5.0º x 5.0º
- 6.0º x 6.0º
- 7.5º x 7.5º
- 10.0º x 10.0º

User select suitable grid from combo box :

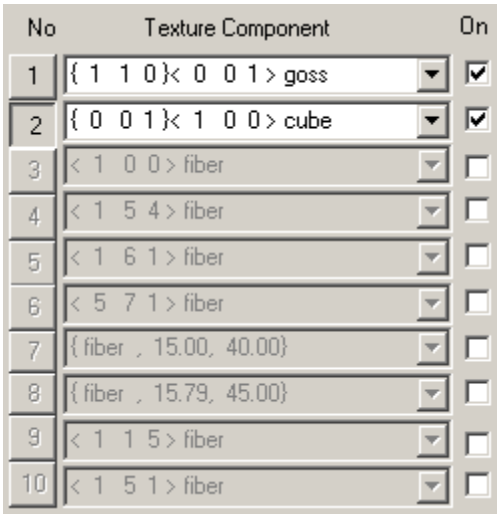
The pictures below shows examples of ODF created for different grids: 10.0º x 10.0º and 1.0º x 1.0º (cubic crystal symmetry, orthorhombic sample symmetry).



Notice*: Work with high resolution ODF (<2.5º) needs high speed graphic card and PC. You should test and find maximal resolution for comfortable work with LaboTex on the your computer (for example: file with ODF for triclinic sample symmetry and triclinic crystal symmetry for grid 1.0º x 1.0º contains about 23millions data when file for the same ODF for grid 5.0º x 5.0º contains about 180 000 data).*

1.7 Texture components

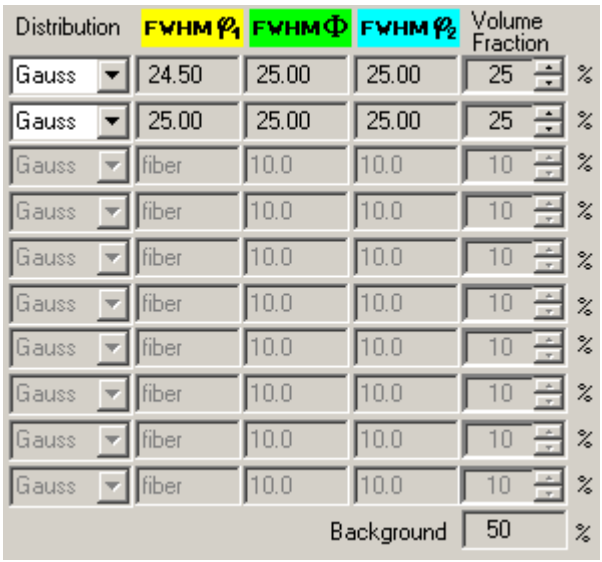
Model ODF can contains up to 10 components. User can add new component click on the appropriate check box. In example on the picture below user has chosen 'goss' and 'cube' components. Components 3 to 10 are non-active in model ODF calculations.



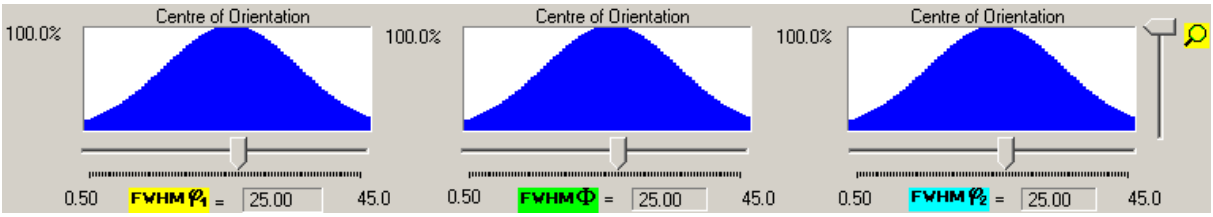
User can change component in suitable combo box for texture component. Combo box contains all components from orientation data base for given crystal symmetry. If you would like to create model with new component then you have to introduce first new component to database. You can to make it in dialog 'Database'. It is available from menu 'Analysis'.

For each component you can choose :

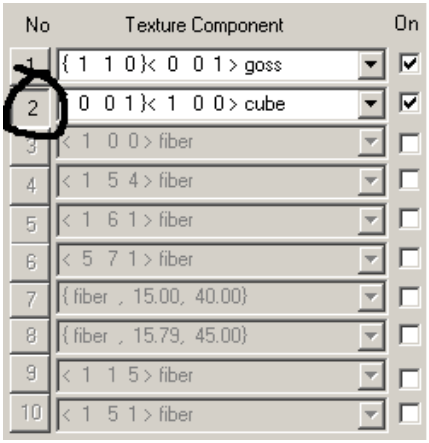
- Type of distribution function;
- FWHM for φ_1;
- FWHM for Φ;
- FWHM for φ_2;
- Volume fraction.



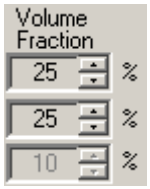
You can choose Gauss or Lorentz distribution function using combo box for given component's. FWHM for each Euler angle you can set using sliders:



LaboTex displays graph with distribution for component which '**No**' button is pressed:



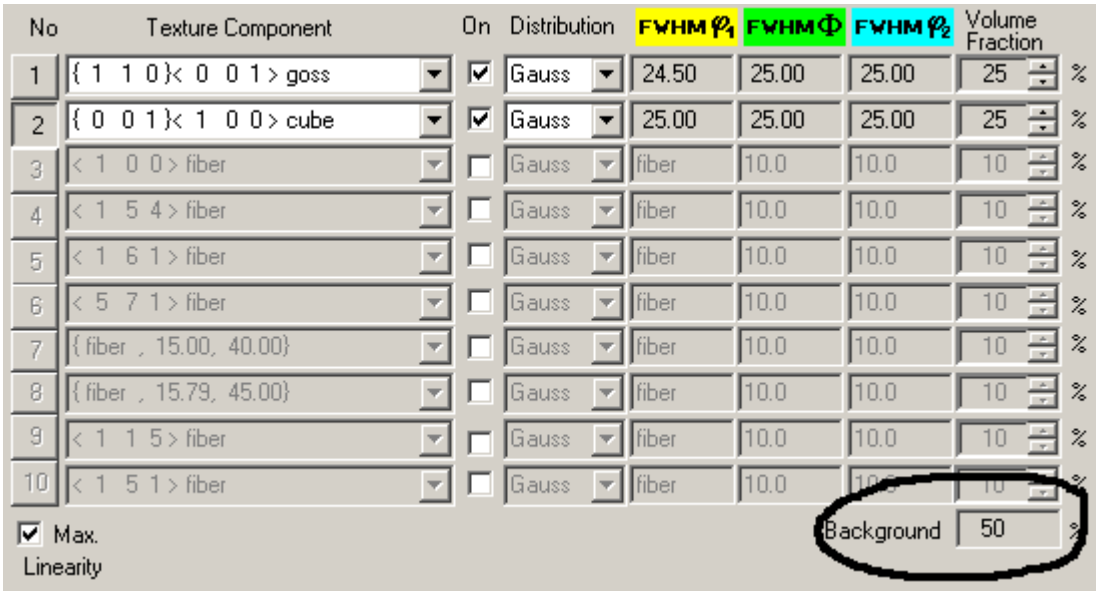
Similarly, FWHM settings are doing for component which '**No**' button is pressed. User should also set volume fraction of texture component in percents. It can be done for each component using vertical scroll bar:



LaboTex calculates automatic volume fraction of background V_B (random orientation component) on the base of volume fraction of all n components :

$$V_B = 100\,\% - \sum_{i=1}^{n} V_i$$

and it write V_B value in 'Background' field in column of 'Volume Fraction'':



1.8 Model calculations

LaboTex in model calculations assumes isotropy of Euler space for Gauss or Lorentz distribution. Exceptions are orientations lying on the Φ=0 plane. These orientations are not 'points' but are 'lines' for $\varphi_1+\varphi_2$=const. in Euler space. In case of cubic crystal symmetry LaboTex shows basic region of ODF which one consists with 3 'true' (fundamental) basic regions ('true basic' regions have non-linear boundary hence they are not used for ODF visualization - for details see for example to: J.W.Flowers, "Volume Fractions of Texture Components of Cubic Materials", Textures and Microstructures, 1983, Vol.5, pp. 205-218), hence each component has at least 3 symmetrically equivalent orientations. If option 'Max. Linearity" is checked then LaboTex build model in 'true' basic region which one has the smallest distortions along Φ axis. ODF in second and third basic region is build on the base of model from first region.

To start model calculation user should press button 'Creation of Model ODF' :

Next LaboTex calculates model ODF. User should choose kind of ODF projection for visualization of calculated ODF:

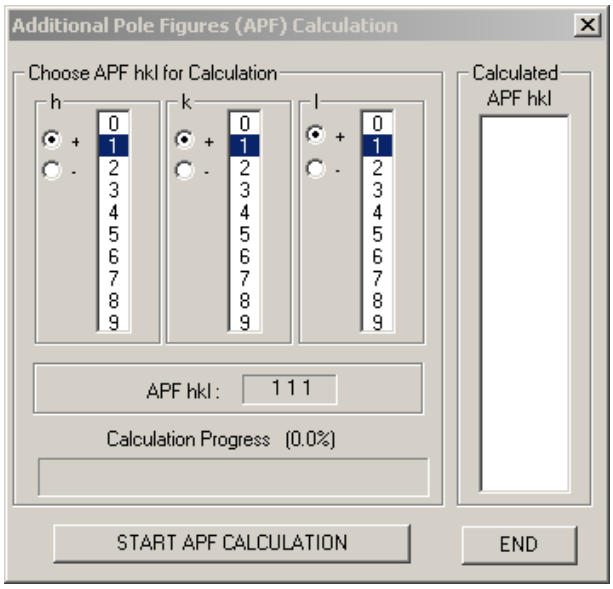
Next user can display ODF in 3D view.

Note: If you would like to compare created model of ODF with other ODF use 'Compare Mode'. If you want to fit model of ODF to your experimental ODF use option in menu 'Analysis', item 'Quantitative Analysis - Model Functions Methods ...".

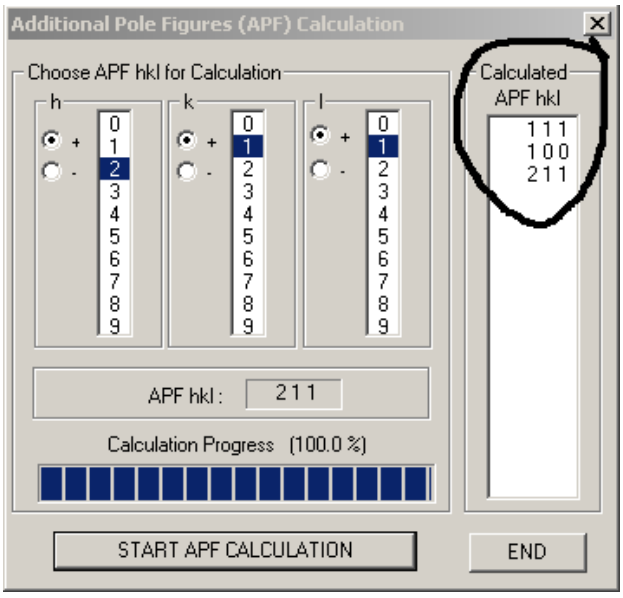
2. Models of Pole Figures and Inverse Pole Figures

When you have done model ODF then you can make calculations of models pole figures analogically as for ODF calculated from experimental pole figures or as for ODF calculated from single orientations data. In menu 'Calculation' are menu items : 'ODF to APF' and 'ODF to INV'. You can also click directly on the icon to start dialog window for calculation of pole figures:

In 'ODF to APF' dialog window you can make calculation of normal pole figures. You only have to choose miller indices h, k, l of pole figure which you want create and next click on the button 'START APF CALCULATION'.



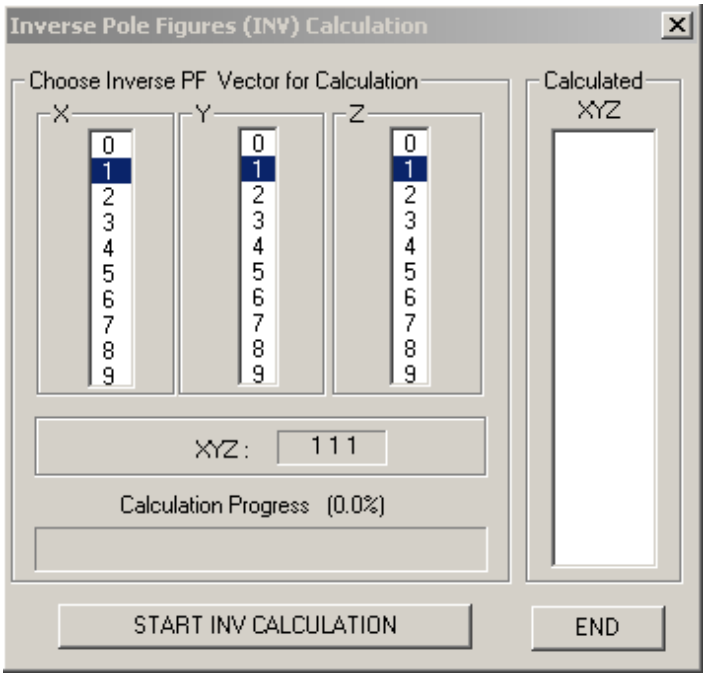
Miller indices of calculated pole figures are displayed on the list as marked below.



When you finish calculation of pole figures then click 'END' button. All your pole figures are always available when you choose APF (Additional Pole Figures) icon on the toolbar. When you click on the '111', '100', '211' icon then LaboTex displays one or more pole figures. If you would like to display pole figures from job number 2 you have to click first on button 'J2' and next you should choose 'APF' icon and finally you should click on the pole figures icons.

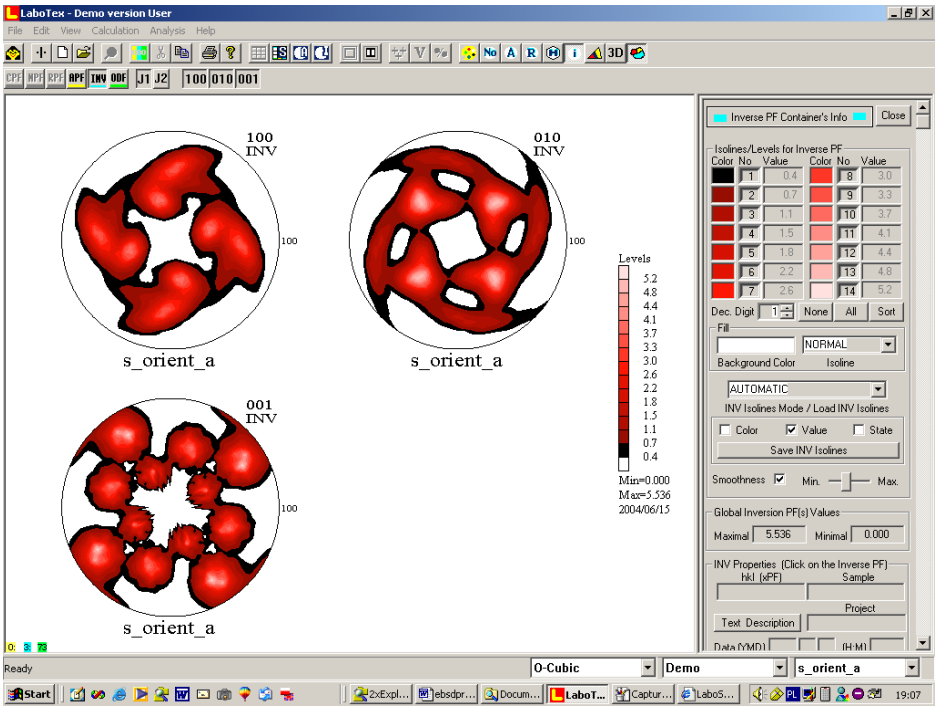
Note: Pole figures for each job are calculated on the base of ODF from this job.

Analogically you can create models of inverse pole figures (menu item : 'ODF to INV'). In this case you have to choose the vector components: X, Y, Z for which LaboTex calculates orientation distribution on the stereogram. The most popular are directions of axis: 001 (ND direction), 010 (TD direction) and 100 (RD/LD direction). Details you can find in Report :"The Nomenclature of Inverse Pole Figures Use in LaboTex" (see: http://labotex.com).



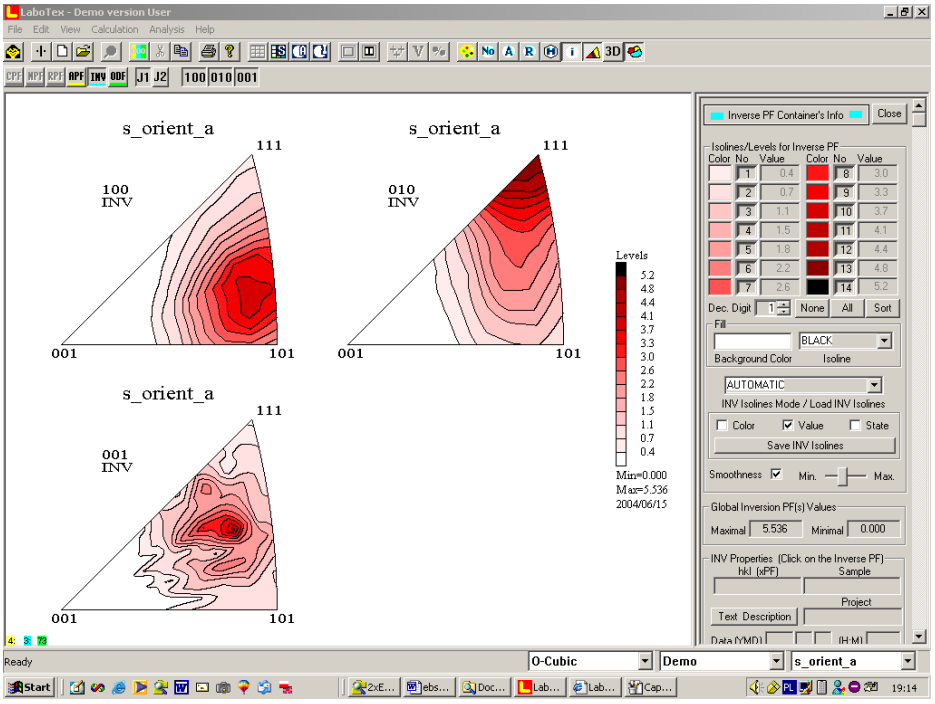
All your inverse pole figures are always available when you choose INV (INVerse pole figures) icon on the toolbar:

When you click on the '001', '100', '010' icon then LaboTex displays one or more complete inverse pole figures:



If you would like display partial inverse pole figure (orientations distribution of a sample axis on a standard stereographic triangle) you should click on the icon with triangle or you should choose item 'Basic Region' in menu 'View'.

When this icon is pressed LaboTex displays partial inverse pole figures in place of complete inverse pole figures:

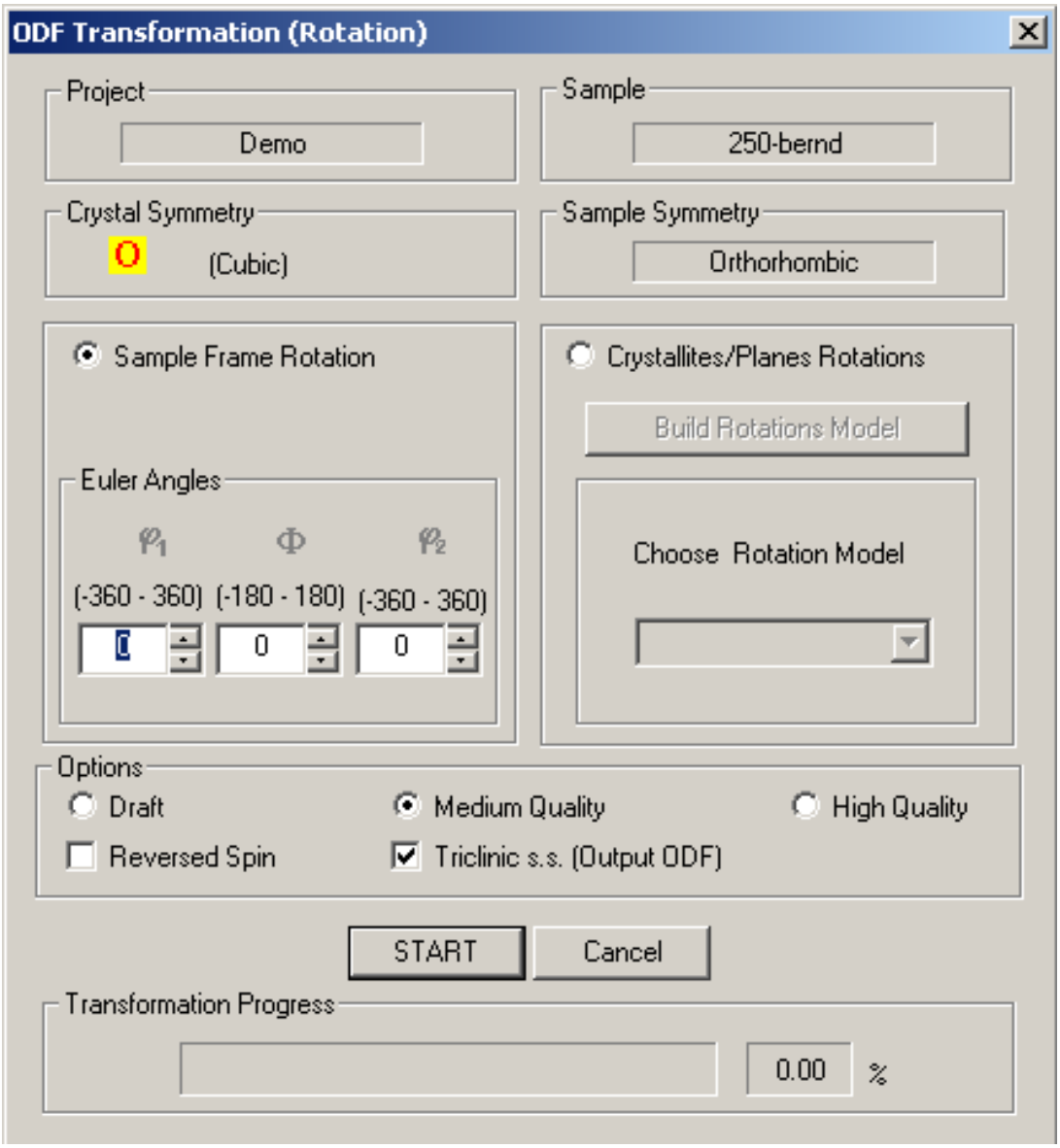


Note: I*f icon for basic region is pressed then analysis icons are grayed.*

3. ODF Transformation

LaboTex calculates new ODF which is result transformation of initial ODF. New ODF is created in new job for sample of initial ODF. There are two kinds of transformations:

- Sample Frame Rotation;
- Crystallites/Planes Rotations.

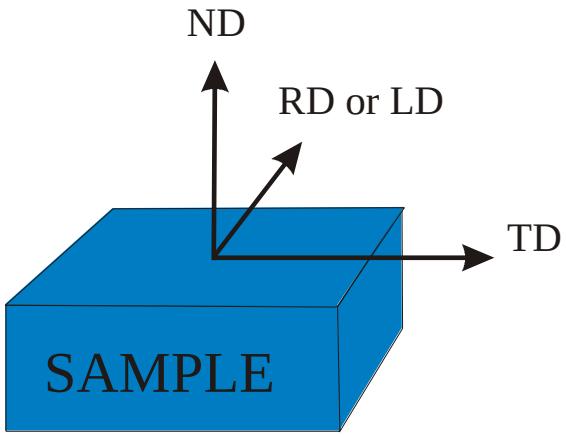


3.1. Sample Frame Rotations

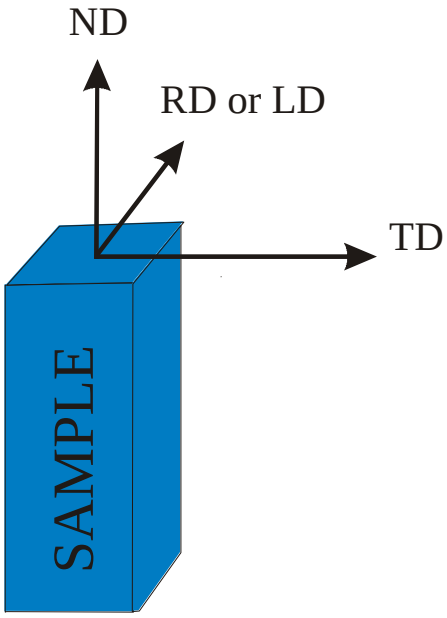
Using dialog: “Sample Frame Rotations” user can rotate the sample frame. This option is very important if user would like to see ODF for other (different) sample position User can change sample symmetry for transformed ODF.

Example 1:

You want see ODF for the perpendicular surface with relation to surface which was measured:

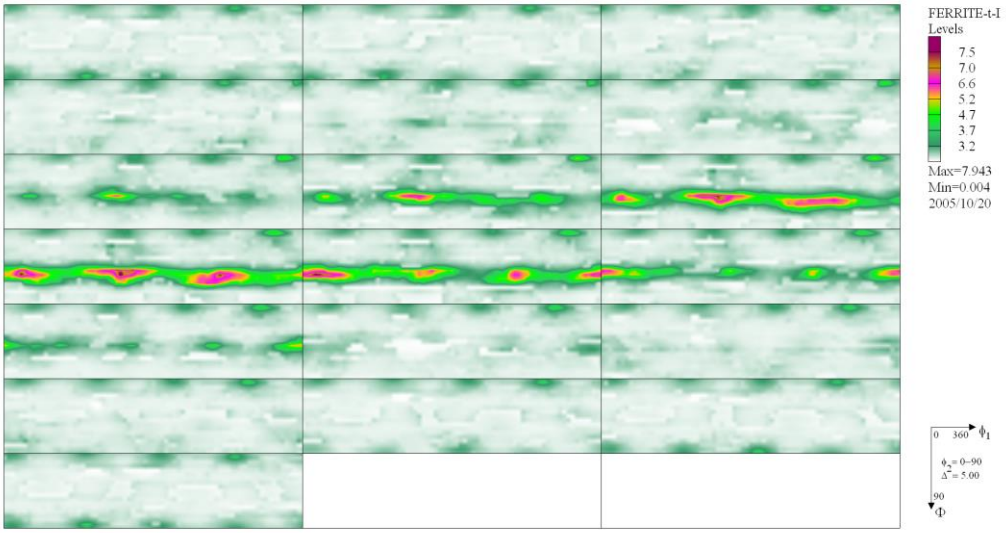


Sample Axis Definition
Initial

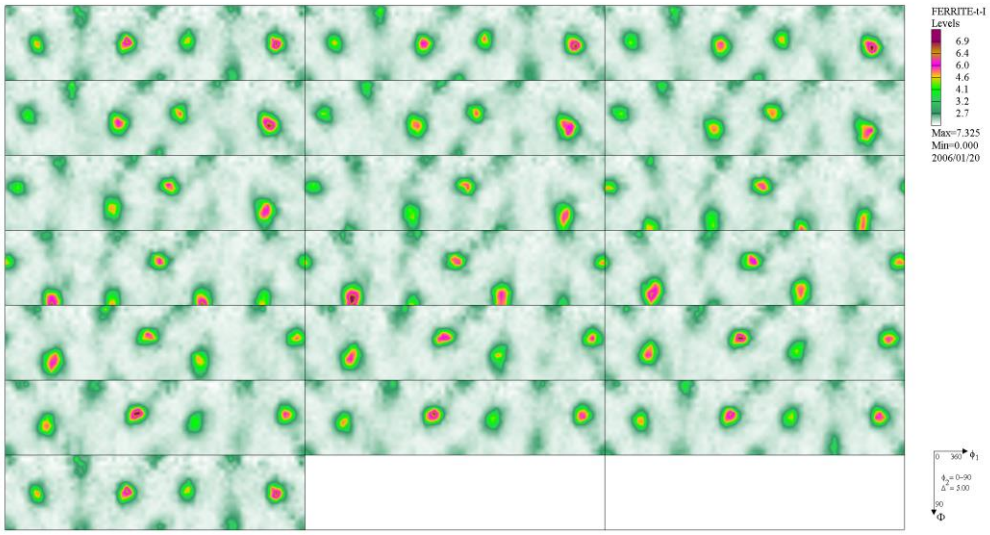


Sample Axis Definition after
Frame Rotation (0,90,0)

ODF for initial axis definition. Sample: Ferrite – triclinic sample symmetry.

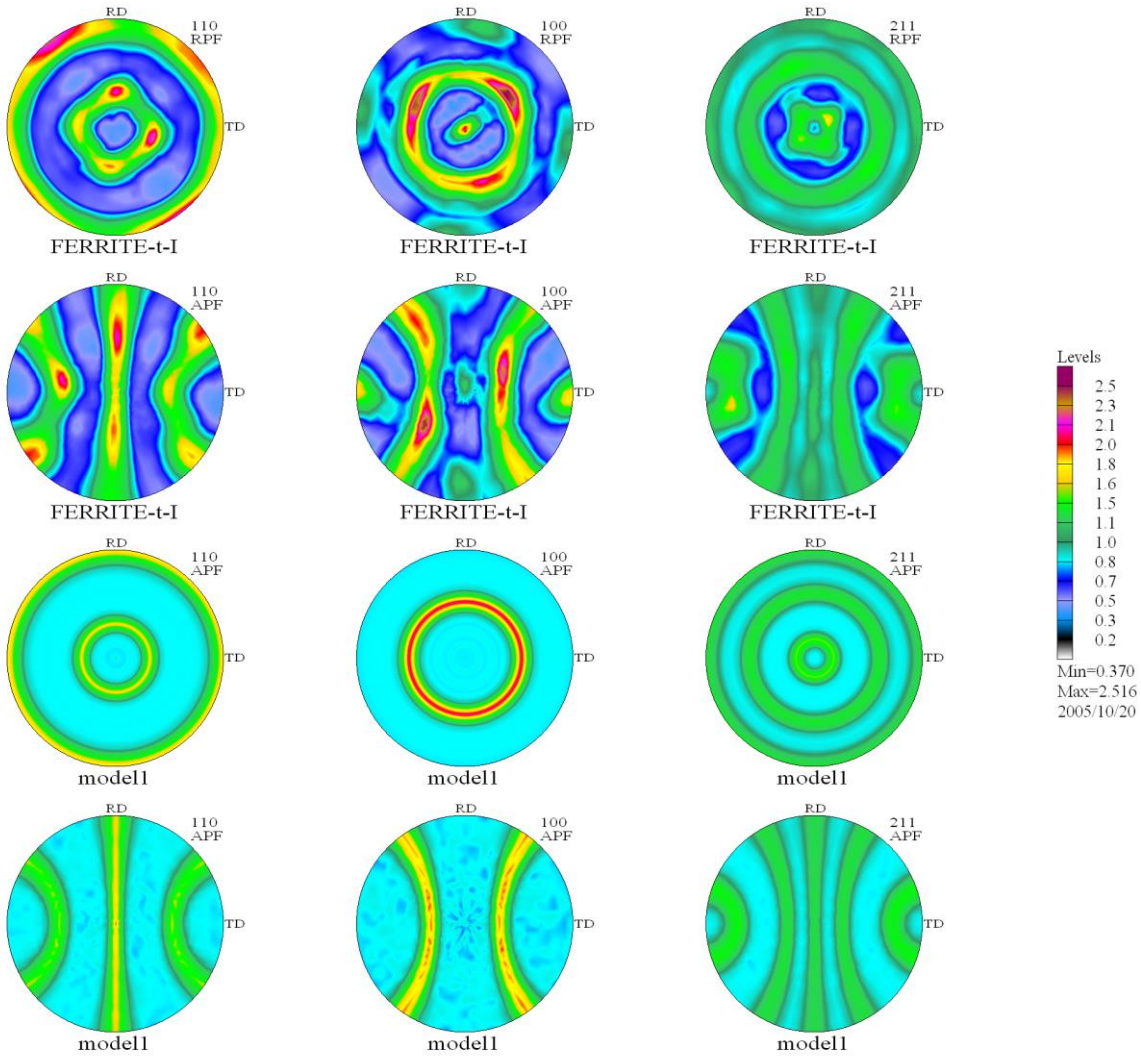


ODF after frame rotation : (0,90,0). Sample Ferrite – triclinic sample symmetry.

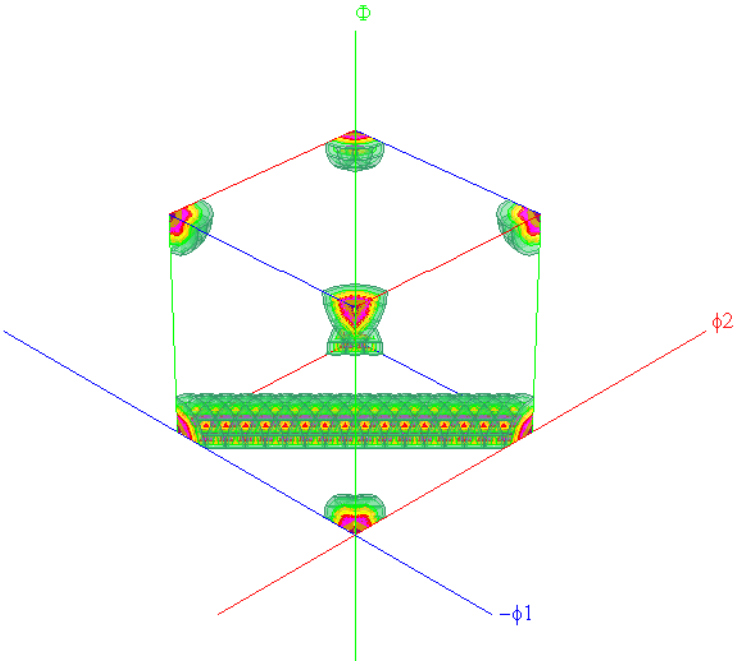


Pole figures:

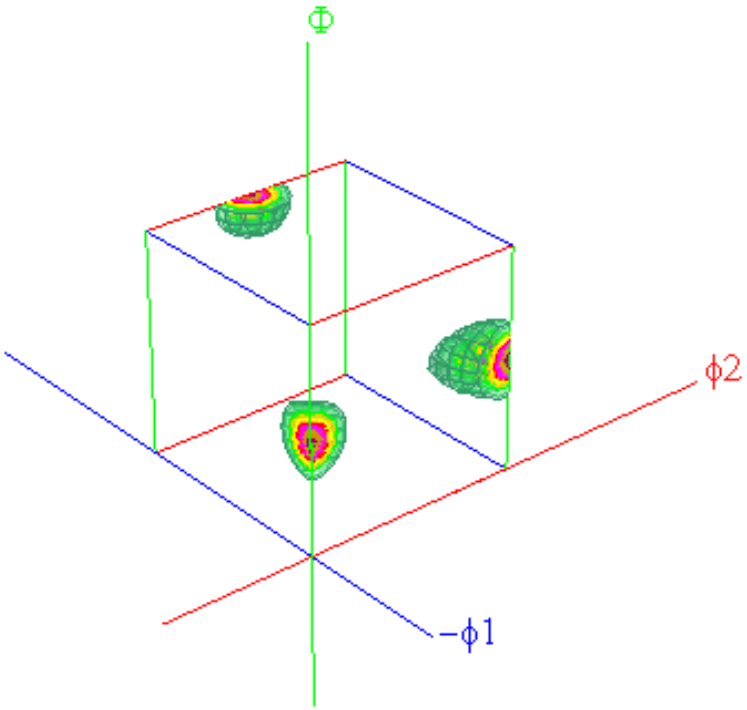
first row: pole figures for sample Ferrite (triclinic sample symmetry),
second row : pole figures calculated from ODF after frame rotation: (0,90,0) for sample Ferrite (triclinic sample symmetry)
third row: pole figures for <111>fiber model
fourth row: pole figures calculated from model ODF after frame rotation: (0.90.0)



Example 2:



Initial ODF (3D Image) – (Cubic component).



Initial ODF (ODF with Cubic component) after transformation of frame (45 degrees, Phi axis) gives ODF with Goss Orientation.

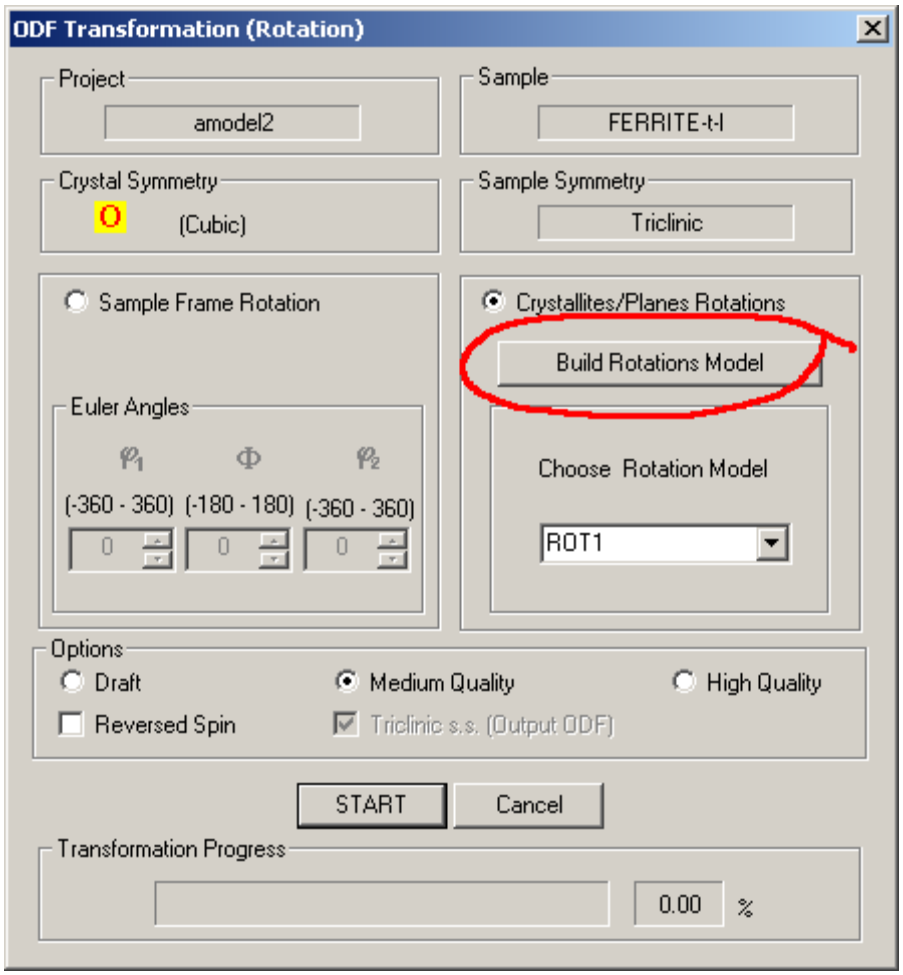
3.2. Crystalites/Planes rotations.

If you would like to make rotation some crystallites in sample and observe change of ODF then you should make this transformation in two steps:

1) Preparation and creations of model of crystallites rotations.
2) Transformation of current ODF using model of crystallites rotations.

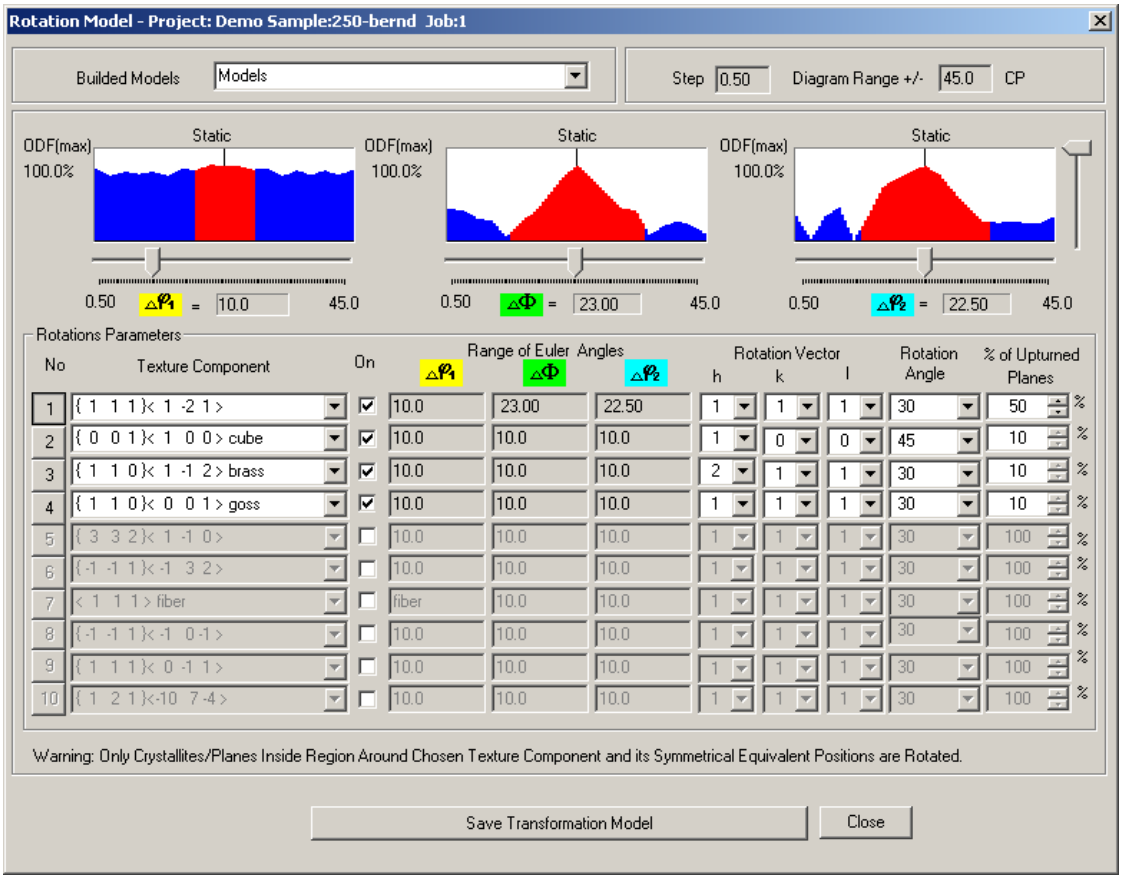
For preparation of model of crystallites rotations you should:

- click on the menu item "**ODF Transformation**" in menu "**Modelling**" and next
- choose radio button "**Crystallites/Planes Rotations**" and finally
- click on the button '**Build Rotations Model"**:



In rotation model you can choose up to 10 texture components for which you set:

- ranges of Euler angle around center of orientation – only crystallites which orientation lies inside marked area of Euler space will be rotated. LaboTex will be automatic to make calculations for all symmetrically equivalent positions of orientation.
- vector "hkl" – crystallites will be rotated around this vector;
- rotation angle – angle about which crystallites will be rotated around ‘hkl’ vektor.,
- percent of rotated crystallites (from 0 to 100%).

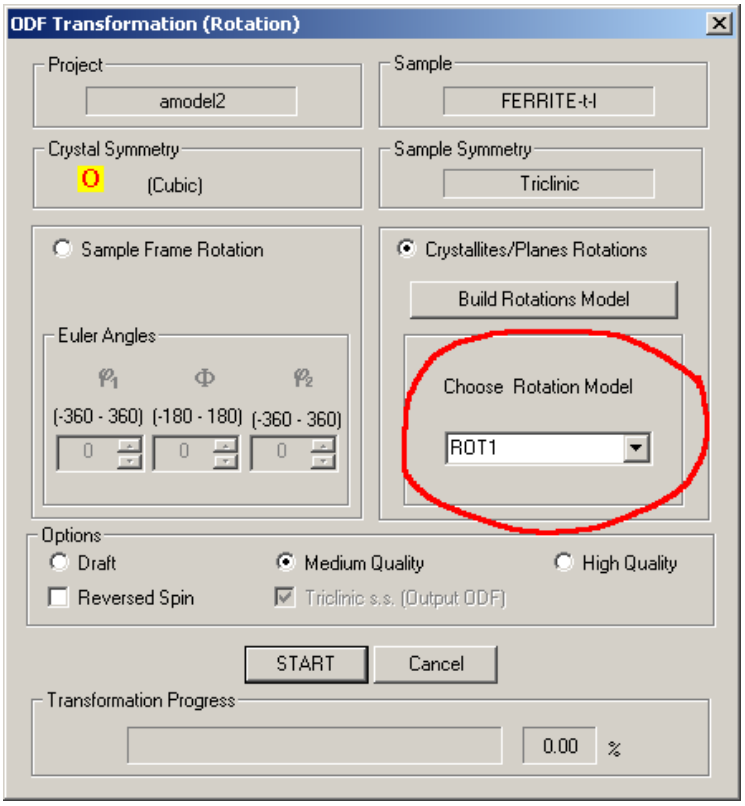


When you choose all parameters of your rotation models then click on the button **“Save Transformation Model”.** You can defined any name for your model.

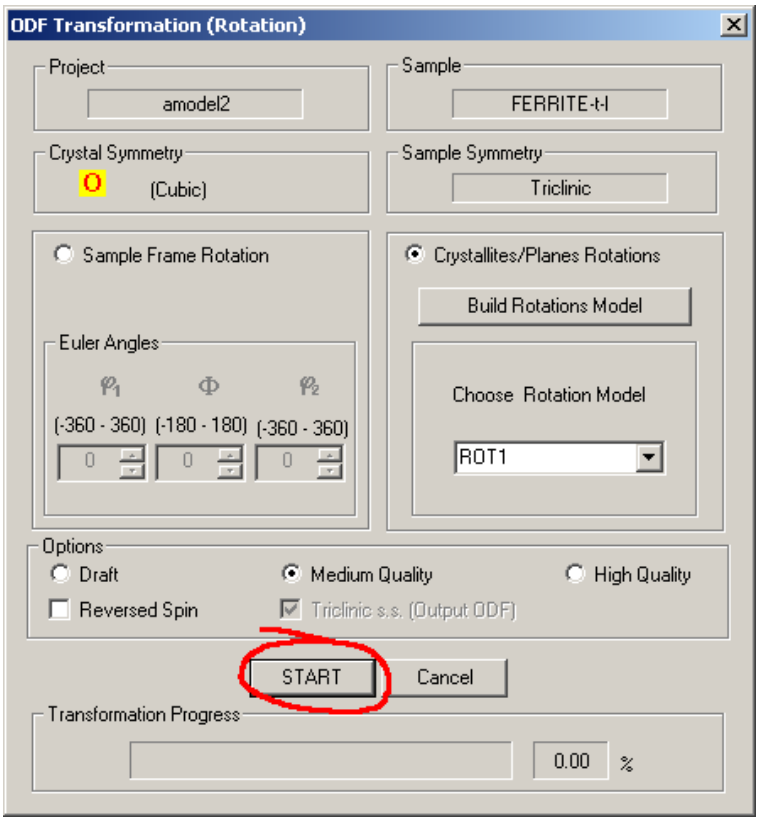
In the second step you should choose rotation model from **“Choose Rotation Model”** combo box.
Next you can choose quality of calculated ODF:

- draft (poor quality ODF – high speed of calculation)
- medium quality (medium quality ODF and medium speed of calculation)
- high quality (high quality ODF and low speed calculation).

You can also change spin of rotations.

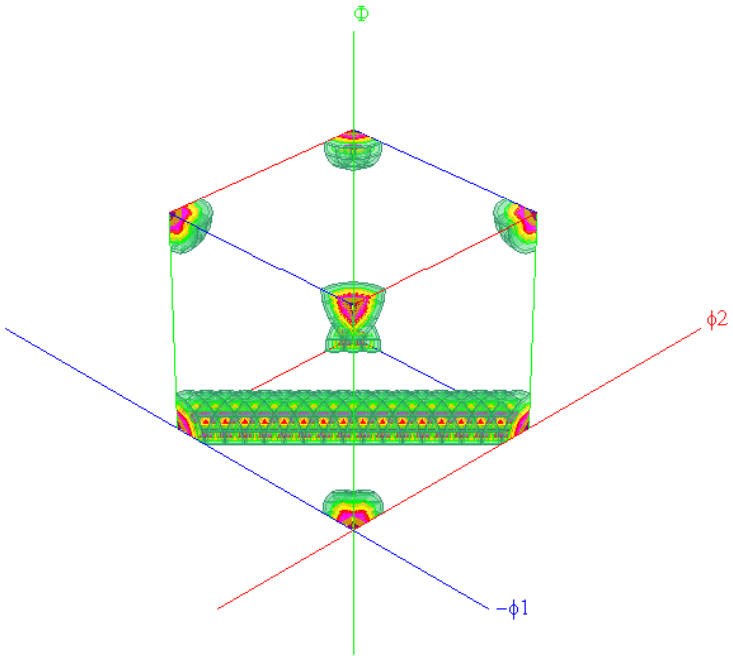


In the last step you start transformation calculation click on the **"START"** button.

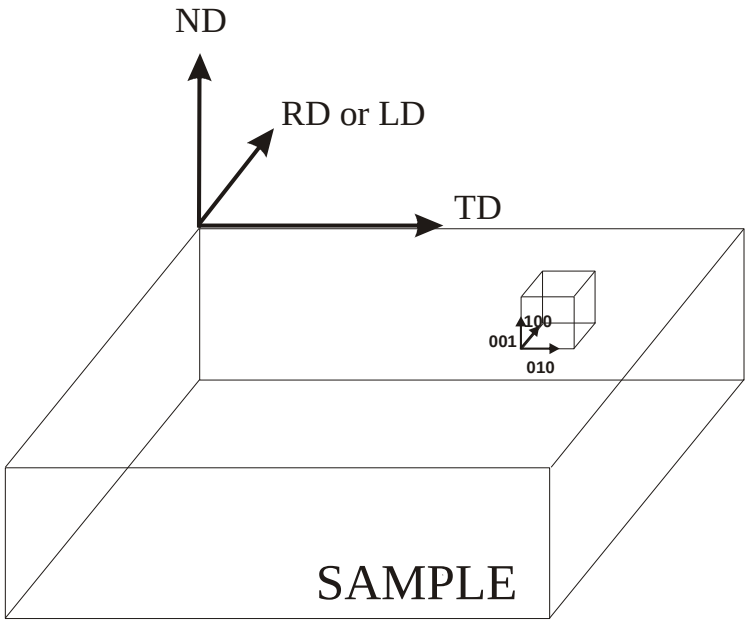


Example:

Build of model ODF using model ODF dialog (Menu "**Modelling**", item "**ODF Model**") with {001}<100> as main component.



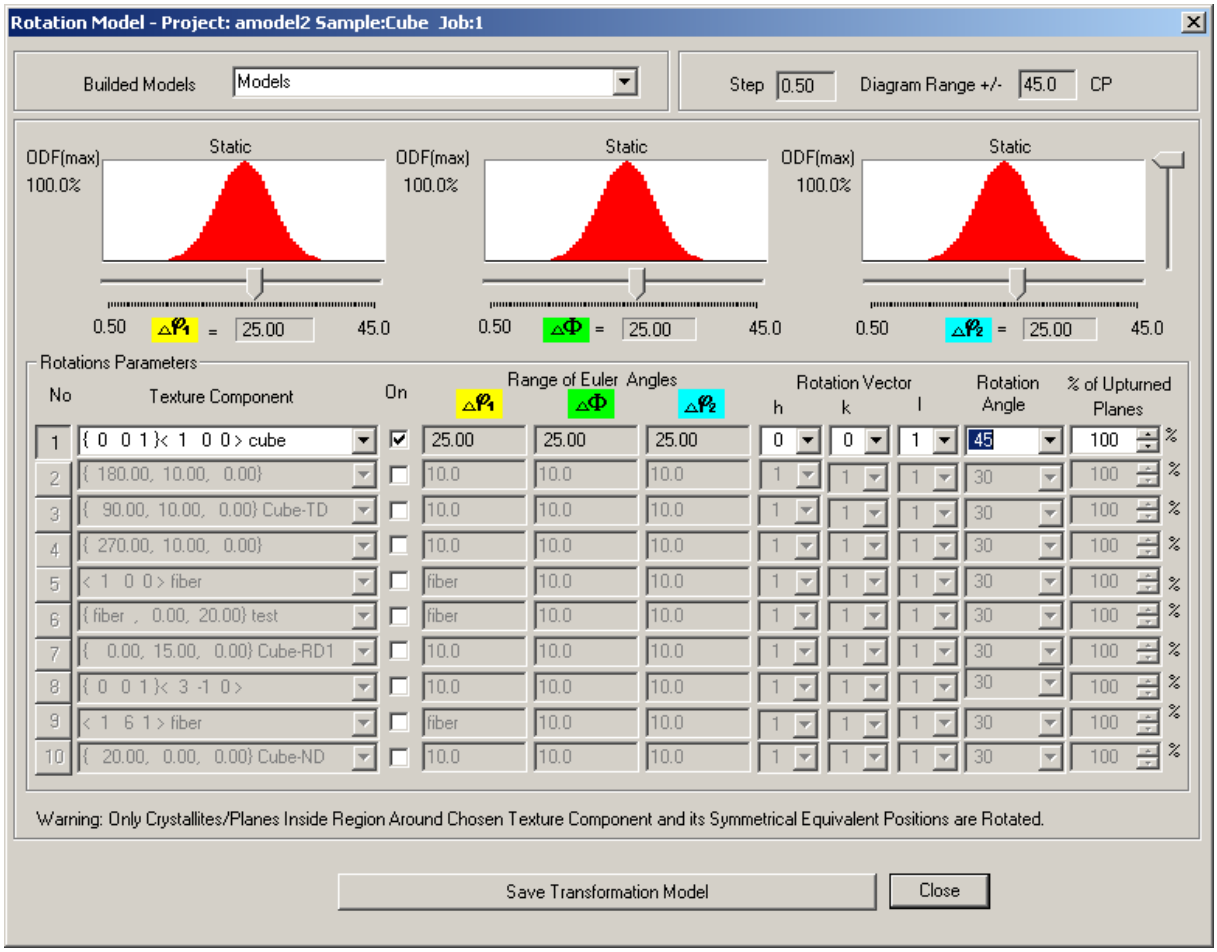
We can show some crystallite with orientation {001}<100> for this model sample :



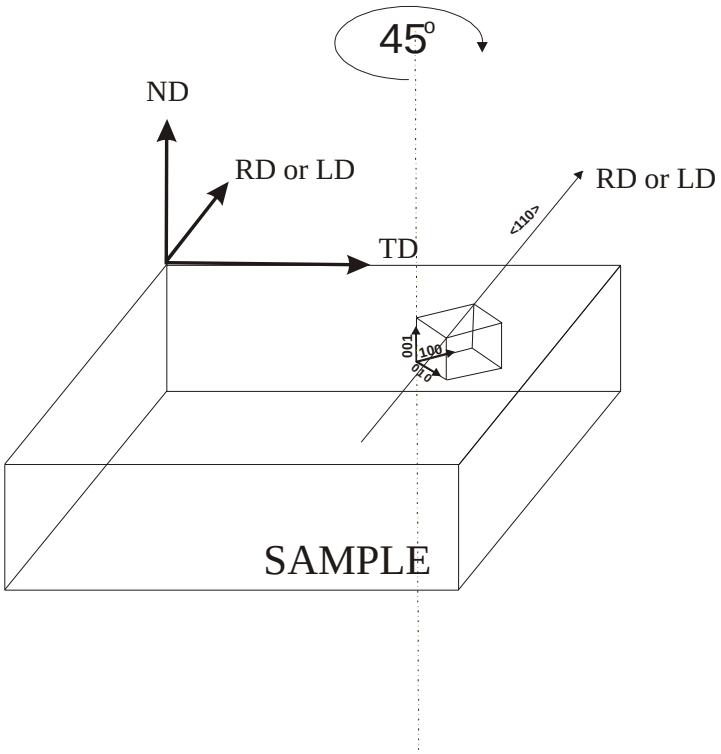
{001} – plane perpendicular to ND , <100> direction parallel to RD/LD

Next we want rotate all crystallites lying near {001}<100> orientation about 45 degrees around vector <001> (<hkl>):

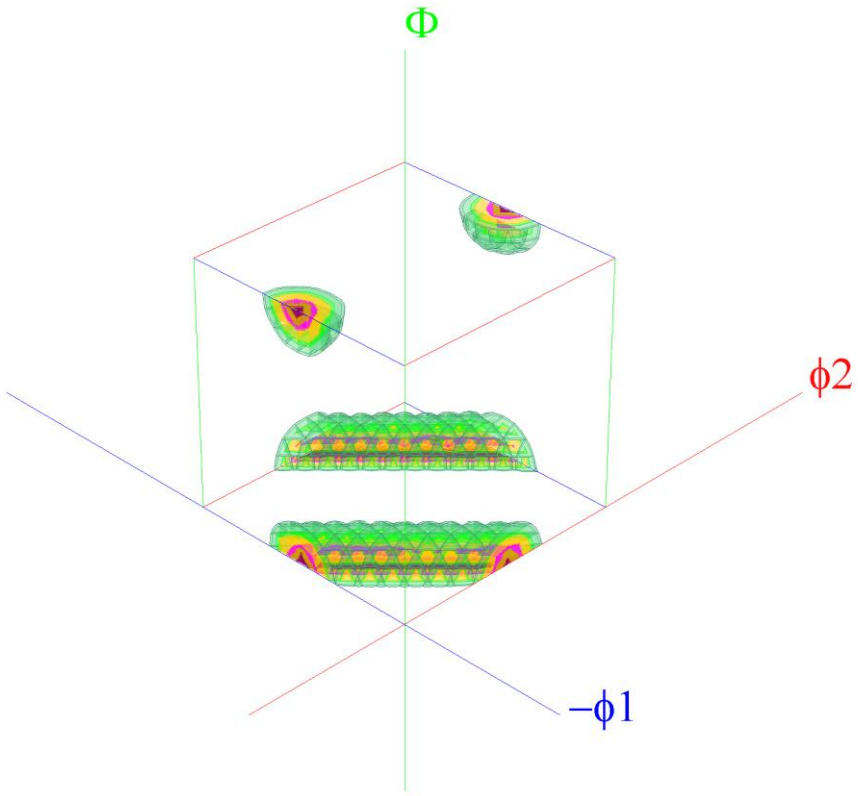
- first we choose {001}<100> from '**Texture Component**' combo box as the No. 1 (No.1 texture component should be '**On**').
- because we want rotate only crystallites lying near {001}<100> component hence we can turn off rest of texture components (No. 2 to No. 10 should be '**Off**")
- choose Euler angles ranges: 25 degrees
- vector <hkl> around all crystallites belong to chosen area of Euler space should be rotate: <001>
- rotate angle = 45 degrees
- percent of crystallites(planes)= 100% (all crystallites in range +/-25degrees for {001}<100> orientation and for all symmetrically points)



So we can show the same crystallite after model rotation <001>45°:



where {001} – plane is perpendicular to ND and <110> direction is parallel to RD/LD



ODF after model transformation: <001>45°

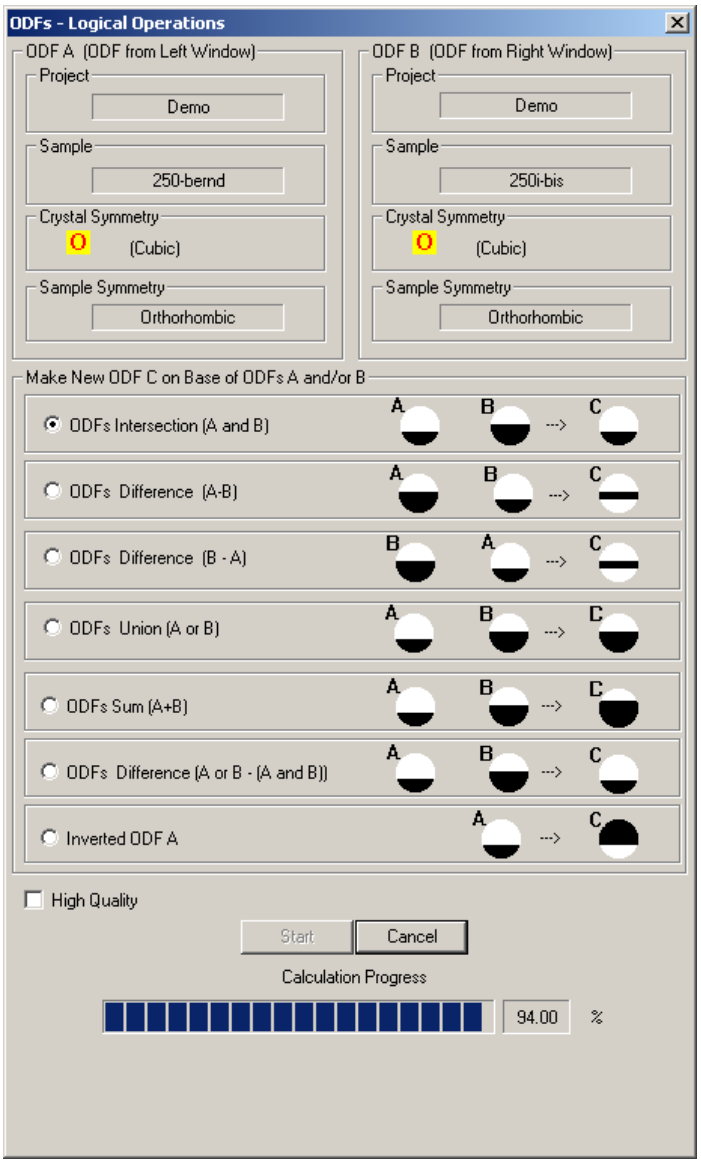
The main component in transformed ODF is {001}<110>.

4. ODFs logical operations (Modelling menu)

ODFs - logical operations. For activate this option user should switch LaboTex to ‘Compare Mode’ and next choose two ODFs for comparison: one in left window and second in right window (LaboTex Compare Mode). On the base these two ODFs (A - from left window and B from right window) LaboTex creates new ODF which is:

- **intersection** of ODF A and ODF B,
- **diference** of ODF A and ODF B (or B-A),
- **union** of ODF A and ODF B,
- **sum** of ODF A and ODF B,
- **ODF difference** : A or B - intersection A and B,
- **inverted ODF** (only for A).

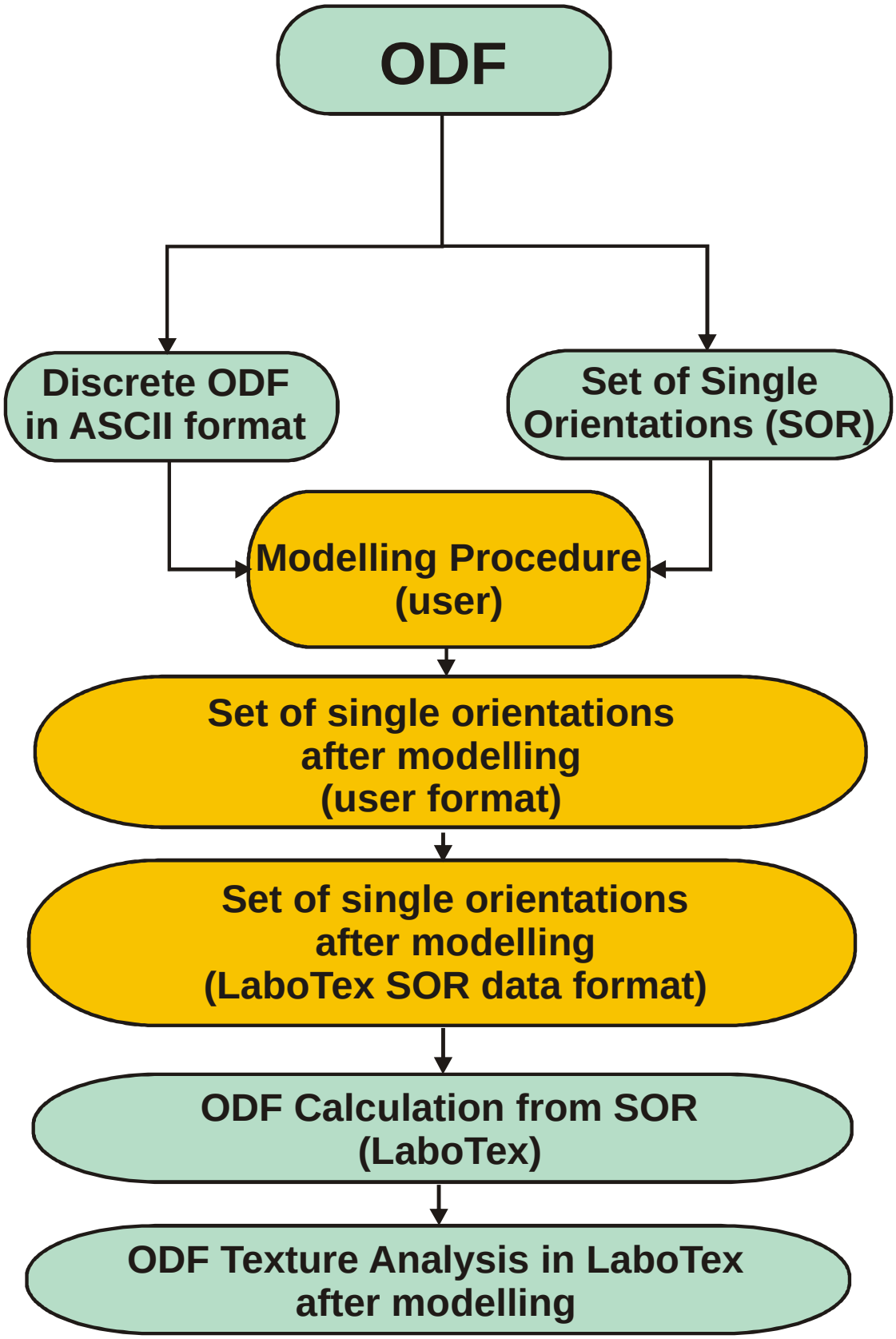
New ODF is created in new Job for sample of ODF A. You can copy and paste these diagrams to other applications or you can made images in 'BMP' ot 'TIF' format (menu 'Edit').



5. ODF modelling using own calculation procedures

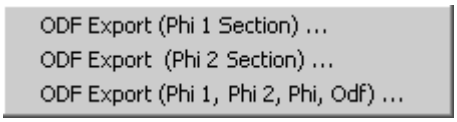
User can use ODF created by LaboTex to own modelling in following ways:

1) exports of ODF data in ASCII format;
2) creates of file with set of single orientation generated on the base of current ODF.



5.1. ODF Export

The option lets on the saving ODF data to the ASC file (option available from menu "**File**"). The user can choose one from among three data formats:



a) **ϕ_1 section - ''ODF Export (Phi 1 Section)...''** :
print to file ϕ_1 section of ODF. First value in first line is a ϕ_1 value. Next data in first line are values of ϕ_2 angle while first column contains values of Φ angle:

```
        ODF projection PHI1
PHI1  PHI2 --->
   PHI
    |       ODF values
    |
    V
```

For example (ODF section for ϕ_1=0):

.0	.0	5.0	10.0	15.0	20.0	25.0	30.0	...	60.0	65.0	70.0	75.0	80.0	85.0	90.0
.0	.90	1.02	1.31	1.72	2.08	2.17	2.08	...	2.05	2.10	1.98	1.61	1.23	.96	.86
5.0	1.80	1.68	1.81	2.30	2.53	2.40	2.01	...	1.97	2.35	2.43	2.06	1.58	.97	.65
10.0	2.17	2.03	2.24	2.73	2.61	2.03	1.40	...	1.20	1.32	1.33	1.14	.93	.65	.48
15.0	2.34	2.19	2.38	2.74	2.26	1.43	.81	...	.49	.48	.41	.32	.27	.20	.16
20.0	2.56	2.32	2.27	2.18	1.48	.81	.42	...	.18	.21	.22	.22	.21	.16	.12
...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...
70.0	2.24	2.24	2.36	2.15	1.47	.81	.42	...	.19	.22	.23	.23	.21	.17	.14
75.0	1.95	2.06	2.50	2.64	2.09	1.32	.75	...	.47	.47	.41	.31	.24	.20	.18
80.0	1.67	1.81	2.34	2.74	2.55	1.98	1.36	...	1.20	1.37	1.41	1.15	.86	.69	.61
85.0	1.25	1.37	1.84	2.43	2.70	2.51	2.06	...	1.97	2.38	2.42	1.97	1.48	1.07	.86
90.0	.88	.99	1.27	1.66	2.03	2.13	2.07	...	2.07	2.13	2.03	1.66	1.27	.99	.88

b) **ϕ_2 section - ''ODF Export (Phi 2 Section)...''**:
Print to file ϕ_2 section of ODF. First value in first line is a ϕ_2 value. Next data in first line are values of ϕ_1 angle while first column contains values of Φ angle:

```
        ODF projection PHI2
PHI2  PHI1 --->
   PHI
    |           ODF values
    |
    V
```

Example is analogically as for ϕ_1 section.

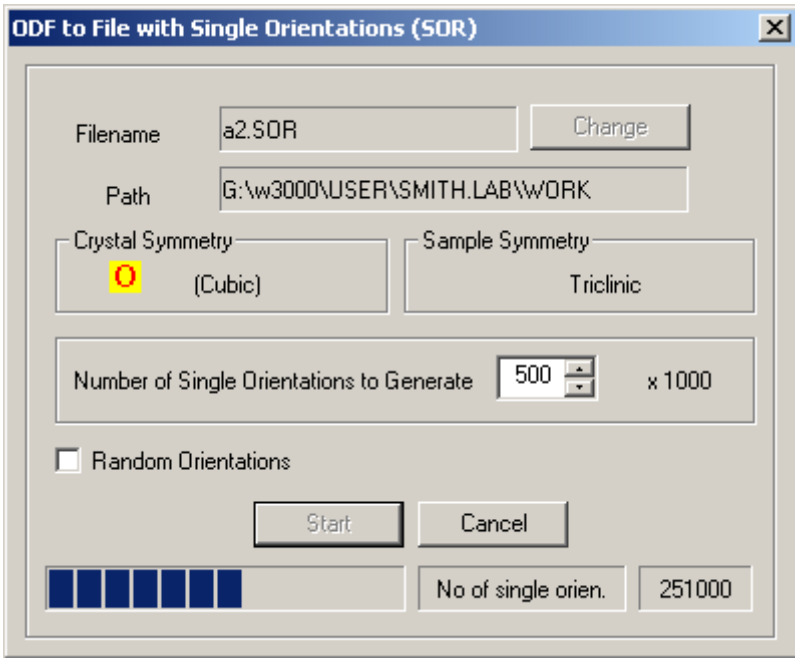
c) **ϕ_1, ϕ_2, Φ, ODF value - "ODF Export (Phi 1 ,Phi 2, Phi, Odf)...**":
Print to file ODF in format: ϕ_1, ϕ_2, Φ, ODF (four values in each line).

For example:

PHI1	PHI2	PHI	ODF
0.00	0.00	0.00	0.592089E+00
5.00	0.00	0.00	0.637786E+00
10.00	0.00	0.00	0.909632E+00
15.00	0.00	0.00	0.553926E+00
20.00	0.00	0.00	0.414515E+00
25.00	0.00	0.00	0.451965E+00
.....	.....	.....	.....

5.2 Set of single orientation on the base of current ODF

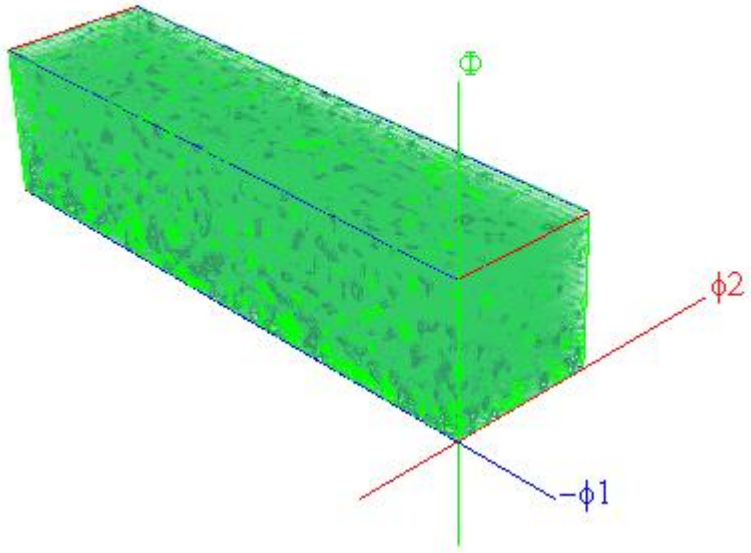
LaboTex can create set of single orientations on the base of current ODF. User can use this set in own modelling procedure and return "SOR" file after modelling. In this manner user receive new ODF after own calculation. On the base of this ODF user can make texture analysis, pole figure calculation volume fraction calculations etc. This option is important for user which modelling deformation (VCS users). User can choose number of single orientations from 10000 to 9999999.



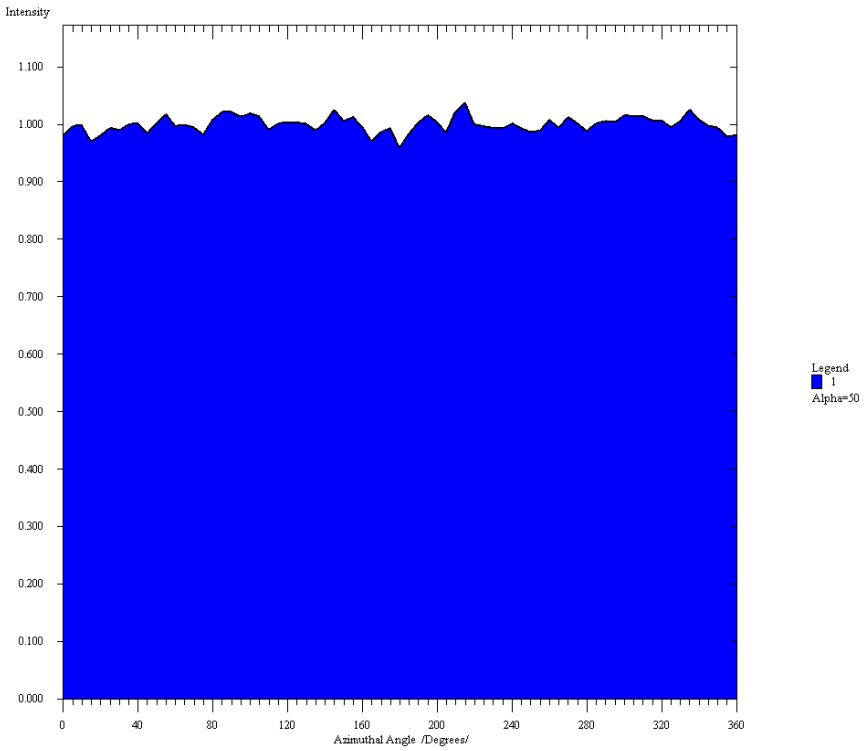
User can also generate random set of single orientation using this option. SOR file creates by LaboTex user can input as a new sample and he can make ODF calculation.

Examples:

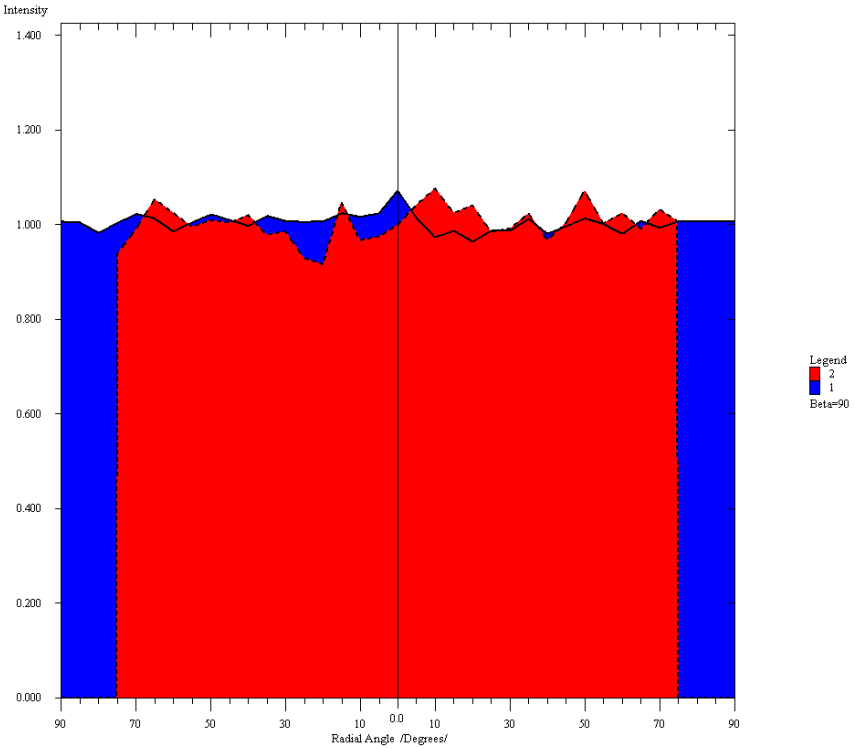
ODF creates on the base set of 500,000 single orientations generates with 'Random' option:



Section of pole figure {111} calculated on the base above 'Random' ODF:



Comparison pole figure for real texure free (random) sample (red) with pole figure generates from 'random' ODF creates on the base set of 500,000 single orientations (blue):



Format of file with single orientations data is very simple:

***filename*.*SOR* – S**ingle **OR**ientation File i.e. experimental**,** single orientation set in LaboTex format
Description of ***filename*.*SOR*** data format:

Line	No of data in line	Description	Type
1 - 2		Arbitrary title	Character
3		Remarks for data in line 4	
4	1	Structure Code (symmetries after Schoenflies): 1 - C_1 (triclinic) 2 - C_2 (monoclinic) 3 - D_2 (orthorhombic) 4 - C_4 (tetragonal) 5 - D_4 (tetragonal) 6 - T (cubic) 7 - O (cubic) 8 - C_3 (trigonal) 9 - D_3 (trigonal) 10 - C_6 (hexagonal) 11 - D_6 (hexagonal)	Integer
4	2	Lattice constant, a (absolute or relative)	Real
4	3	Lattice constant, b (absolute or relative)	Real
4	4	Lattice constant, c (absolute or relative)	Real
4	5	Lattice angle, α in degrees	Real
4	6	Lattice angle, β in degrees	Real
4	7	Lattice angle, γ in degrees	Real
4	8	Step for output ODF (grid cells). Permissible values (deg): 1.0, 1.2, 1.25, 1.5, 2.0, 2.5, 3.0, 3.75, 5.0, 6.0, 7.5, 10.0*	Real
4	9	*Weight* for data (1 – present, 0 – absent)	Integer
4	10	Angle Unit: 0 – deg, 1 – rad	Integer

4	11	Angle Convention: 0 – Bunge 1 – Roe	Integer
5 to the end	1	ϕ_1	Real
5 to the end	2	Φ	Real
5 to the end	3	ϕ_2	Real
5 to the end	[4]	Weight (optionally) (if parameter *weight* in line 4 is 1)	Real

Note: Real and integer input data must be separated in line by one or more spaces.