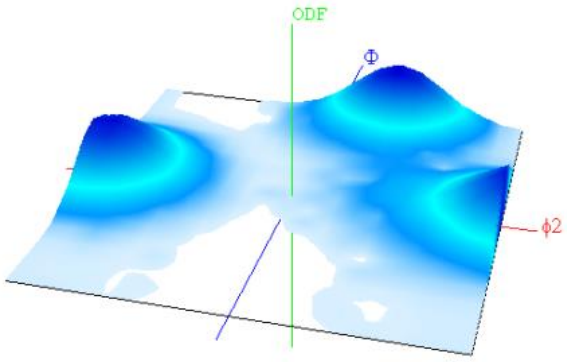
LABSOFT

LaboTex

Version 3.0

The Texture Analysis Software for Windows



Determination of Volume Fraction of Texture Components Using LaboTex - Model Functions Method

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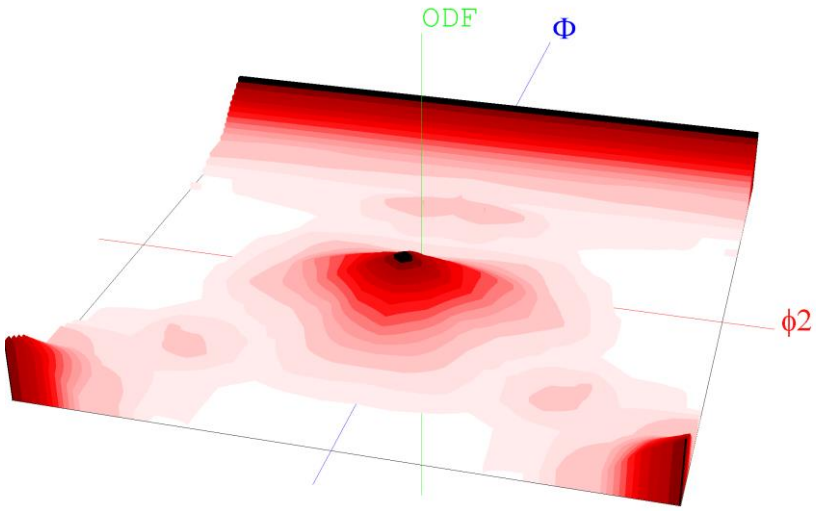
This is an example on how to use LaboTex to determine of volume fraction of texture components. Analysed ODF with axial sample symmetry is shown in the picture below:



Step 1 - Texture Components

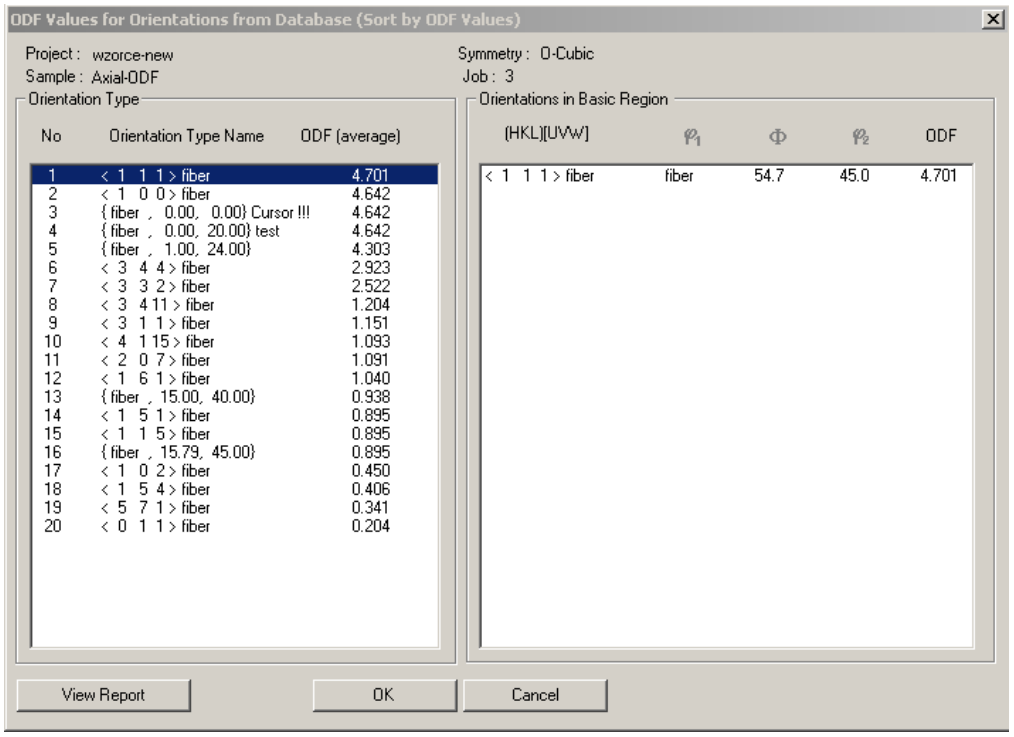
In first step we have to find main texture components of ODF. For this purpose we use orientation analysis :

We can use both methods : automatic and manual.

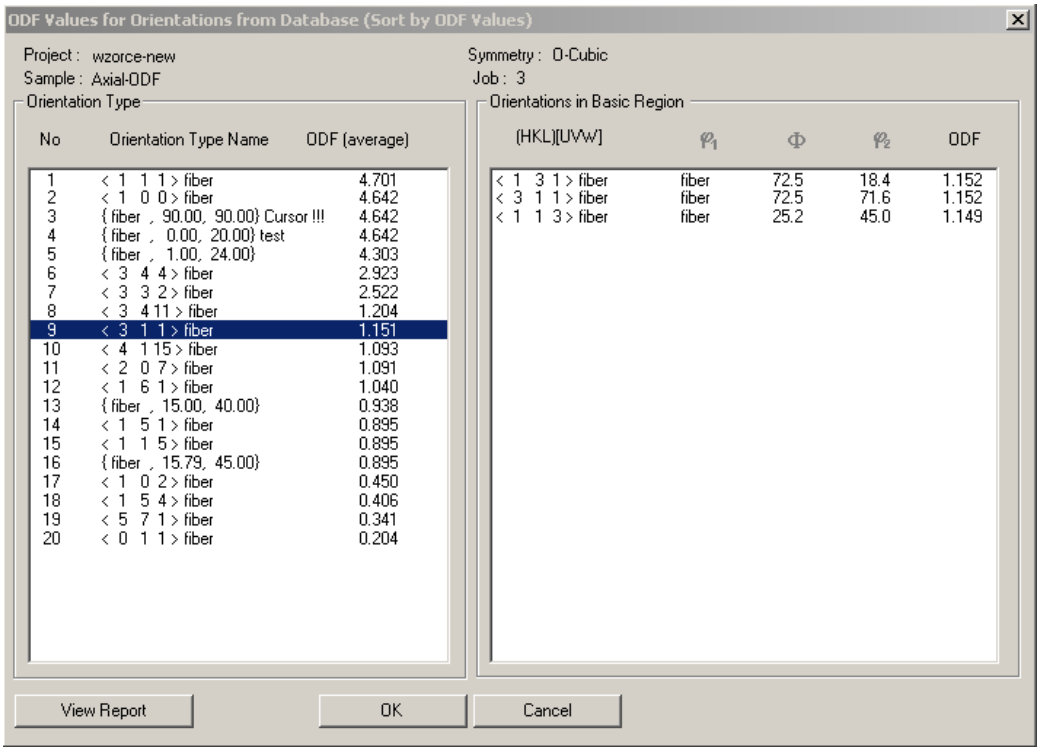
Automatic method (SORT)

In automatic method LaboTex use texture components from database. First LaboTex calculates average ODF values (arithmetic mean) for each components from database on the base of ODF values for all symmetrically equivalent orientations of component. In the next step LaboTex sorts average ODF values for all components from database. When you press 'SORT' button

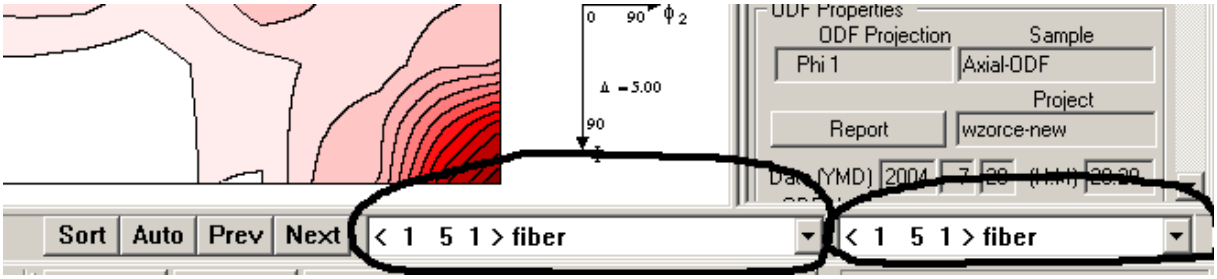
then you can see all components from database and their average ODF values.



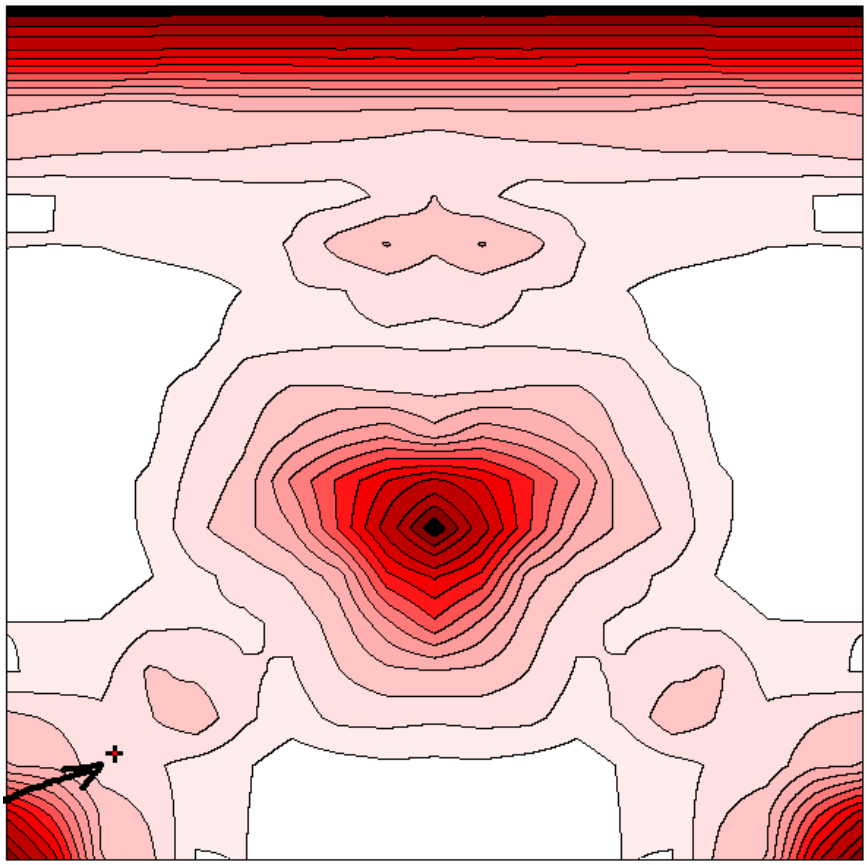
In the list from right side you can see ODF values for each symmetrically equivalent orientations of component. There is only one orientation for ***<111>fiber*** component (***<111>fiber*** component has not symmetrically equivalent orientations).
When you click on the ***<311>fiber*** component you can see 3 symmetrically equivalent orientations, their ODF values and Euler angles:



Next, you can check whether all maxims in analyzed ODF are described by texture components. In marked area (picture below – area from left) is the Combobox in which you can change the active texture component. The second Combobox (in area from right) allows you to change of the symmetrically equivalent orientations for active component.



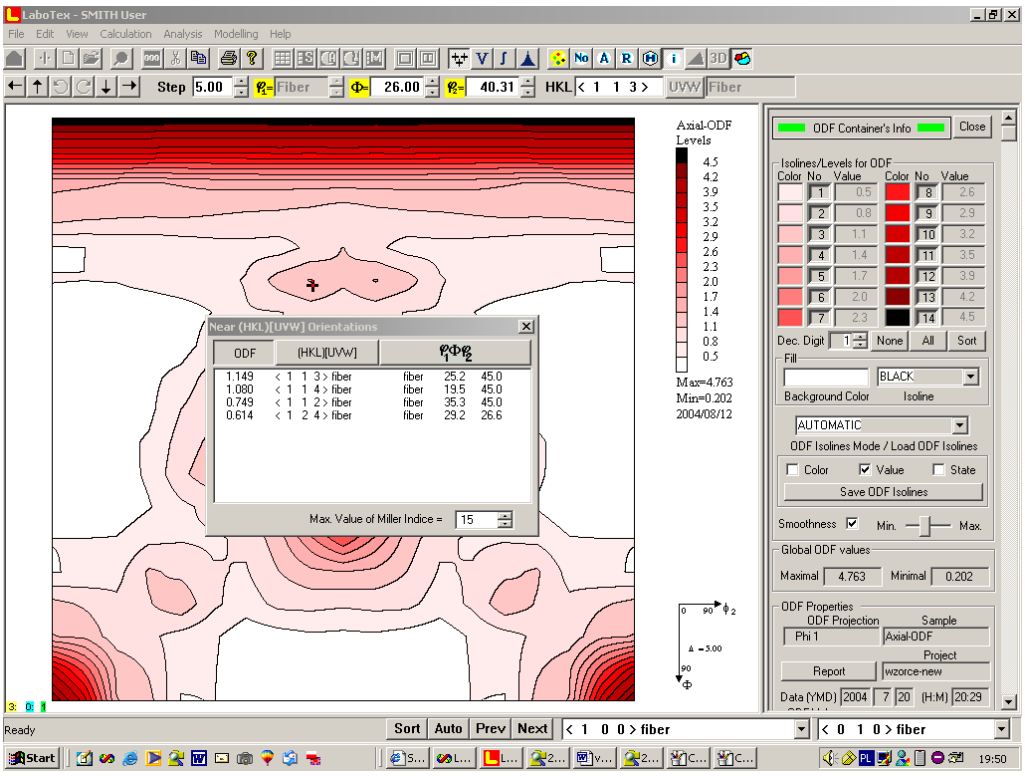
LaboTex displays cross mark (+) in place where lies in ODF projection selected orientation for active component.



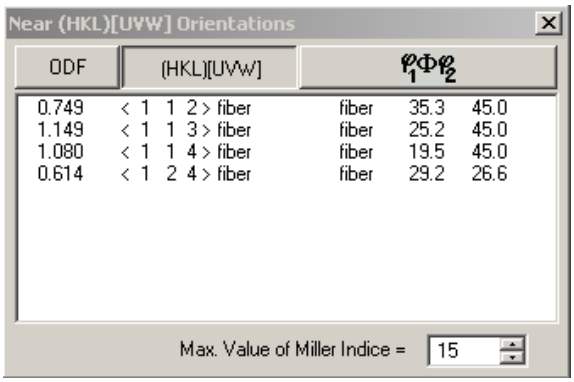
LaboTex displays only one cross mark for one symmetrically equivalent orientation. If you would like see place in the ODF where lies other symmetrically equivalent orientation then you choose it from Combobox. Analogically, you can change texture component which is displaying by LaboTex. When you have found maxim which is not described by components from your database in LaboTex then you should find this component using manual method. Next you should add this component to your database in LaboTex.

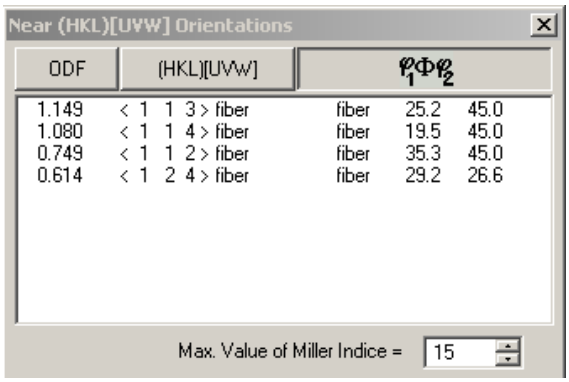
Manual method

You can use *"Near {HKL}<UVW> Orientations"* dialog for finding of components by manual method. You should click left mouse button in local or global maxim of ODF in which you would like find texture component. You can also choose item *"Near {HKL}<UVW> Orientations"* from menu *'Analysis'* :



LaboTex display near orientations sort by: ODF value (image above), miller indices (image below - left) or misorientation (image below - right). You can change type of sort by click in appropriate button.



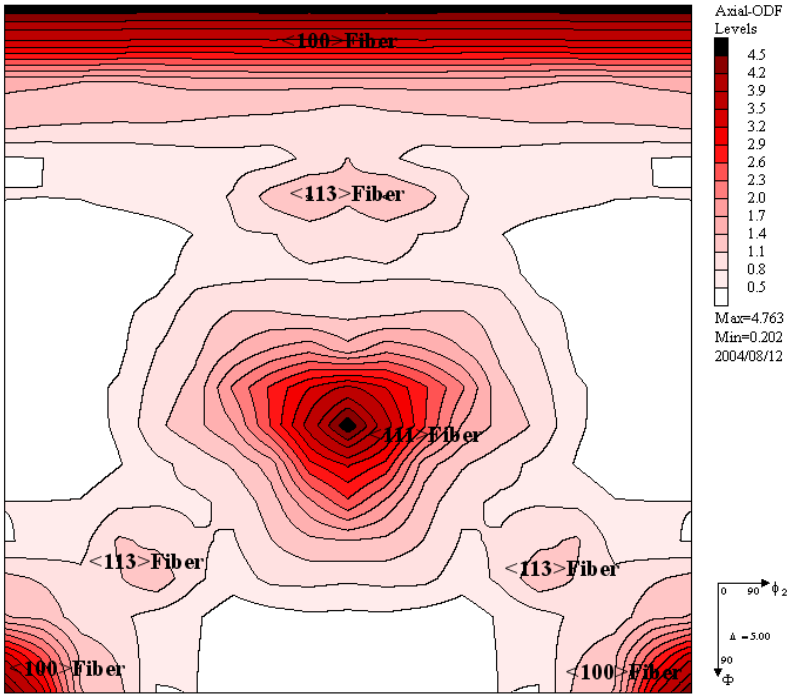


You can also change maximal value of miller indices.

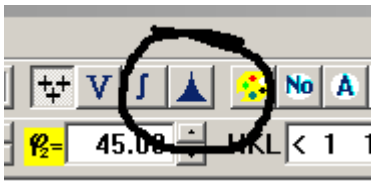
Step 2 - First approximation

After step 1 we have found that we can describe all maxims of analyzed ODF using 3 components:

- <111> Fiber (none symmetrically equivalent orientations)
- <113> Fiber (3 symmetrically equivalent orientations)
- <100> Fiber (2 symmetrically equivalent orientations+orientation for Φ=0)



You can open dialog for determination of volume fraction of texture component by model function method using the icon as below:



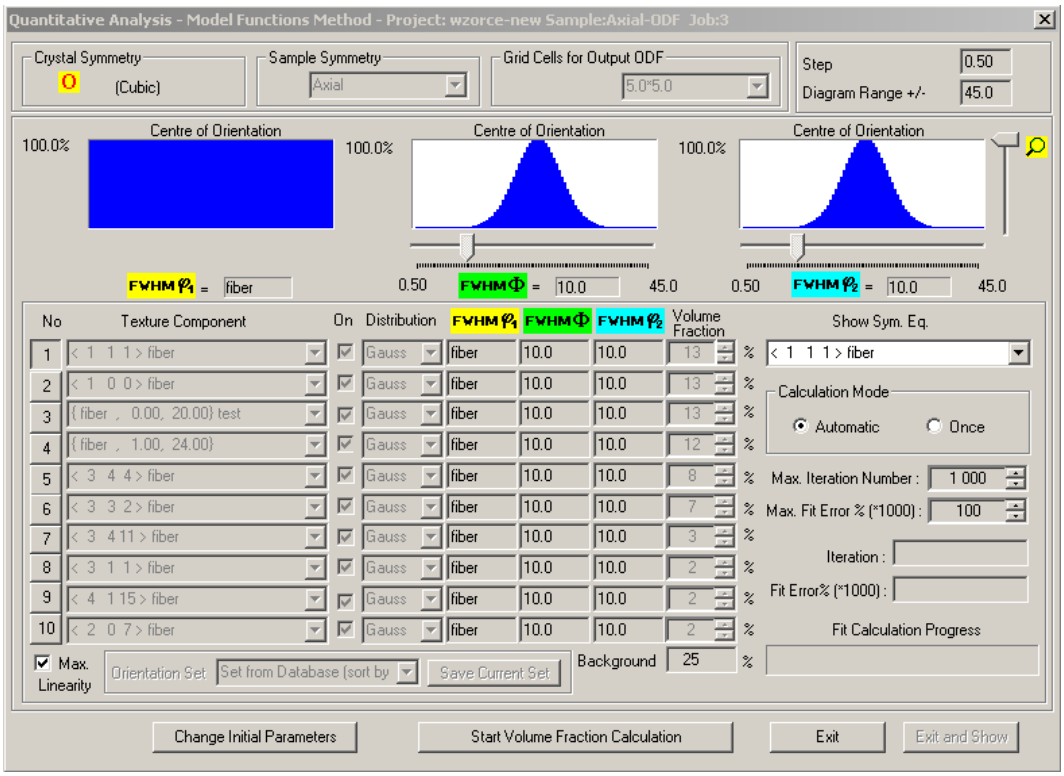
or you can use a suitable item from menu '*Analysis*'.
Dialog window help you in least-squares fitting of the model functions to your ODF and in creations of model ODF nearest to the experimental ODF. LaboTex automatic use in calculation following parameters from analyzed experimental ODF:

- crystal symmetry;
- sample symmetry;
- cell parameters;
- grid cell.

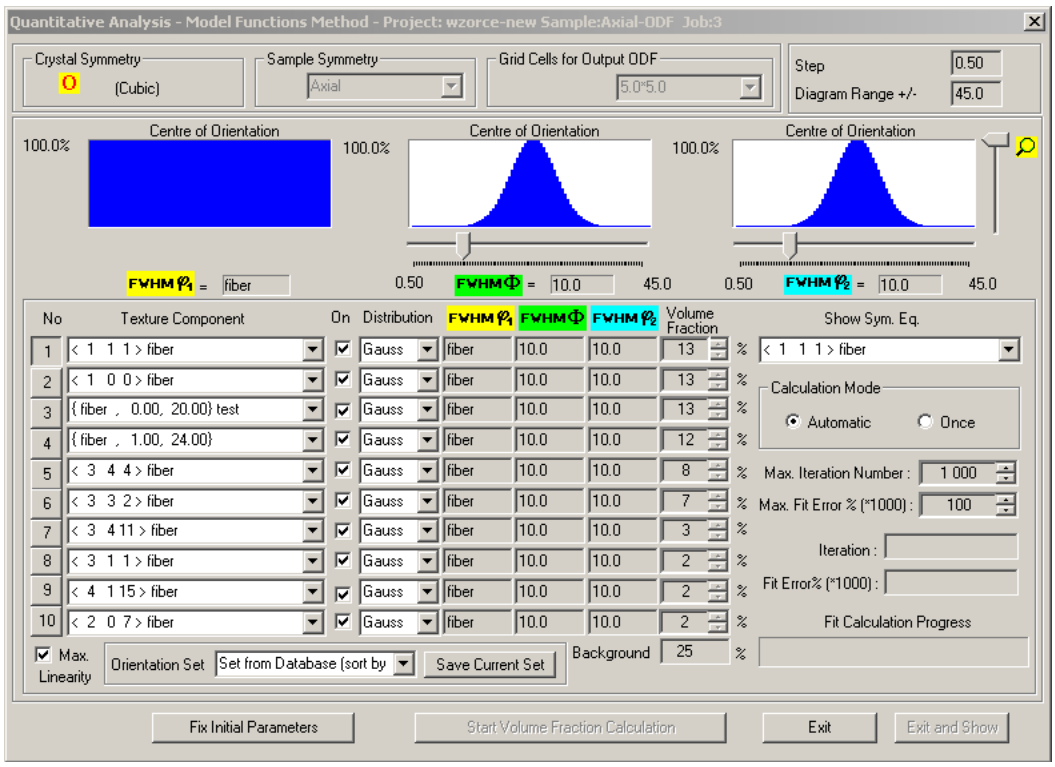
These parameters are grayed and user can't change them.
When you start dialog window LaboTex calculates average ODF values for components and sort components using average ODF values. Hence component No. 1 is the component which has the greatest average ODF value. LaboTex fill also initial parameters for model functions:

- distribution (set to '*Gauss*');
- FWHM for Θ_1, Φ and Θ_2 (all set to 10.0 degrees);
- Volume fraction and background (initial values set on the base of average ODF values of components).

You can start calculations or you can change initial parameters by click mouse on the suitable button.



When you click mouse on the '*Change Initial Parameters*' then the new options are available.

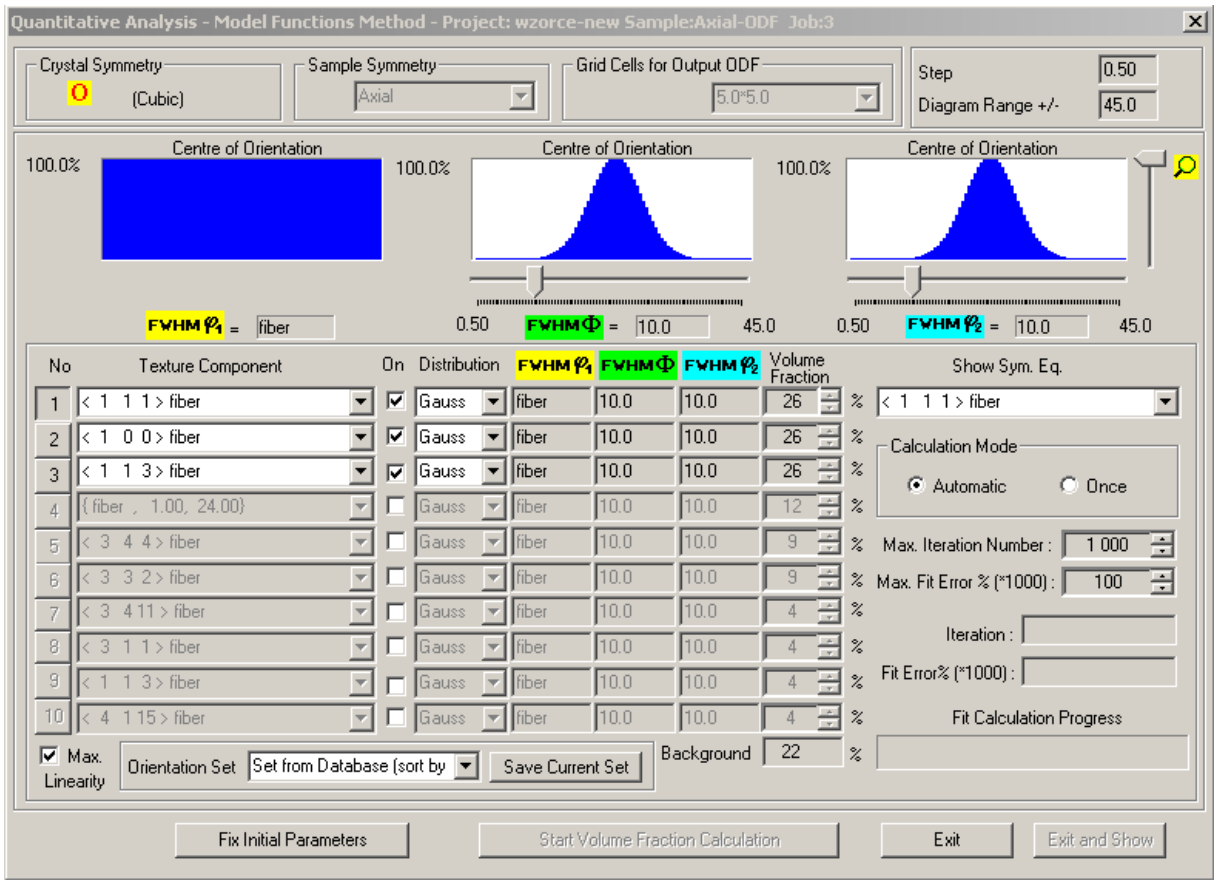


You can change:

- texture component (using suitable Combobox);
- turn on/off component from calculations (using suitable Checkbox);
- set kind of distribution (Gauss or Lorentz);
- set initial FWHM for each Euler angle;
- set initial volume fraction of component.

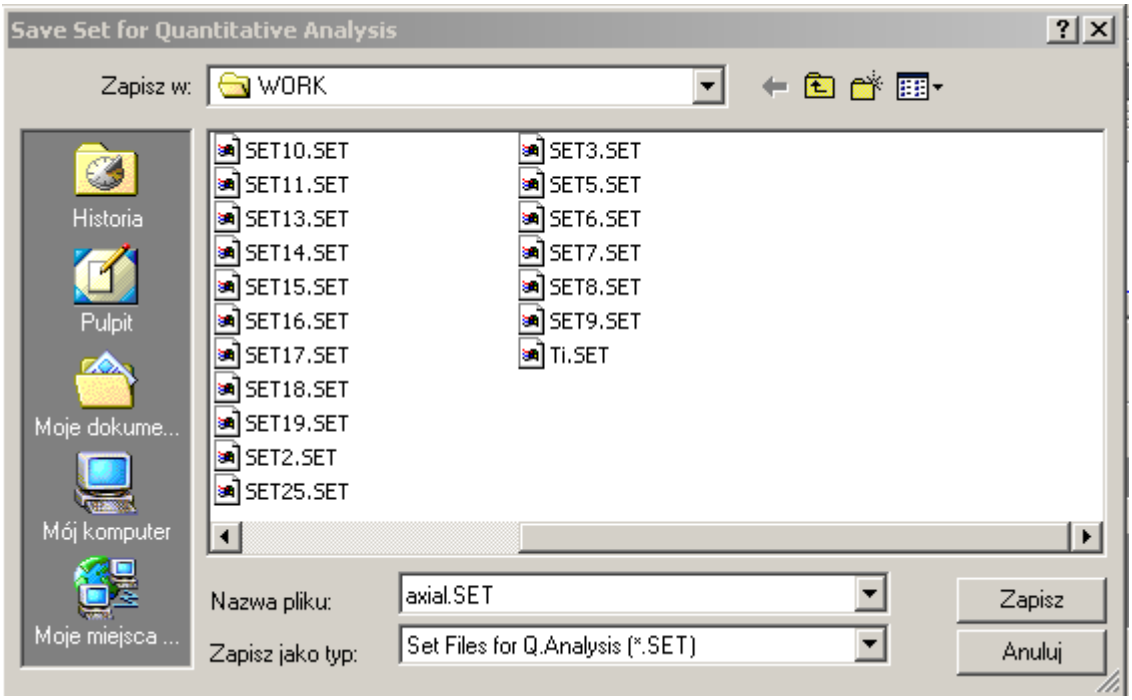
Three diagrams in dialog window show model function for each Euler angle for choosen component. You can change selection of component by click mouse on the *'No.'* button. In case of axial sample symmetry only Φ and Θ_2 Euler angles are essential and available. You can magnification plot of model function by change of slider position.

Now, you should set texture components which you have found in previous step. First two components, proposed by LaboTex are good (LaboTex prompts: <111>fiber and <100>fiber). You should change only component No. 3 and next you should turn off components number 4 to 10 from further calculations.



You can save current set of components by click mouse on the "*Save Current Set*" button:

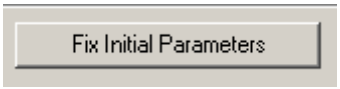
You can accept file name proposed by LaboTex or you can set other file name - for example '*axial.SET*':



LaboTex remembers this set and you can input this set from the list of Combobox:

The default set (set proposed by LaboTex when dialog starts) is set build on the base of the database sort by ODF value:

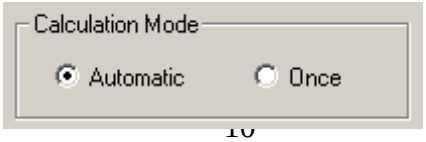
When you have finished setting up of initial parameters you should click on the "*Fix Initial Parameters*" button :



Now you can set up last two parameters of fitting calculation:

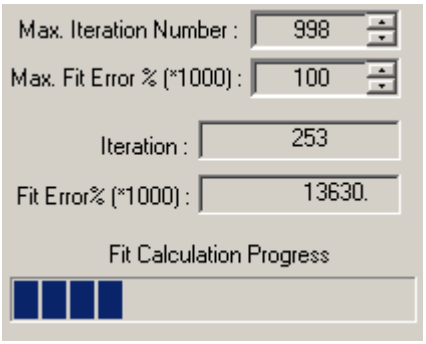
- Maximal Number of Iteration (default is 1000);
- Maximal Fit Error in percent (where fit error is relative error between model and experimental ODF). You should input to LaboTex value of error multiply by 1000 (default is 100 => 0.1%).

These parameters are essential when LaboTex is in 'Automatic' mode. This mode is default .



In this mode LaboTex finish calculation when number of iteration is greater than maximal number of iteration or when fit error is lower than maximal fit error. The second mode of fitting calculation is '*Once*'. In this mode LaboTex creates model ODF on the base of initial parameters of selected texture components and next it calculates and displays the fit error. User can change initial parameters and he can start calculation once more. This is a 'manual' method of fitting. You can start fitting calculation by click on the "*Start Volume Fraction Calculation*" button:

LaboTex displays number of iteration and fit error during calculation. You can also observe fit calculation progress:



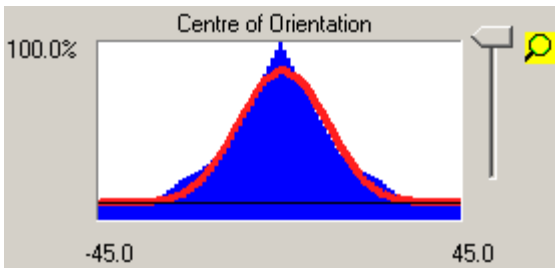
Click on the "Calculation Break" button to break calculation in any moment:

Next you can change initial parameters and start calculation once more.
When LaboTex has finished calculation it displays diagrams for each Euler angle, where LaboTex shows comparison between model and experimental ODF. There are two mode for comparison diagrams:

- Normal (*'Norm.'*);
- Difference (*'Diff.'*).

You can change mode by click mouse on the button *'Norm.'* or *'Diff.'*.
In '*Norm.*' mode LaboTex displays diagrams using colors:

- blue (blue area) - for experimental ODF around of center of symmetrically equivalent orientation of component (diagrams are for each Euler angle);
- red (red line) - for model ODF;
- black (black line) - for background of the model ODF ('*random*' texture component).



In 'Diff.' mode LaboTex displays diagrams using color:

- blue (blue area) - for common area of experimental and model ODF;
- red (red line) - for non-common area of experimental and model ODF;
- black (black line) - for background of the model ODF.

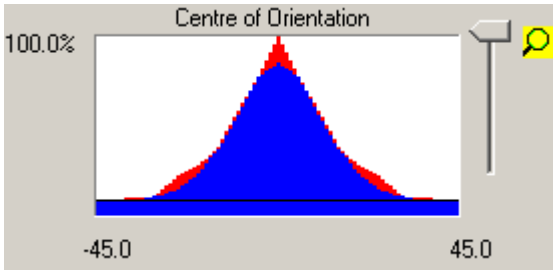


Figure below shows complete dialog window with diagrams for <111> fiber component in 'Norm.' mode.

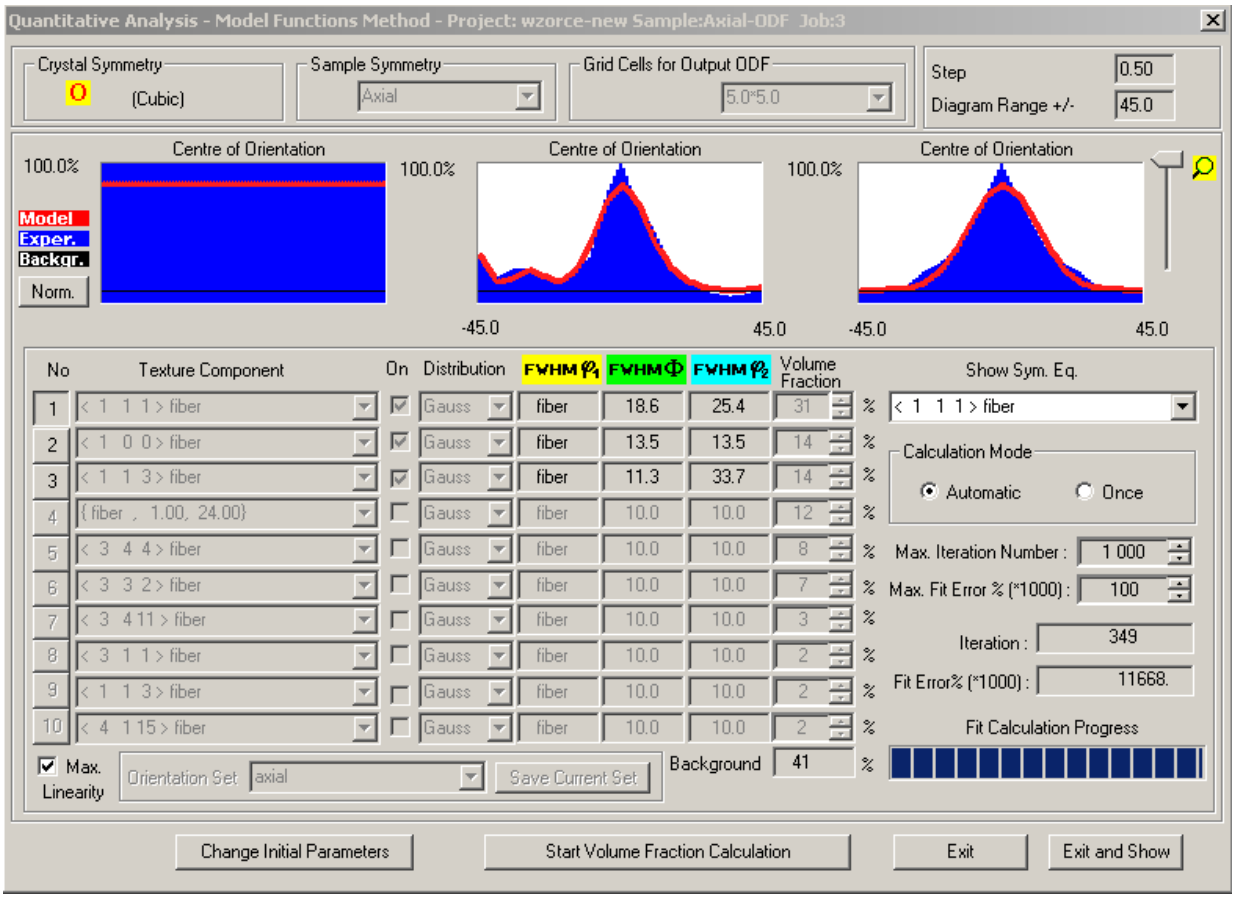
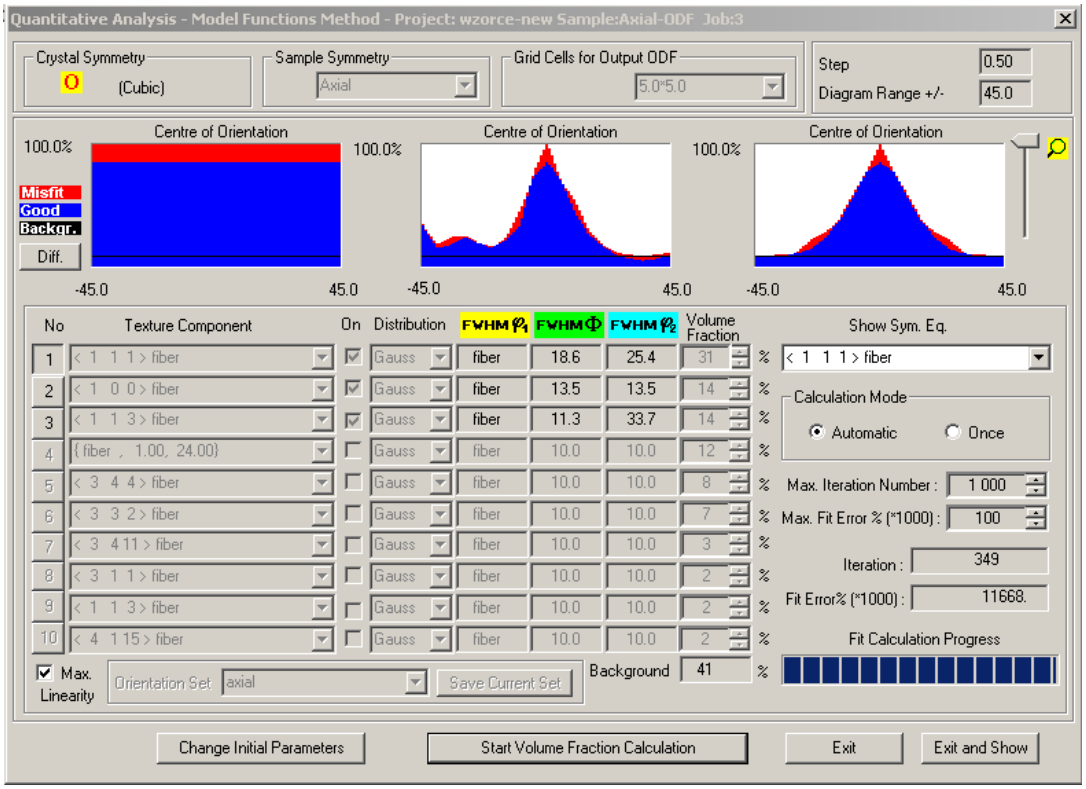
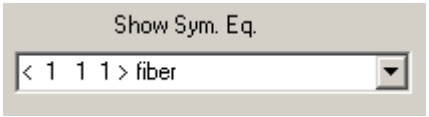


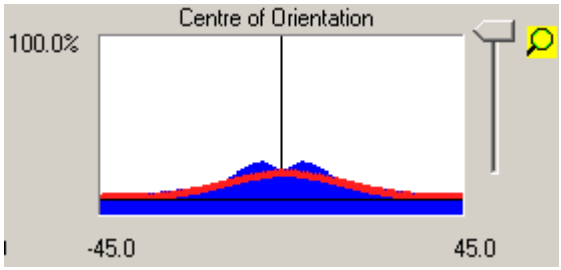
Figure below shows complete dialog window with diagrams for <111> fiber component in 'Diff.' mode.



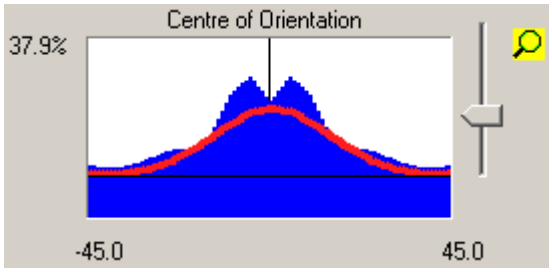
You can choose any symmetrically equivalent orientation from the "*Show Sym. Eq.*" Combobox to display the comparison diagrams:



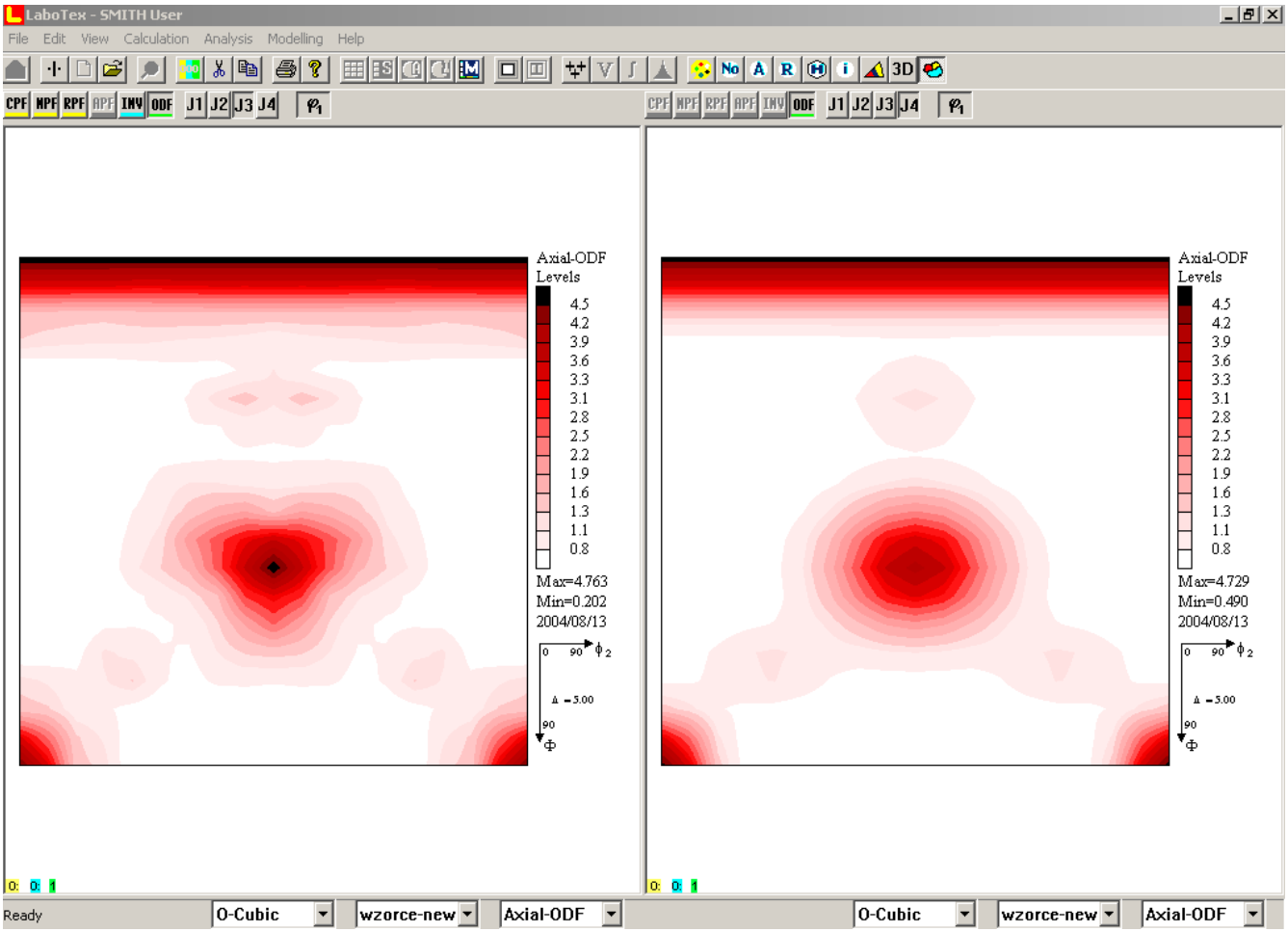
Component *<113>fiber* is weak in comparison with *<111>fiber*, hence quality of diagrams is bad.



You can change magnification of component plot using slider. Value in left corner (37.9%) of diagram shows on the percent of maximal ODF value.

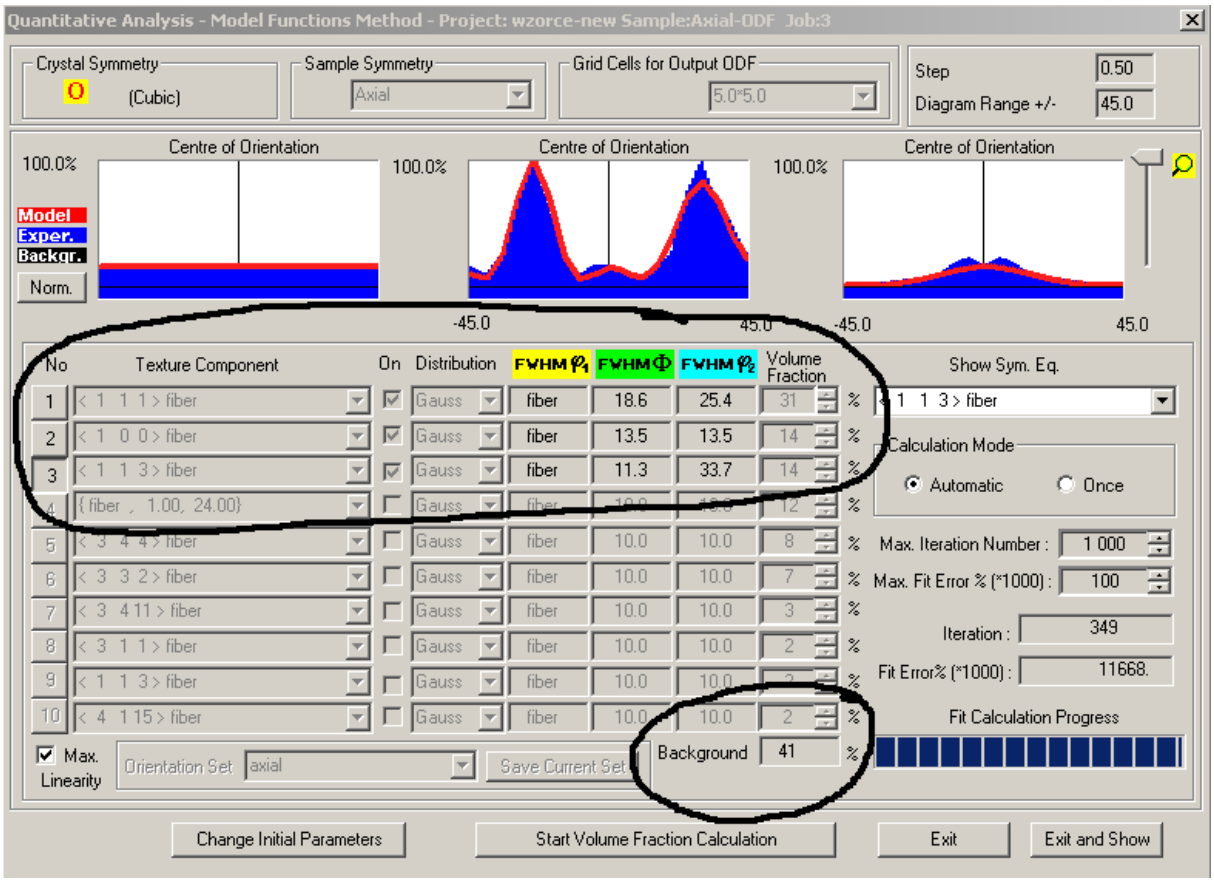


The comparison between 'experimental' and calculated ODF for *<113>fiber* component exhibits that experimental ODF is more complicated. In next approximation of ODF we should assume presence of two components instead of *<113>fiber* component. Model and experimental ODF are very similar as you can see this in the picture below:



You can find calculated model ODF in last job for current sample (in example shown above it is job No.4).

You can find in dialog window calculated parameters: FWHM, volume fraction and background (see marked area in the figure below):

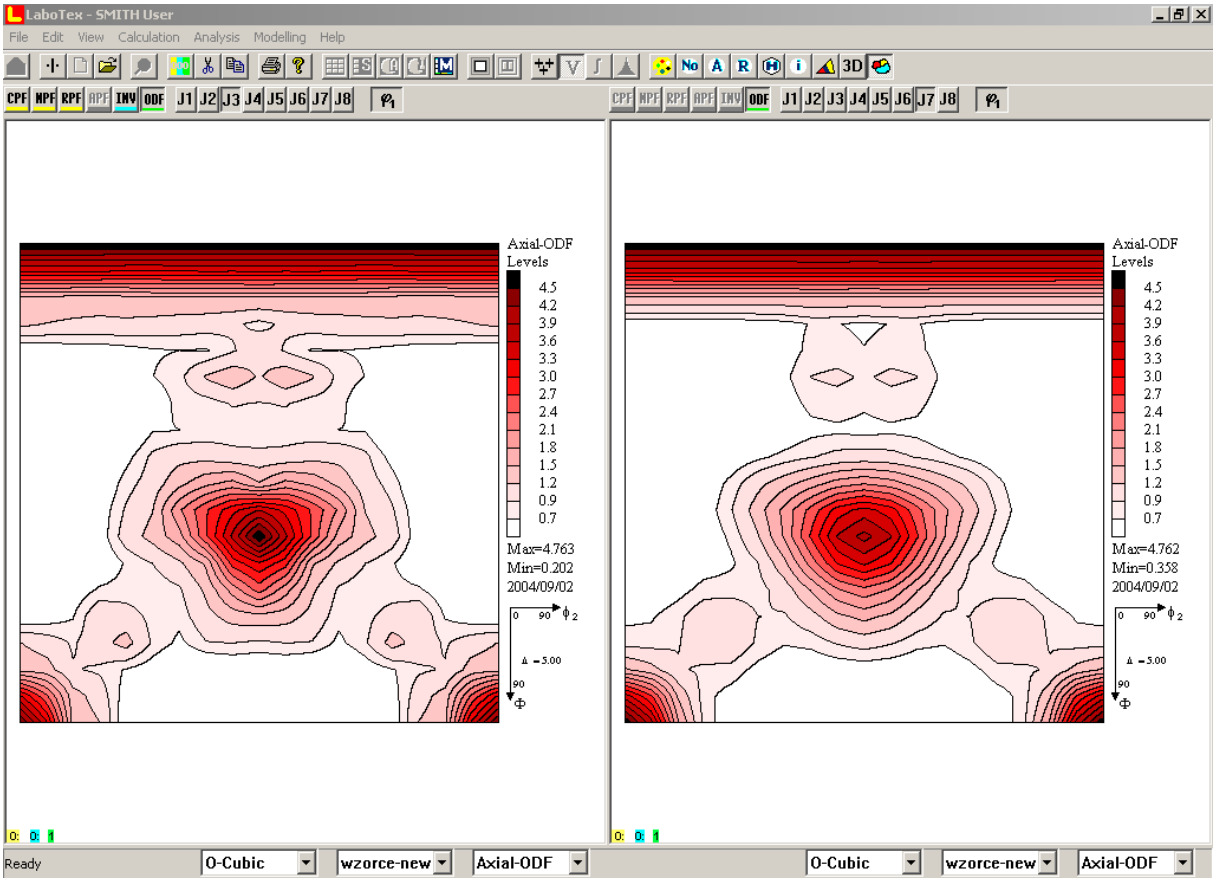


Calculation report is available after save of fitted model. LaboTex displays this report when you click right mouse button on the model ODF. You can print or copy this report:

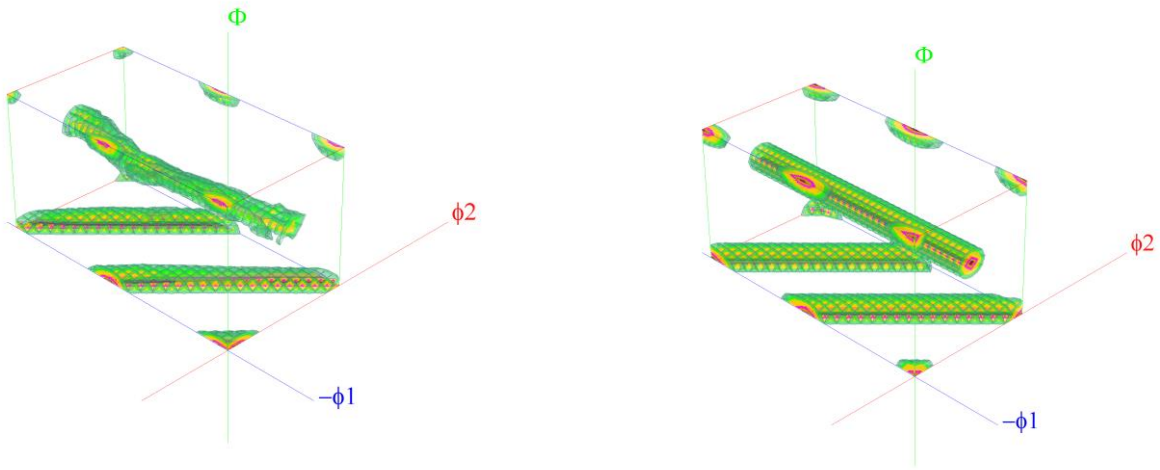
```
LaboTex - Texture - Quantitative Analysis Report
User: SMITH
Project: Ferritic
Sample: Axial-ODF
Job: 4
Date:2004/08/14
Time:18:42:11


_____________________________________________________________
Volume       FWHM    FWHM   FWHM
Fraction     Phi1     Phi    Phi2              Orientation
_____________________________________________________________
Component No 1  - Distribution :Gauss
  30.1      fiber   18.9   24.7            <1   1   1 > fiber
Component No 2  - Distribution :Gauss
  12.7      fiber   13.0   13.1            <  1   0   0 > fiber
Component No 3  - Distribution :Gauss
  8.2       fiber   11.2   19.0            <  1   1   3 > fiber
_____________________________________________________________
  48.99     Background Volume Fraction
```

Step 3 to N - Second to N approximation

You can add new components (or take place one component by two components) and build more complicated model of the ODF on the base of differences between calculated and 'experimental' ODF from previous step. In the picture below is shown new approximation of 'experimental' ODF with components: *<111>fiber*, *<100>fiber*, *<113>fiber* and with new components: <122>fiber and <3 4 11>fiber (fit error decrease with 11.7% to 10.2%).

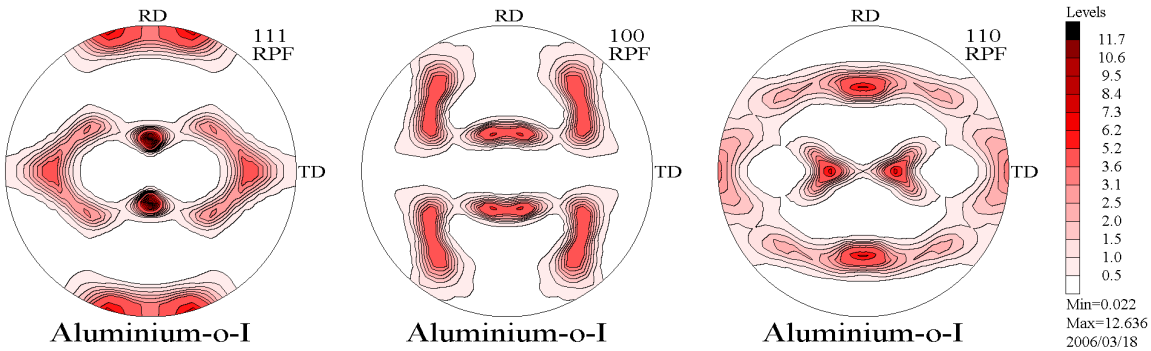


Similary, you can make calculation for the 'experimental' ODF with other sample symmetry. The example below for monoclinic sample symmetry shows 'experimental' ODF for rolled ferritic stainless steel (left) and model ODF (right) fitted by LaboTex. Model ODF assumes only presence of *{001}<100>* (cube) and *<111>fiber* texture components.



Example 2
Aluminium Sample

We can find texture component model which describes experimental pole figures. This is an example on how to use LaboTex to determine of volume fraction of texture components by analysed of pole figures and ODF:



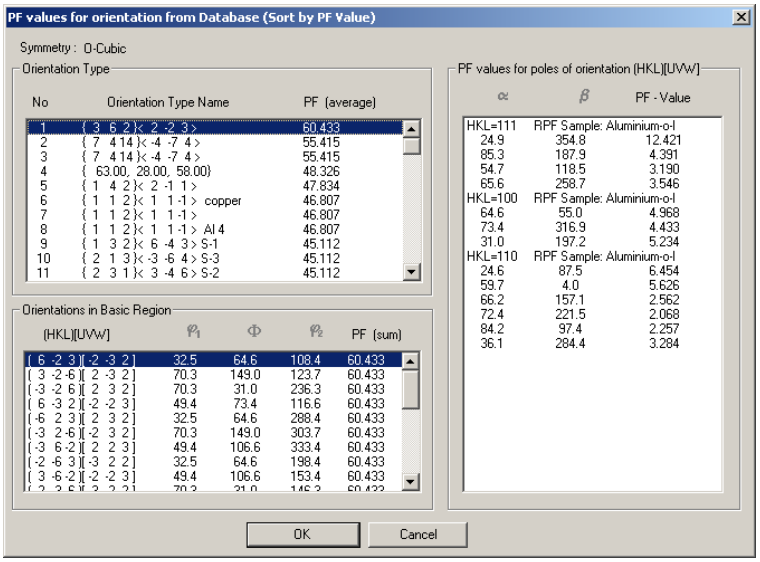
In first step we have to find main texture components. For this purpose we use orientation analysis:

We can use both methods : automatic and manual.

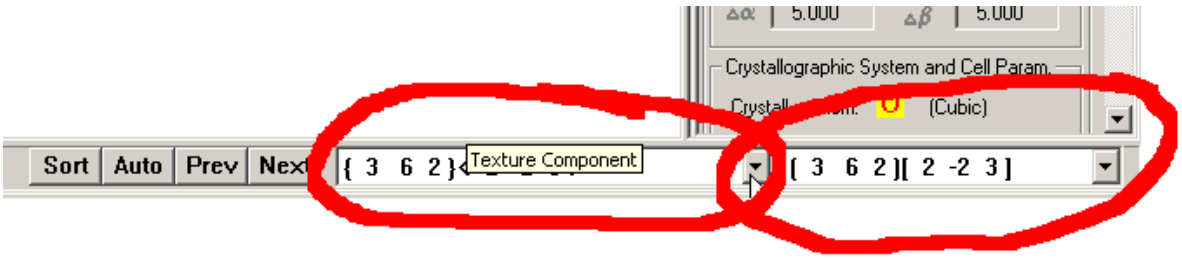
Automatic method (SORT)

In automatic method LaboTex use texture components from database. First LaboTex calculates average pole figures values (arithmetic mean from poles) for each components from database on the base of pole figure values for all symmetrically equivalent orientations of component. In the next step LaboTex sorts average pole figures values for all components from database. When you press 'SORT' button

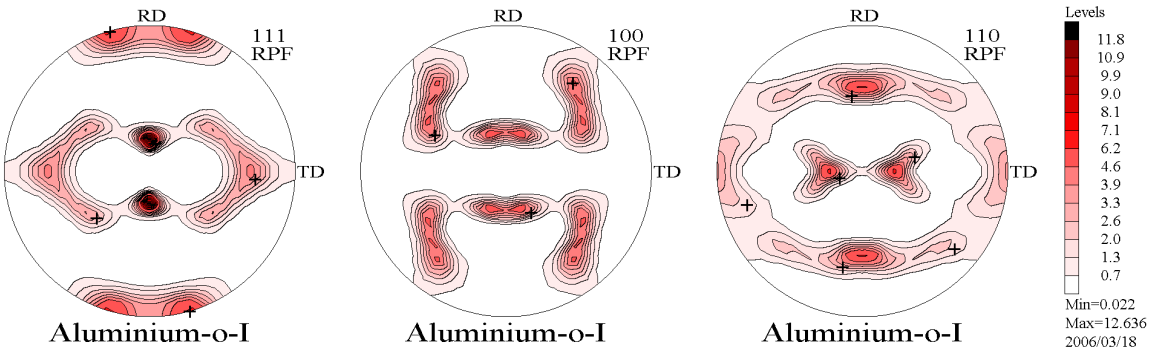
then you can see all components from database and their average pole figues values.



In the lists from left side you can see average pole figure values for component (top list) and pole figure values for each symmetrically equivalent orientations of component (sum from all poles, bottom list). In the list from right side you can see values for each pole of component. (when you click on the symmetrical equivalent of component). When you have more than one pole figures chosen in container then LaboTex shows average values for poles from all pole figures. Next, you can check whether all maxims in analyzed pole figures are described by texture components.



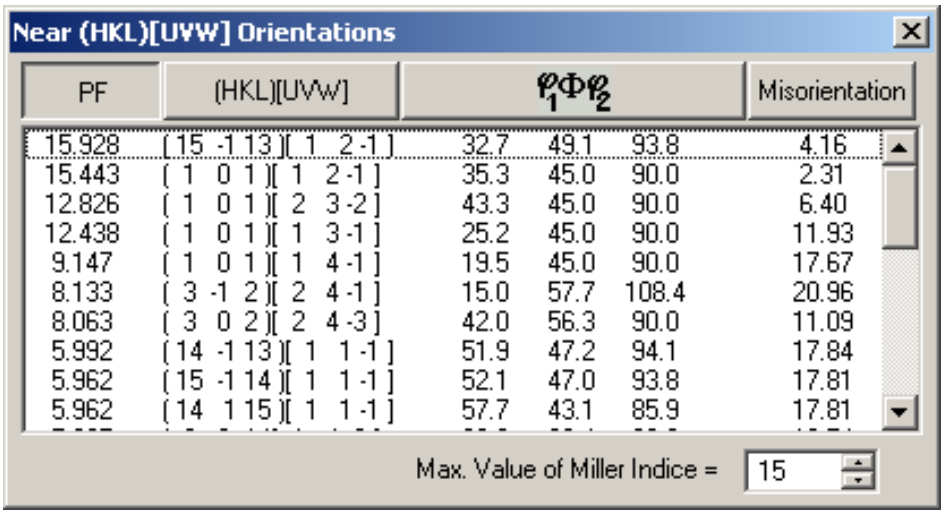
LaboTex displays cross mark (+) in place where lies poles for selected orientation of active komponent ({132}<6-43> in case below):



LaboTex displays only cross marks for one symmetrically equivalent orientation. If you would like see place in the ODF where lies other symmetrically equivalent orientation then you choose it from Combobox. Analogically, you can change texture component which is displaying by LaboTex. When you have found maxim which is not described by components from your database in LaboTex then you should find this component using manual method. Next you should add this component to your database in LaboTex.

Manual method

You can use *"Near {HKL}<UVW> Orientations"* dialog for finding of components by manual method. You should click left mouse button in local or global maxim of pole figure in which you would like find texture component. You can also choose item *"Near {HKL}<UVW> Orientations"* from menu *'Analysis'* :



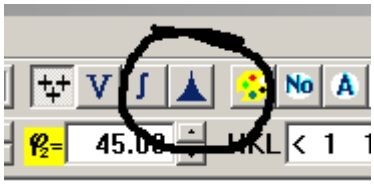
LaboTex displays near orientations sort by average value for poles of pole figures, miller indices or misorientation. You can change type of sort by click in appropriate button.

First approximation

After step 1 we have found that we can describe maxims of analyzed pole figures using components:

- { 1 3 2 }< 6 -4 3 >
- { 1 1 2 }< 1 1 -1 >
- { 1 4 6 }< 2 1 -1 >
- { 1 1 0 }< 1 -1 2 >
- { 1 2 3 }< 4 1 -2 >
- { 1 1 0 }< 0 0 -1 >

Next you should open dialog for determination of volume fraction of texture component by model function method using the icon as below:



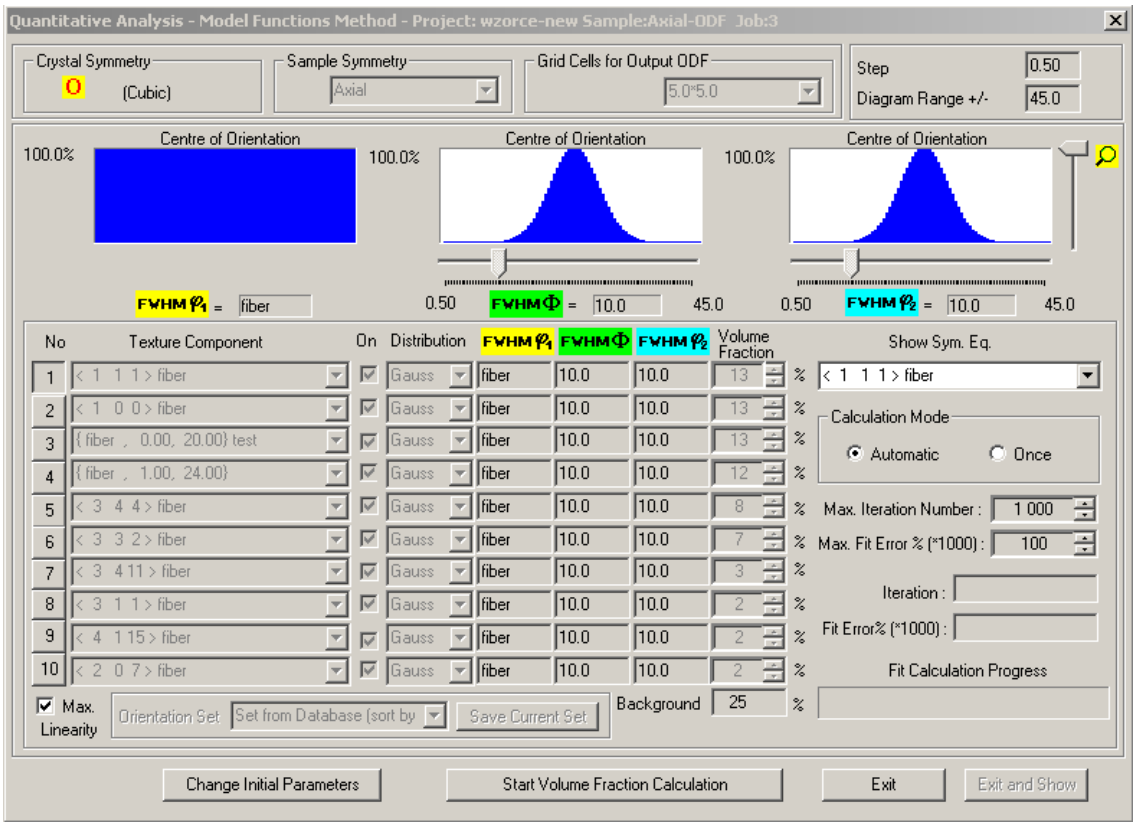
Dialog window help you in least-squares fitting of the model functions to your ODF and in creations of model ODF nearest to the experimental ODF. LaboTex automatic use in calculation following parameters from analyzed experimental ODF:

- crystal symmetry;
- sample symmetry;
- cell parameters;
- grid cell.

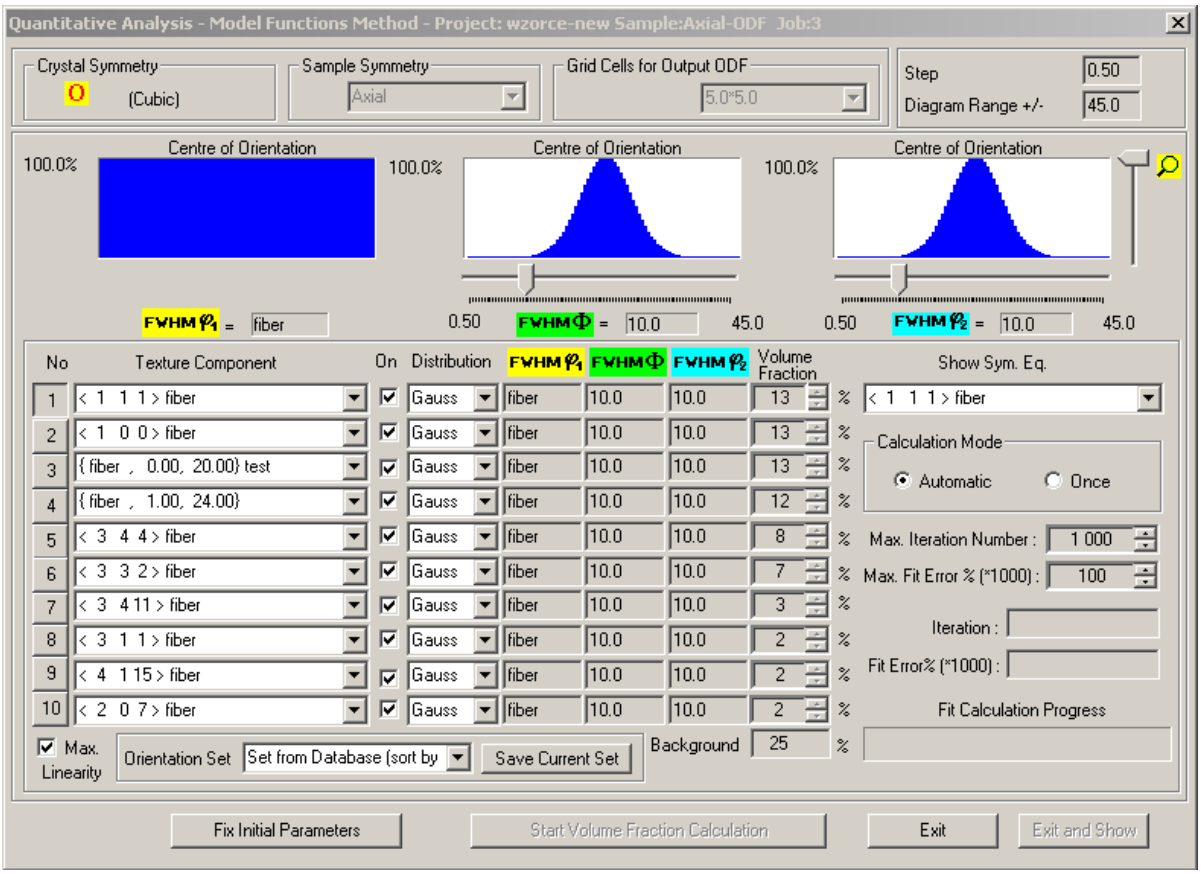
These parameters are grayed and user can't change them.
When you start dialog window LaboTex calculates average ODF values for components and sort components using average ODF values. Hence component No. 1 is the component which has the greatest average ODF value. LaboTex fill also initial parameters for model functions:

- distribution (set to '*Gauss*');
- FWHM for Θ_1, Φ and Θ_2 (all set to 10.0 degrees);
- Volume fraction and background (initial values set on the base of average ODF values of components).

You can start calculations or you can change initial parameters by click mouse on the suitable



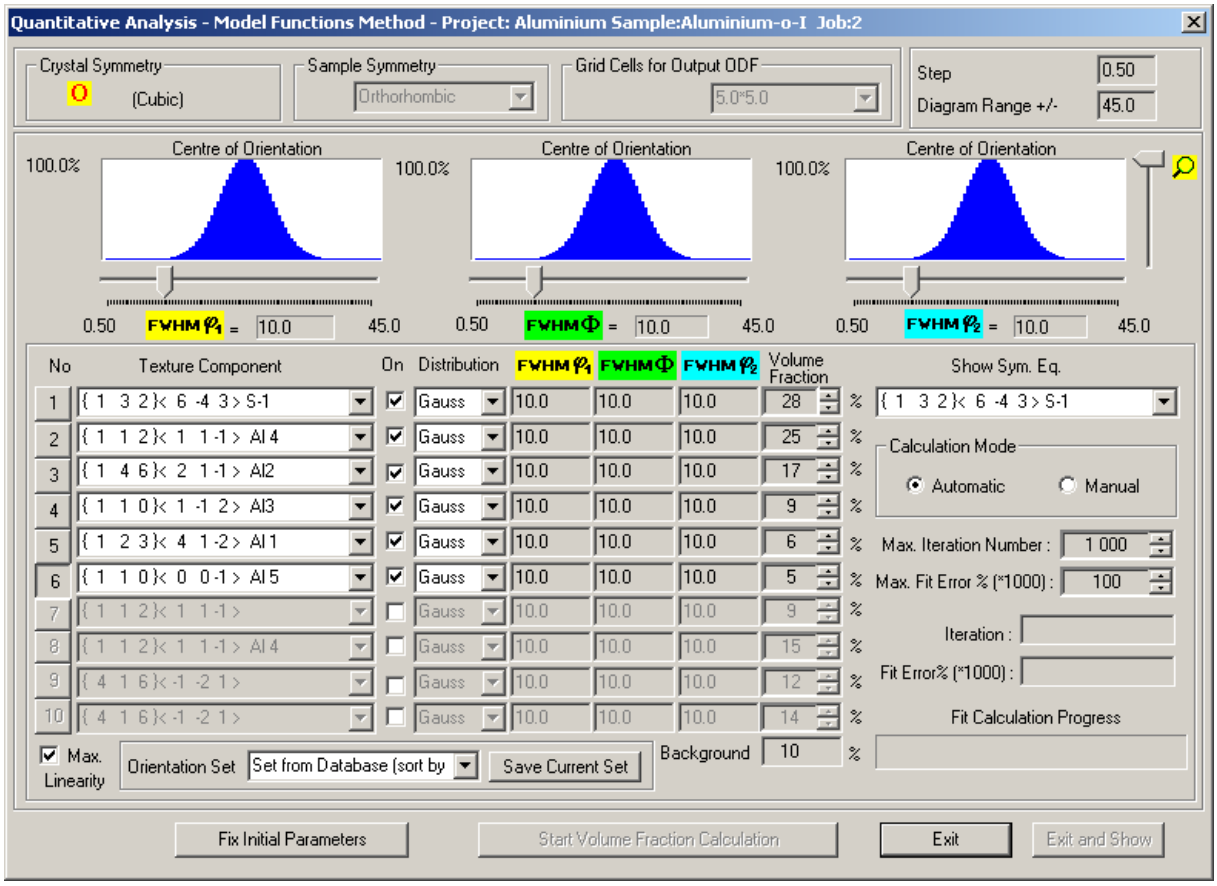
When you click mouse on the '*Change Initial Parameters*' then the new options are available.



You can change:

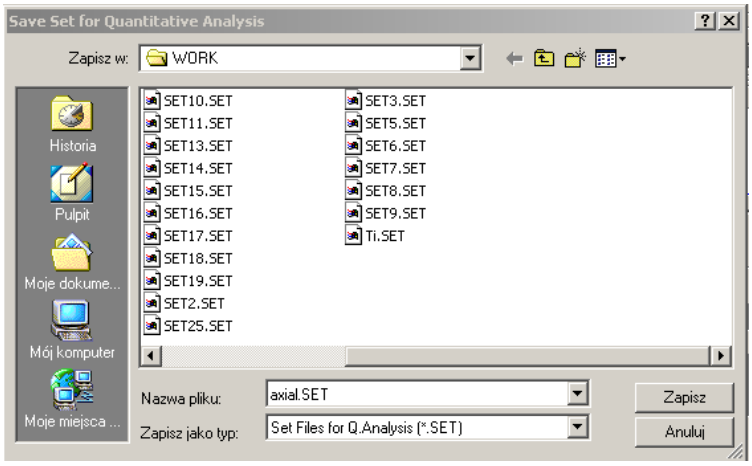
- texture component (using suitable Combobox);
- turn on/off component from calculations (using suitable Checkbox);
- set kind of distribution (Gauss or Lorentz);
- set initial FWHM for each Euler angle;
- set initial volume fraction of component.

Three diagrams in dialog window show model function for each Euler angle for chosen component. You can change selection of component by click mouse on the *'No.'* button. In case of axial sample symmetry only Φ and Θ_2 Euler angles are essential and available. You can magnification plot of model function by change of slider position.
Now, you should set texture components 1 to 5 which you have found in previous step. Next components 6-10 you should turn off from further calculations.



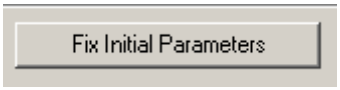
You can save current set of components by click mouse on the "*Save Current Set*" button:

You can accept file name proposed by LaboTex or you can set other file name - for example '*axial.SET*':



LaboTex remembers this set and you can input this set from the list of Combobox. The default set (set proposed by LaboTex when dialog starts) is set build on the base of the database sort by ODF value:

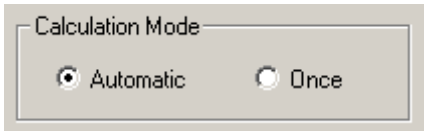
When you have finished setting up of initial parameters you should click on the "*Fix Initial Parameters*" button :



Now you can set up last two parameters of fitting calculation:

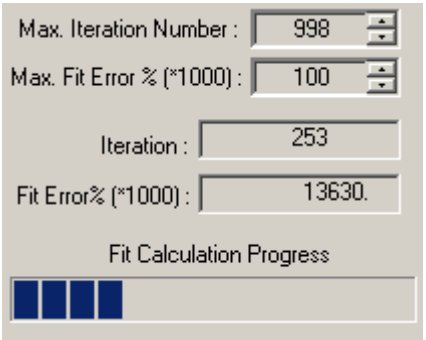
- Maximal Number of Iteration (default is 1000);
- Maximal Fit Error in percent (where fit error is relative error between model and experimental ODF). You should input to LaboTex value of error multiply by 1000 (default is 100 => 0.1%).

These parameters are essential when LaboTex is in 'Automatic' mode. This mode is default .



In this mode LaboTex finish calculation when number of iteration is greater than maximal number of iteration or when fit error is lower than maximal fit error. The second mode of fitting calculation is '*Once*'. In this mode LaboTex creates model ODF on the base of initial parameters of selected texture components and next it calculates and displays the fit error. User can change initial parameters and he can start calculation once more. This is a 'manual' method of fitting. You can start fitting calculation by click on the "*Start Volume Fraction Calculation*" button:

LaboTex displays number of iteration and fit error during calculation. You can also observe fit calculation progress:



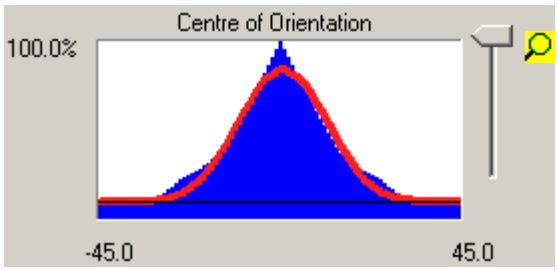
Click on the "Calculation Break" button to break calculation in any moment:

Next you can change initial parameters and start calculation once more.
When LaboTex has finished calculation it displays diagrams for each Euler angle, where LaboTex shows comparison between model and experimental ODF. There are two mode for comparison diagrams:

- Normal (*'Norm.'*);
- Difference (*'Diff.'*).

You can change mode by click mouse on the button *'Norm.'* or *'Diff.'*.
In *'Norm.'* mode LaboTex displays diagrams using colors:

- blue (blue area) - for experimental ODF around of center of symmetrically equivalent orientation of component (diagrams are for each Euler angle);
- red (red line) - for model ODF;
- black (black line) - for background of the model ODF ('*random*' texture component).



In 'Diff.' mode LaboTex displays diagrams using color:

- blue (blue area) - for common area of experimental and model ODF;
- red (red line) - for non-common area of experimental and model ODF;
- black (black line) - for background of the model ODF.

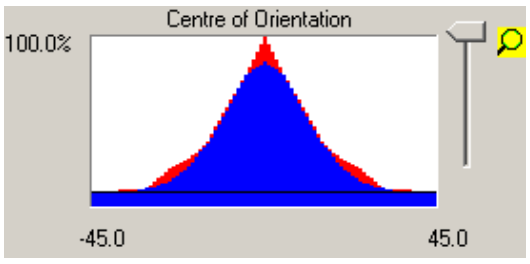


Figure below shows complete dialog window with diagrams for {1 4 6}<2 1 -1> component in 'Norm.' mode.

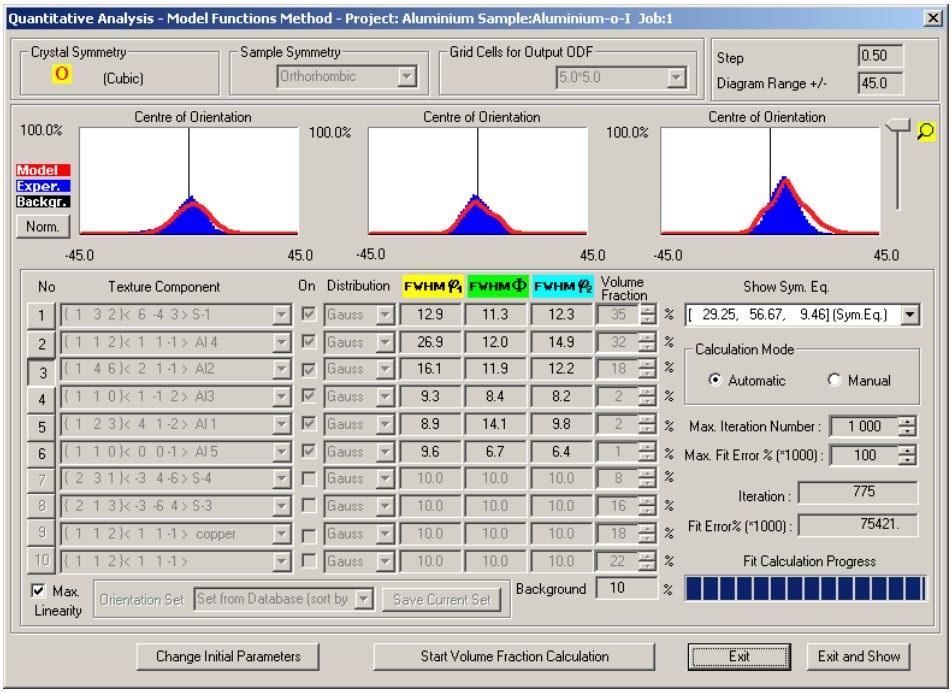
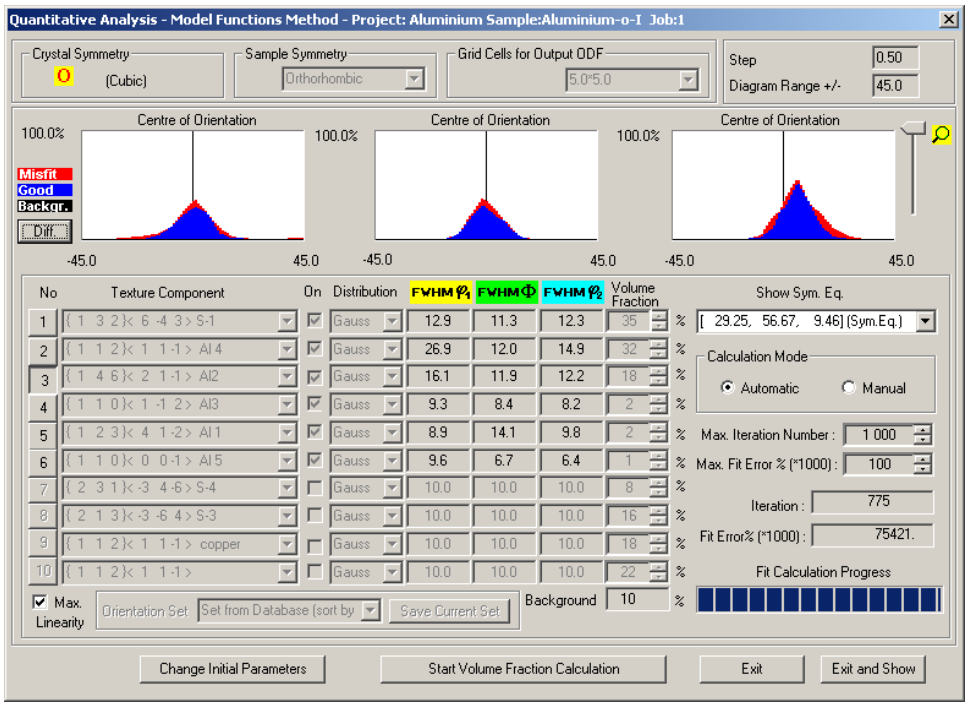
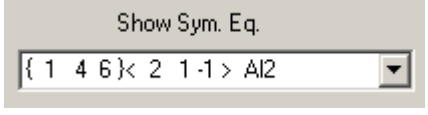


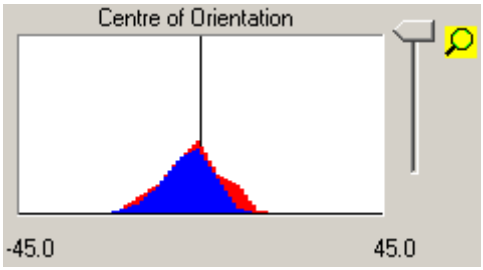
Figure below shows complete dialog window with diagrams for {1 4 6}<2 1 -1> component in 'Diff.' mode.



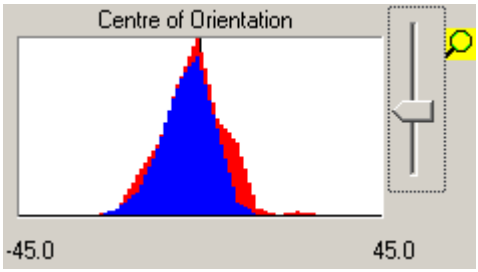
You can choose any symmetrically equivalent orientation from the "*Show Sym. Eq.*" Combobox to display the comparison diagrams:



Component {1 4 6}<2 1 -1> is weak in comparison, hence quality of diagrams is bad.



You can change magnification of component plot using slider. Value in left corner (41 %) of diagram shows on the percent of maximal ODF value.



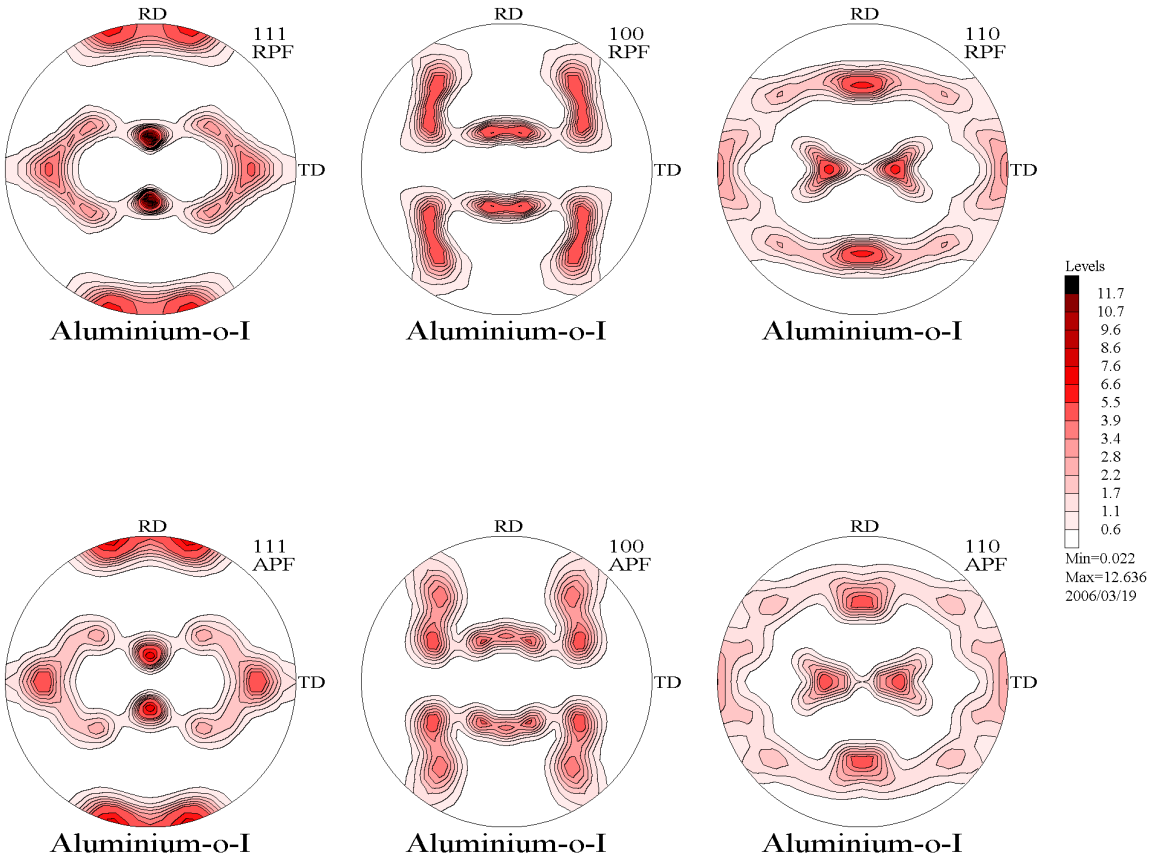
The comparison between 'experimental' and calculated ODF for component {1 4 6}<2 1 -1> component exhibits that experimental ODF is more complicated. In the next approximation of ODF we can correct this difference.
Finally, we receive results calculation:

LaboTex - Texture - Quantitative Analysis Report
User: Ozga
Project: Aluminium
Sample: Aluminium-o-I
Job: 2
Date:2006/03/18
Time:18:28:32

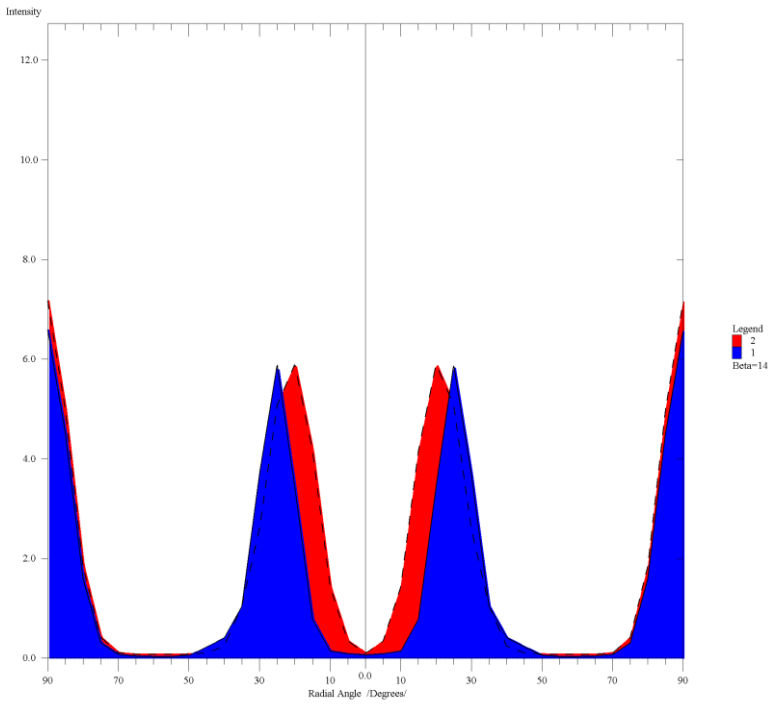
Volume Fraction	FWHM Phi1	FWHM Phi	FWHM Phi2	Orientation
Component No 1 - Distribution :Gauss				
37.4	12.6	12.0	12.5	{ 1 3 2 }< 6 -4 3 > S-1
Component No 2 - Distribution :Gauss				
34.5	29.7	11.9	15.7	{ 1 1 2 }< 1 1 -1 > Al 4
Component No 3 - Distribution :Gauss				
18.2	19.0	12.2	13.6	{ 1 4 6 }< 2 1 -1 > Al2
Component No 4 - Distribution :Gauss				
2.3	9.6	10.4	10.5	{ 1 1 0 }< 1 -1 2 > Al3
Component No 5 - Distribution :Gauss				
0.1	5.9	9.3	9.1	{ 1 2 3 }< 4 1 -2 > Al 1
Component No 6 - Distribution :Gauss				
0.4	6.2	11.7	6.3	{ 1 1 0 }< 0 0 -1 > Al 5

6.98 Background Volume Fraction

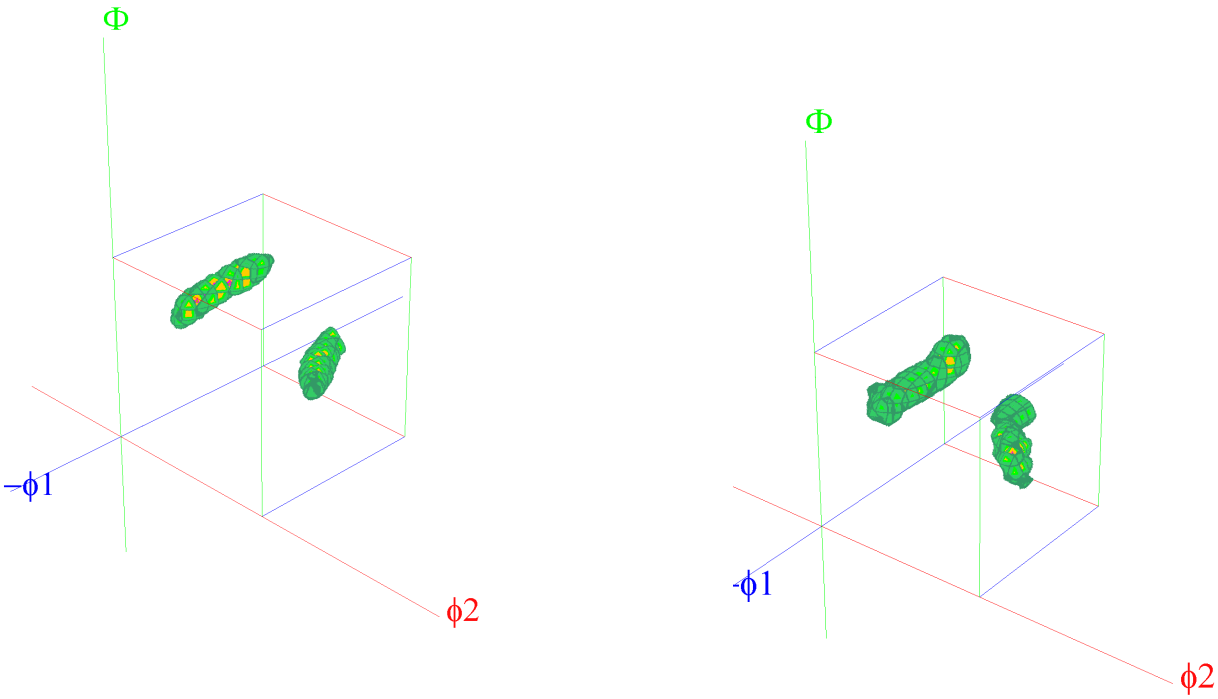
Next we can do pole figures calculation from model ODF and we can make comparison between experimental (first row) and model pole figures (second row).



We can also makes comparison between sections of pole figures as on the example below for (111) pole:



“Experimental” (from left) and model ODF (from right):



You can add new components (or take place one component by two components) and build more complicated model on the base of differences between calculated and 'experimental' pole figures or ODFs from previous step