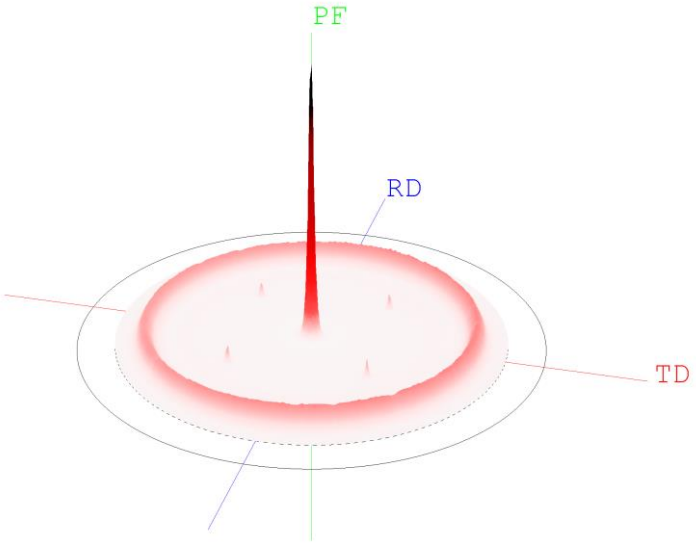
LABSOFT

LaboTex

Version 3

The Texture Analysis Software for Windows



Pole Figures: Registration and Plot Conventions

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Release 3.0

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CONTENTS

1. Pole Figure: Definition

The most popular techniques for texture measurement are X-Ray and neutron diffraction. The polycrystalline specimen contains many grains (crystallites) in which atoms form a three-dimensional periodic arrangement. Each grain has a unique orientation and in each grain we can indicate different crystallographic planes. In diffraction techniques, we can choose planes such as {111}, {100} or other planes, which give the diffraction peak, by fixing the 2θ angle in the source-counter system and next, we can make a measurement of the intensities diffracted by these selected planes for different positions of the source-counter system, with respect to the sample. In LaboTex, the results of the texture measurement are plotted by means of the stereographic projection and the created plots are referred to as pole figures. For example, we get the pole figure {111} when we choose the 2θ angle for {111} planes. Consequently, pole figures show the statistical distribution of the normal to the given {hkl} plane.

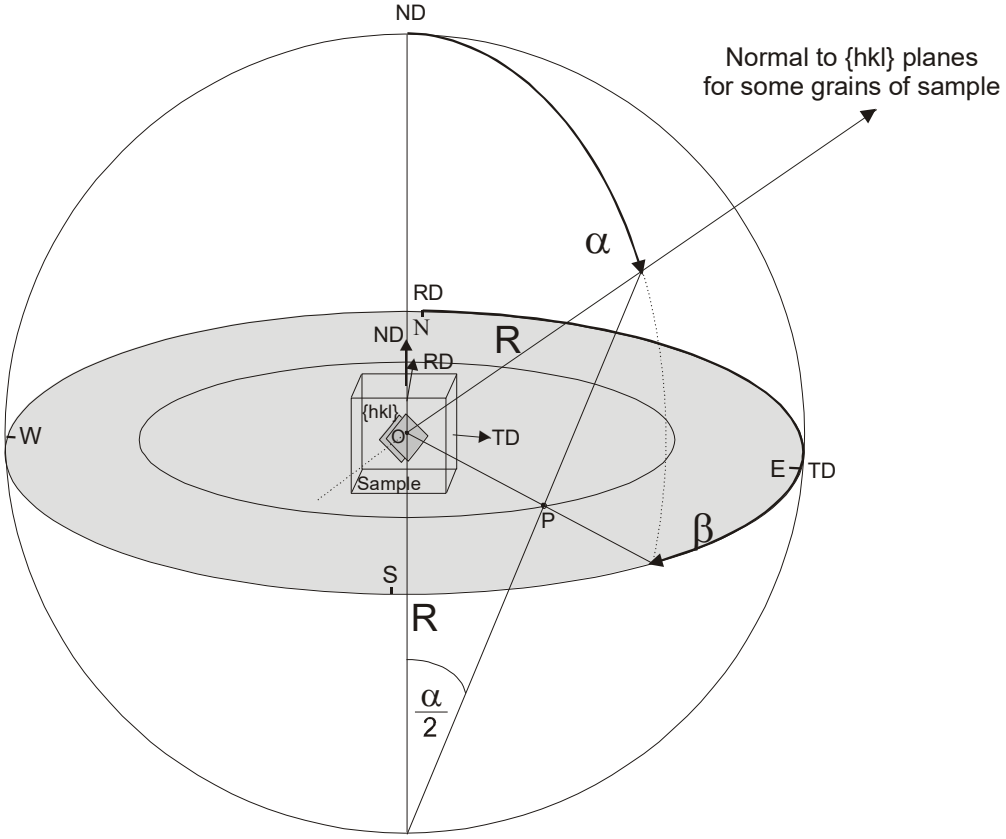


Fig. 1 The principle of using the stereographic projection to create a pole figure in LaboTex.

In LaboTex, pole figures are characterized by the angles α and β, where the α ranges (angular or radial) are from 0º at the center to 90º at the edge, and the β ranges (azimuthal) are from 0º to 360º. The definitions of the α and β angles are shown in Figure 1. The point where the {hkl} plane normal intersects the sphere (the point defined by the α and β angles) is projected in the pole figure in point P, hence $\overline{OP} = R \cdot tg(\frac{\alpha}{2})$ (see Figures 1 and 2).

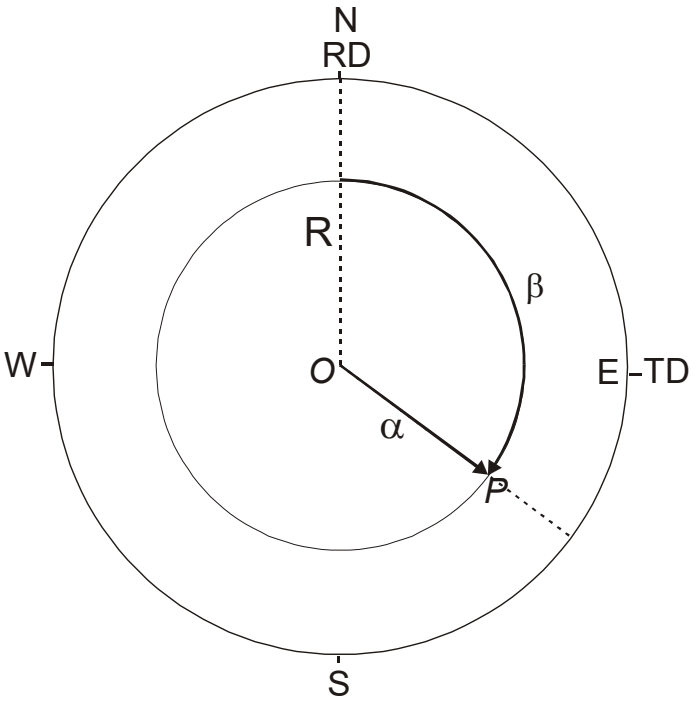


Fig. 2 Pole figure with point P and angles α, β defined in Figure 1.

2. Pole Figure: Measurements

In practice, the source-counter system is non-moving and different measurement positions (α, β) are made by sample rotations (see for Figure 3).

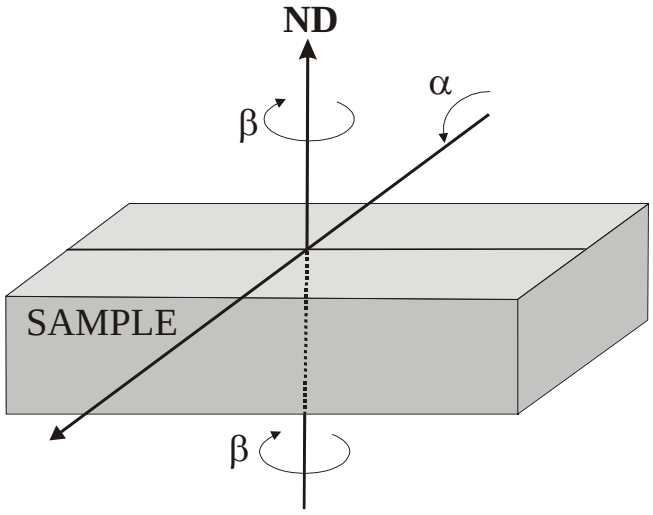


Fig.3 Pole figure measurements by sample rotations.

The traditionally applied registration method of the pole figure is based on the equiangular (regular) measurement grid (Δα=Δβ). LaboTex also inputs the data for equal azimuthal and radial steps (see Figure 4). The measurement grid should be one from: 1. ,2. ,1.2 ,1.25 ,1.5 ,2. ,2.5 ,3. ,3.75, 5. ,6. ,7.5 , 10 degrees and it can also be: 1.8 ,2.25 ,3.6 ,4.5, but with the exception of the trigonal and hexagonal crystal lattice symmetry. The step size should depend on the degree of the preferred orientation. Strong texture needs a smaller grid (for details see the report "Volume Fraction Calculation").

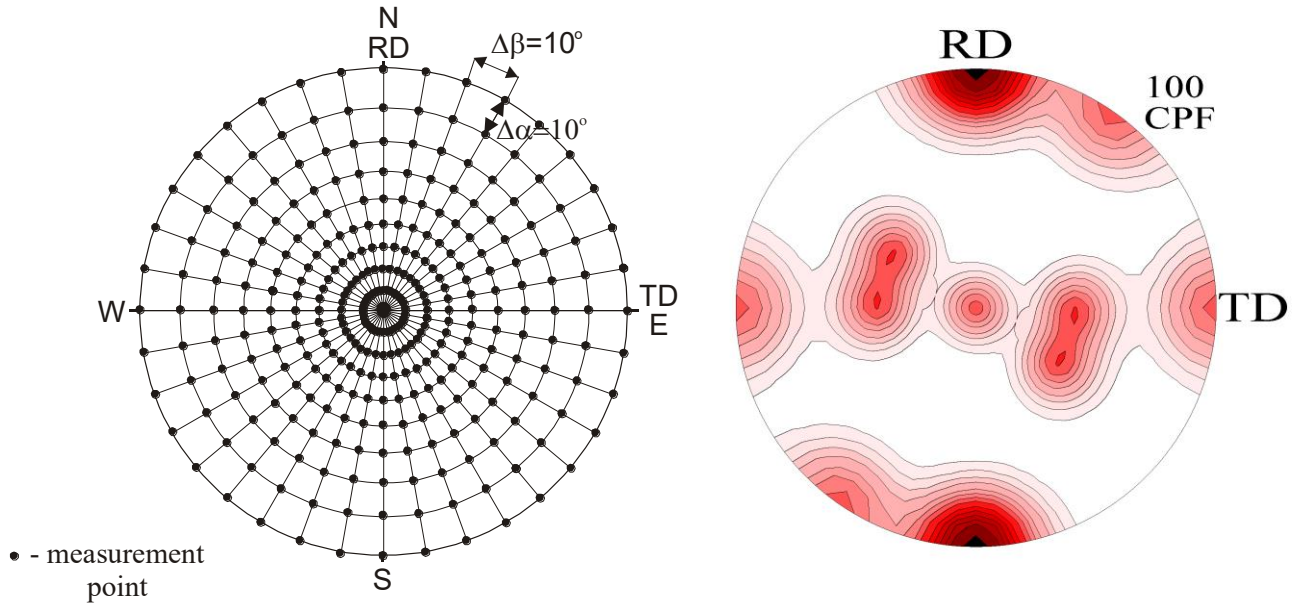


Fig. 4 Measurement of a complete pole figure.
(Left) - Example of an equiangular measurement grid for a pole figure (left), $\Delta\alpha=\Delta\beta=10^o$.
(Right) - Example of a complete pole figure.

LaboTex can also input the data for different azimuthal and radial steps, but in this case, the azimuthal step is adjusted to the radial step by the linear interpolation of the pole figure data (see Figure 5 and Figure 6 – the radial step for the data of the defocusing correction has to be the same as for the pole figures). LaboTex informs the user when it has made an adjustment from the azimuthal step to the radial step:

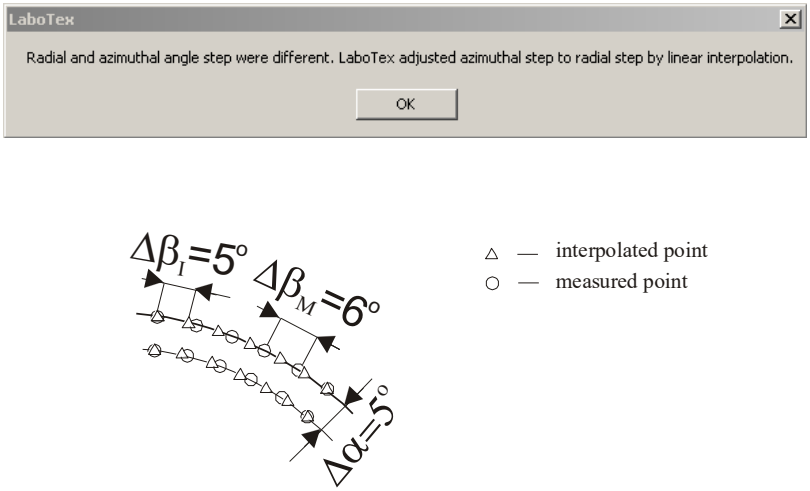


Fig. 5 Example of an adjustment of the measure azimuthal step ($\Delta\beta_M=6^o$) to the radial step ($\Delta\alpha=5^o$) by means of the linear interpolation for a non-equiangular measurement grid ($\Delta\beta_I$ - step for interpolated points). Input grid : $\Delta\alpha=5^o$, $\Delta\beta_M=6^o$; Output grid : $\Delta\alpha=5^o$, $\Delta\beta_I=5^o$.

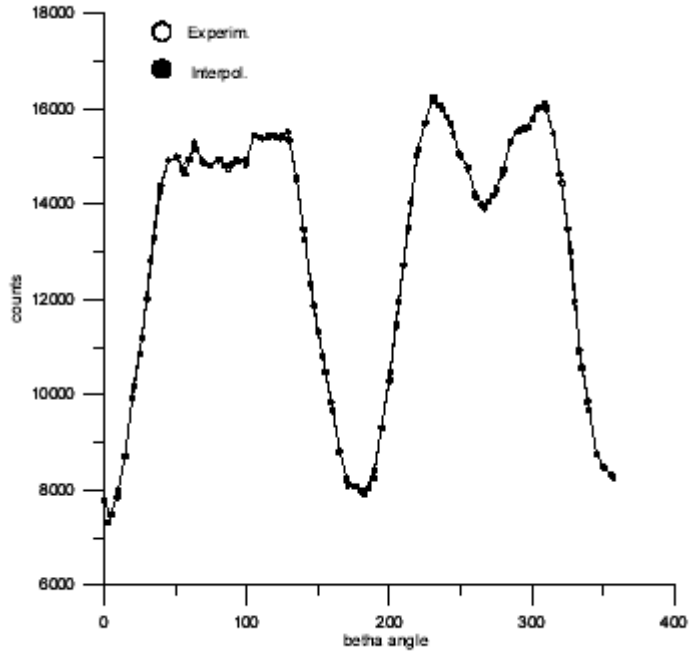


Fig. 6 Example of data adjusted by the linear interpolation for a non-equiangular measurement grid. Radial angle (α) constant, azimuthal angle (β) in the range from 0 ° to 360 °.

A correct measurement of complete pole figures is impossible by means of one technique. For the transmission technique (neutron diffraction, X-ray diffraction for polymers), correct measurements for the radial angle of about '0' are not accessible, hence the data from the transmission technique start from α>0. Figure 7 shows an example of the measurement grid and measurement ranges for the transmission technique.

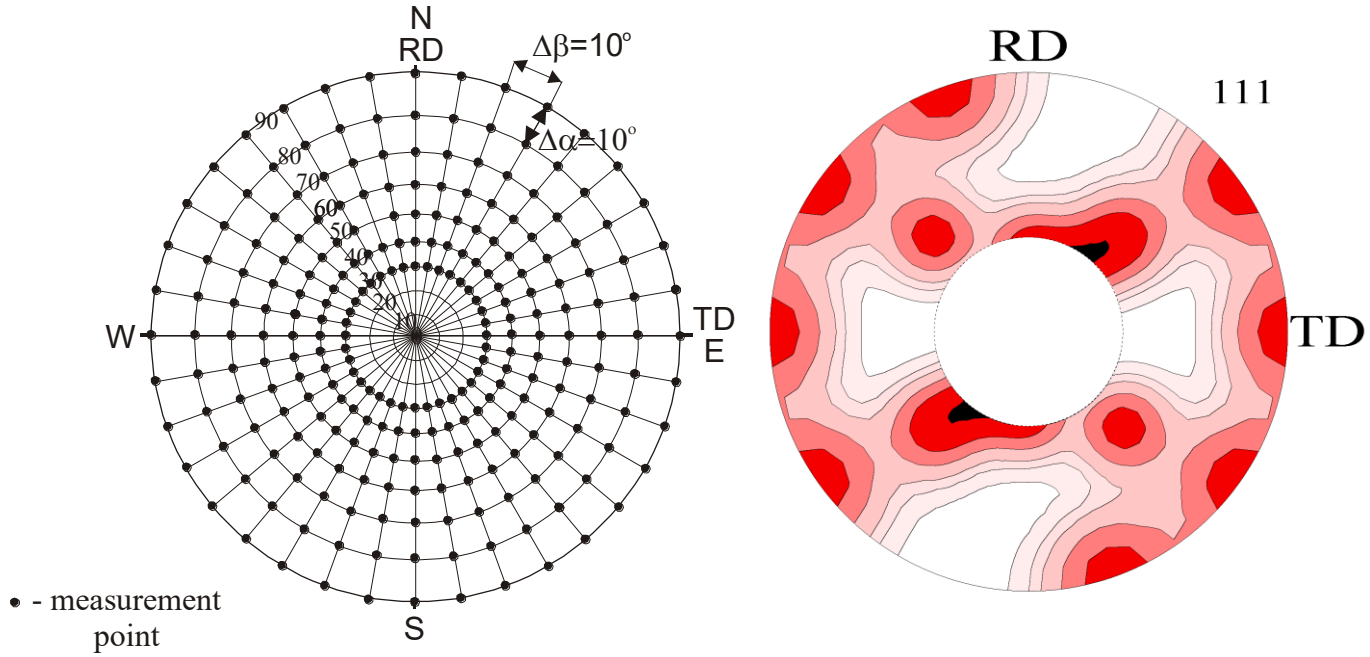


Fig. 7 Transmission technique. (Left) - Example of an equiangular measurement grid for an incomplete pole figure (α=30 to 90°, β= 0 to 360°, equiangular measurement grid Δα=Δβ=10°). (Right) - Example of an incomplete pole figure.

For the **reflection technique** (X-ray diffraction), the measurement fails when the radial angle approaches the '90' degree, as the sample plane and the diffracted beam are parallel for the 90 degree (see Figure 8). Hence the proper data from the reflection technique are for $\alpha<90$.

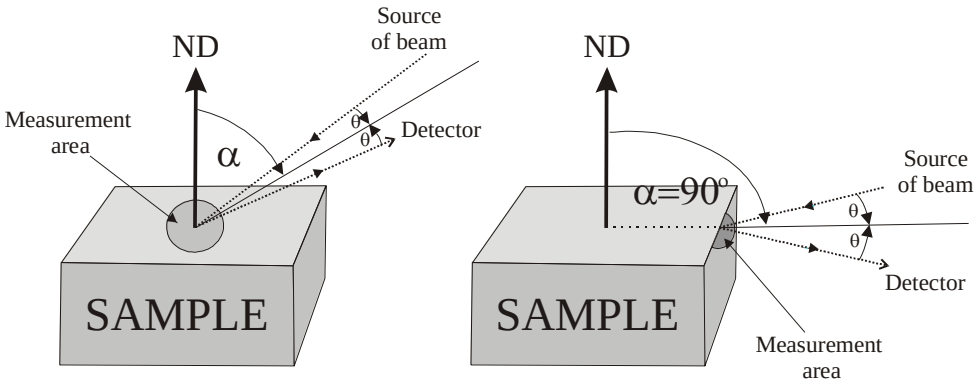


Fig. 8 Reflection technique. Illustration of the problematic measurements for the radial angle close to '90' degrees.

Figure 9 shows an example of the measurement grid and measurement ranges for the reflection technique.

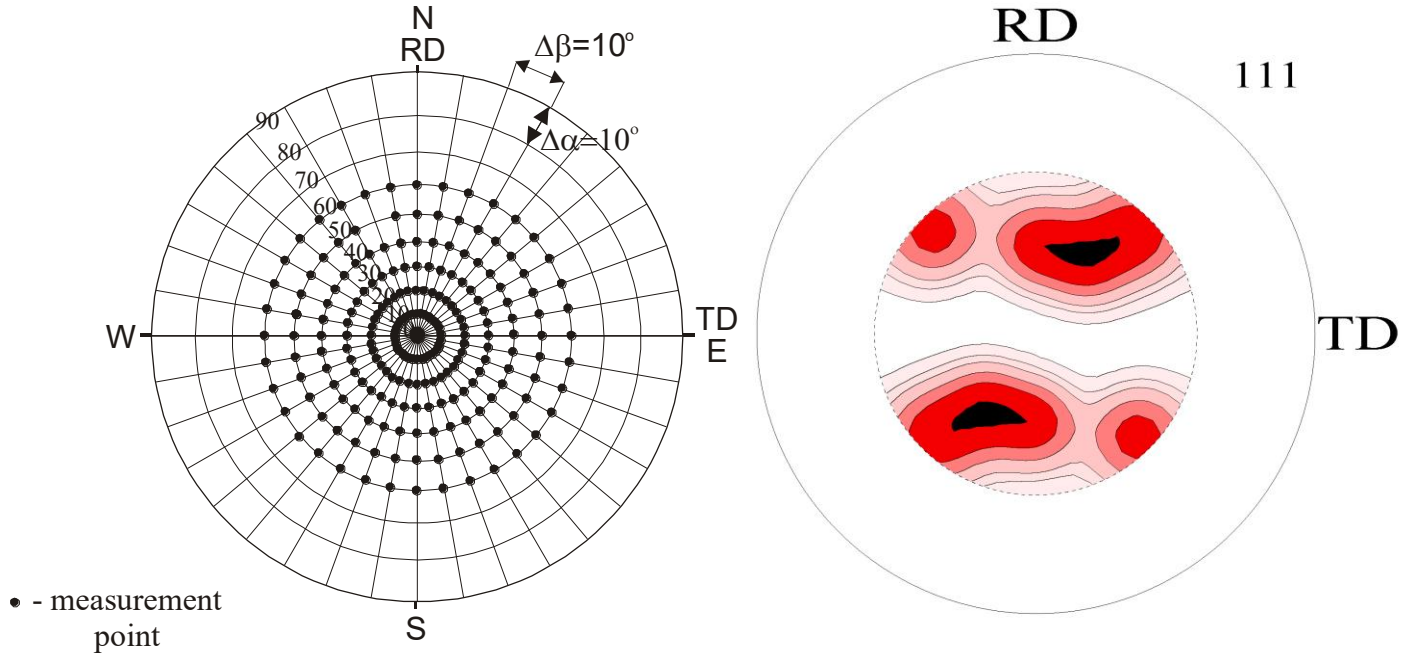
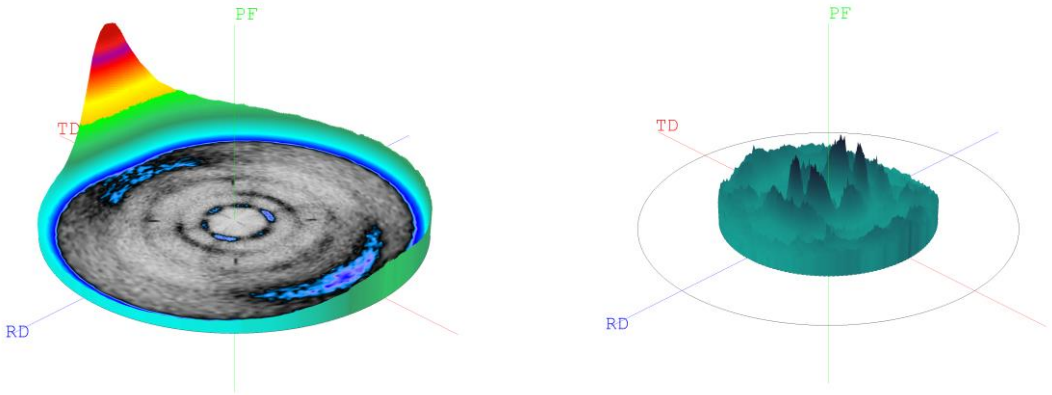


Fig. 9 Reflection technique. (Left) - Example of an equiangular measurement grid for an incomplete pole figure (α=0 to 60°, β= 0 to 360°, equiangular measurement grid: $\Delta\alpha=\Delta\beta=10°$). (Right) - Example of an incomplete pole figure.



A) B)

Fig. 10 Reflection technique. A) Deformation at α close to the 90 degree. Example of a complete pole figure (α=0 to 90º, β= 0 to 360º) B) The same measurement as in A) but in the range: α=0 to 60º (incomplete pole figure) and with a different factor of normalization.

Figure 10 shows an example of deformation of the complete pole figure for the reflection technique at α close to the 90 degree.

A similar deformation of the pole figure can be a result of a bad assumption of the convention for the radial angle when the pole figure is plot. Some data formats do not use the α angle measured from the centre of the pole figure (i.e. α=0 is in the centre of the pole figure) but they use the convention where α=90 is in the centre of the pole figure. You can find a similar problem with the UXD file format. In this case, please reverse the data input for α /choose : **Edit ⇒ LaboTex Option ⇒ Data Format ⇒ UXD - Bruker (reversed radial direct)/.**

If you use the area detector or the position sensitive detector, then the software for your detector should make a transformation of the integrated intensities from the diffractometer coordinate system {2θ, ω,γ,χ,φ) into the pole figure angles (α,β). Basic information about this transformation, as well as about measurements with area detectors and position sensitive detectors can be found in:

- H.J.Bunge, K.Klein, Z.Metallkunde, 6, 465 (1996);
- L.Wcislak, H.J.Bunge, "Texture Analysis with Position Sensitive Detector", Cuvillier Verlag, Gottingen (1996).

When the interplanar spacings in the layer of the deposit and in the substrate are close for some planes (the diffraction peaks overlap - Fig. 11), then we can observe the presence of the substrate texture in the pole figure for the deposit. This effect can also be observed in the case of bulk multiphase samples.

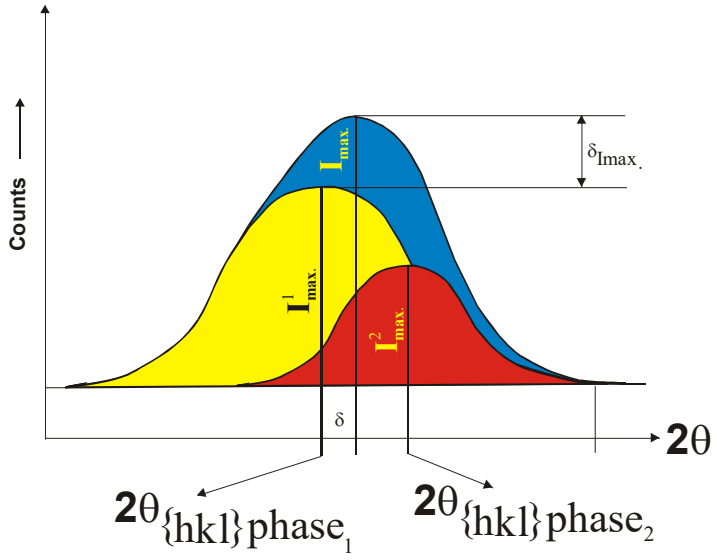


Fig. 11 The observed (resultant) profile of the diffraction peak (blue) in the multiphase system where the peaks overlap (the profile of the diffraction peak for phase 1 (yellow), the profile of the diffraction peak for phase 2 (red)).

This effect can be observed especially when the substrate has a strong texture. For example, the peak for (220) Si (2Theta 47.37) interferes with (111) Cu (2Theta 43.34). The pole figure shown in Figure 11a additionally contains four small peaks. These peaks come from the monocrystal substrate.

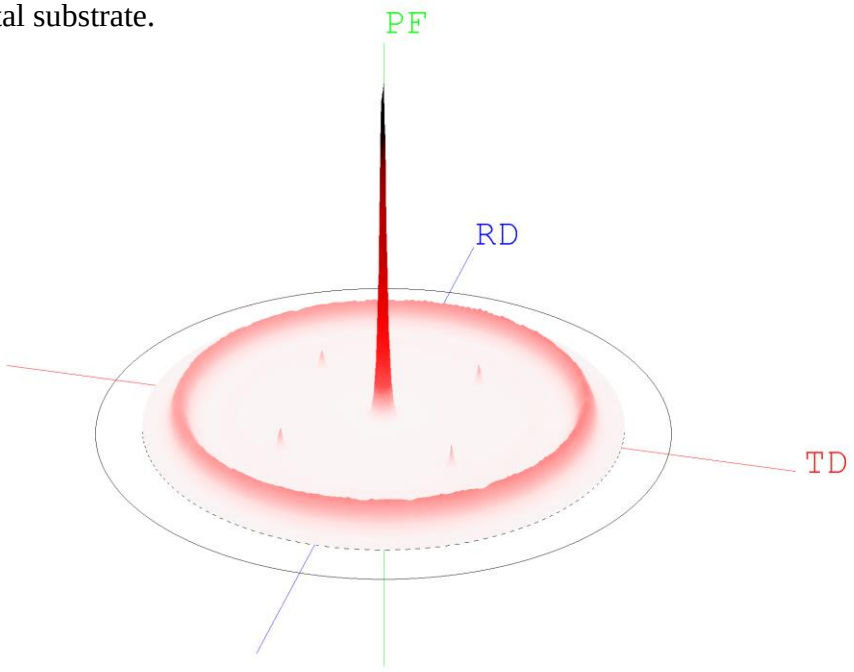
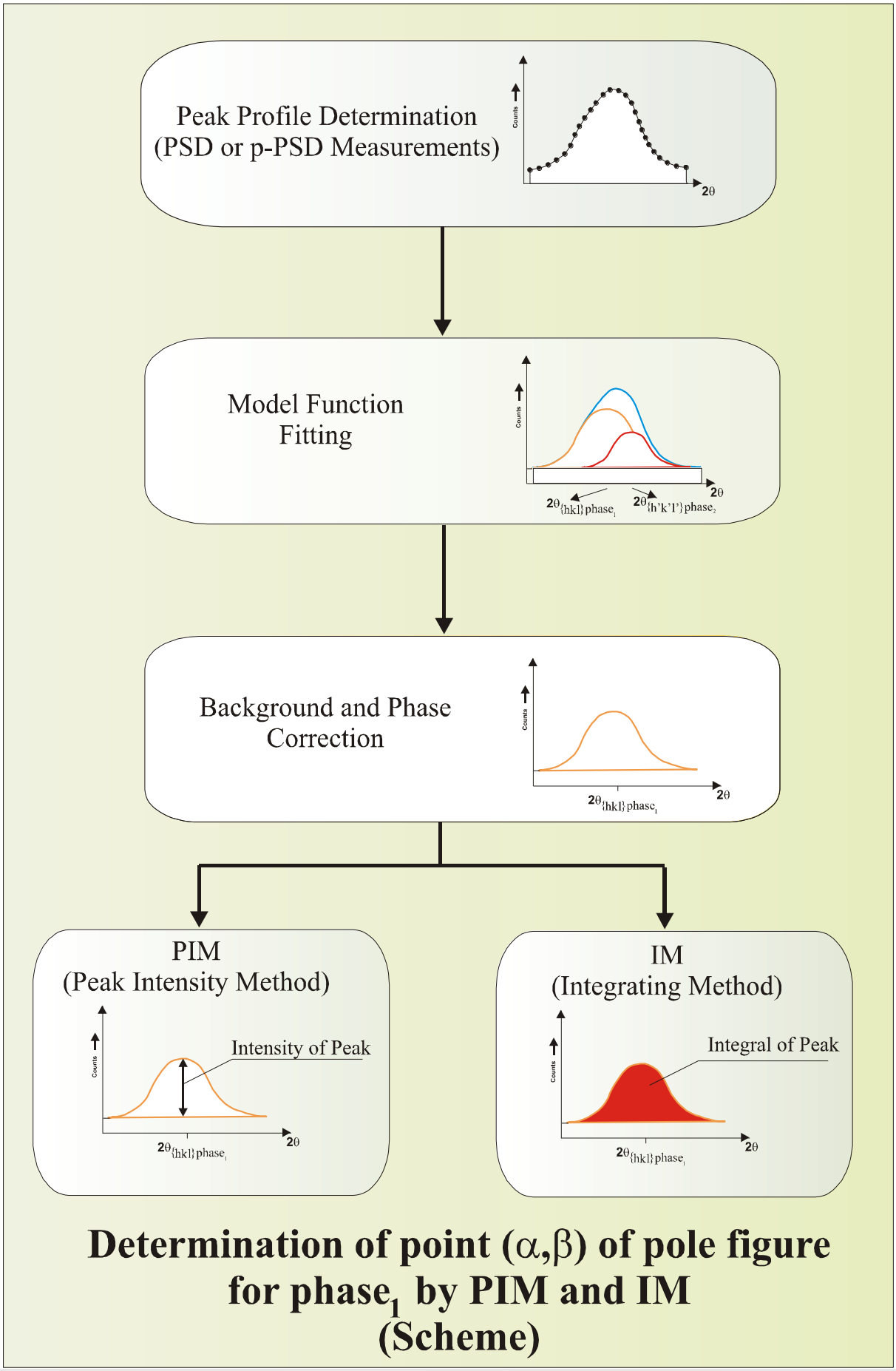


Fig. 11a Reflection technique. The presence of the peaks from the substrate (four peaks in the centre, the Cu layer on the monocrystal of Si).

In the case when the diffraction peaks overlap, we should apply the profile analysis (such as the PIM or IM technique - see the table at the following page) for extracting the point (α,β) of the pole figure.



Determination of point (α,β) of pole figure for phase$_1$ by PIM and IM (Scheme)

3. Pole Figure: Measurements and Sample Symmetry

When we are sure that the pole figure's sample symmetry is higher than triclinic, then we can make a measurement in a smaller range of the β angle. Below, we can see examples of complete pole figures with different sample symmetries (left) and examples of the measurement grids for each sample symmetry (right):

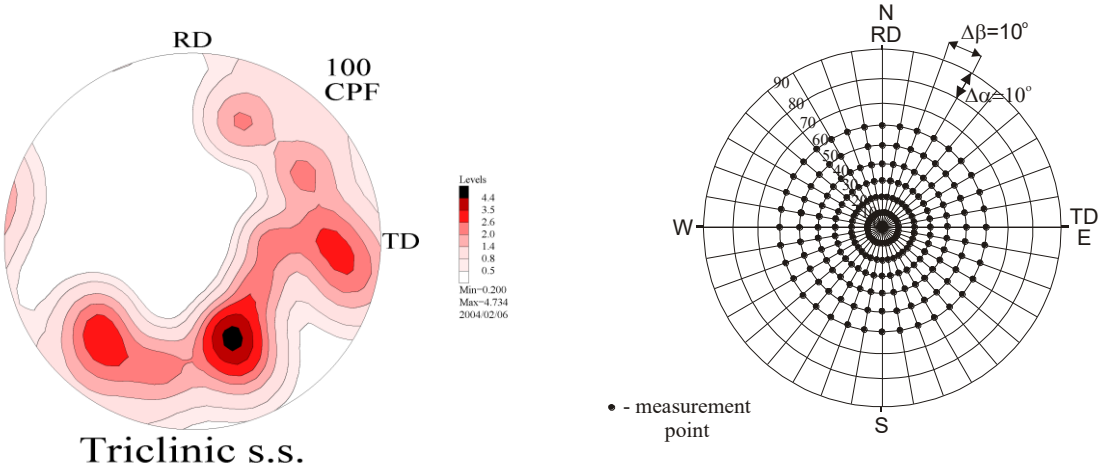


Fig. 12 Triclinic Sample Symmetry: β = 0^0 to 355^0 or 0^0 to 360^0 (Symmetry element C_1)

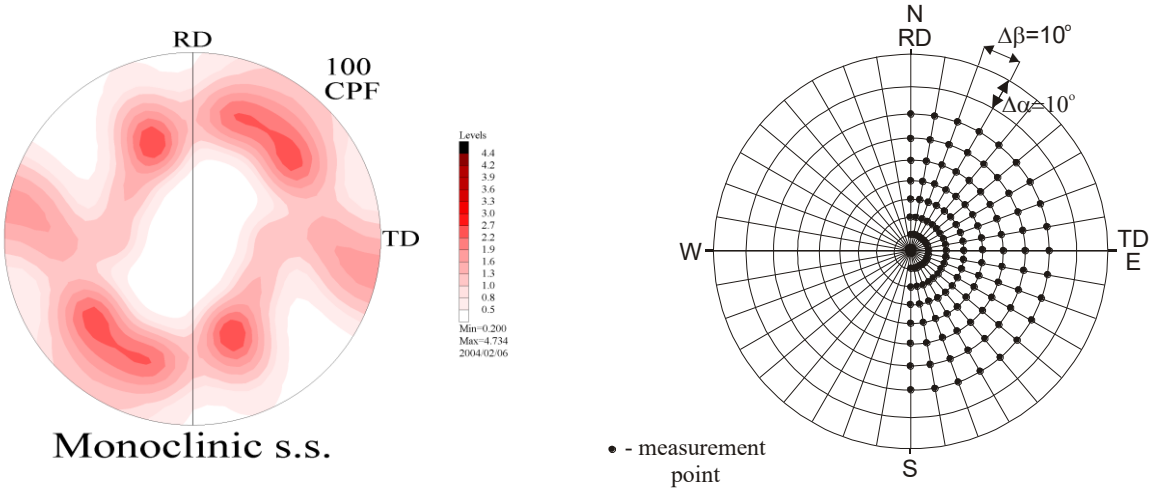


Fig. 13 Monoclinic Sample Symmetry: β = 0^0 to 180^0 (Symmetry element C_2)

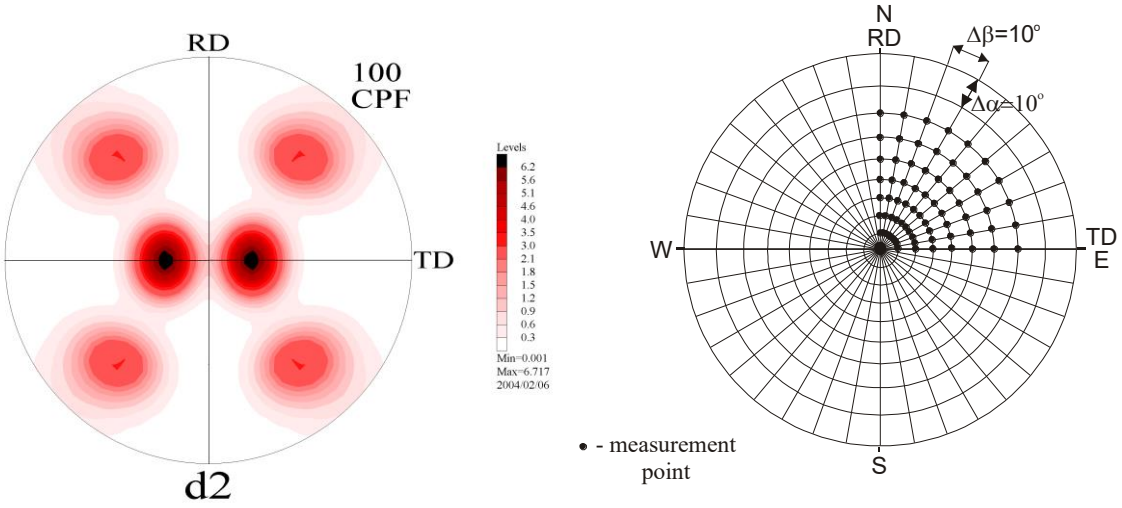


Fig. 14. Orthorhombic Sample Symmetry: $\beta = 0^0$ to 90^0 (Symmetry elements: C_2 m)

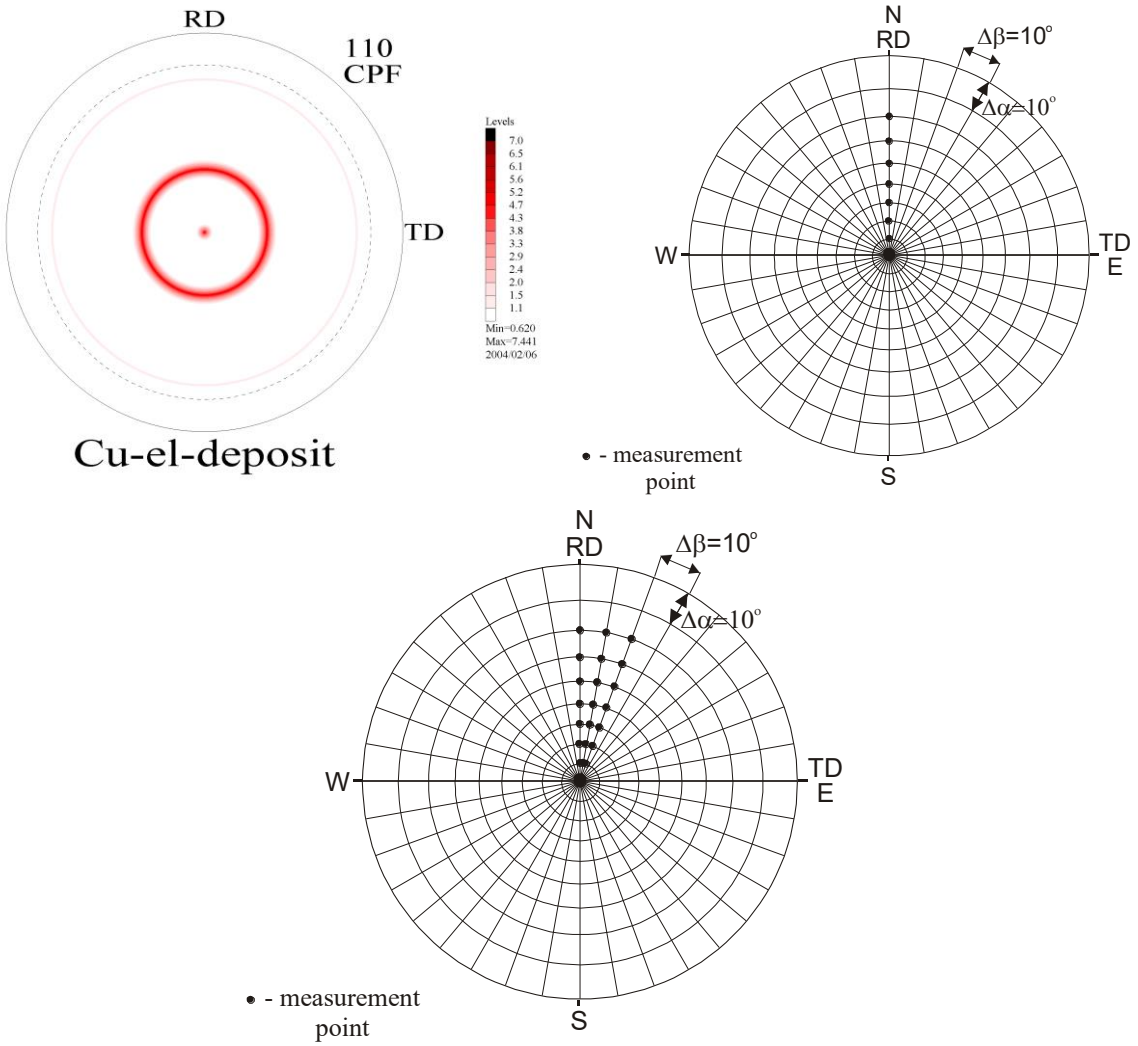
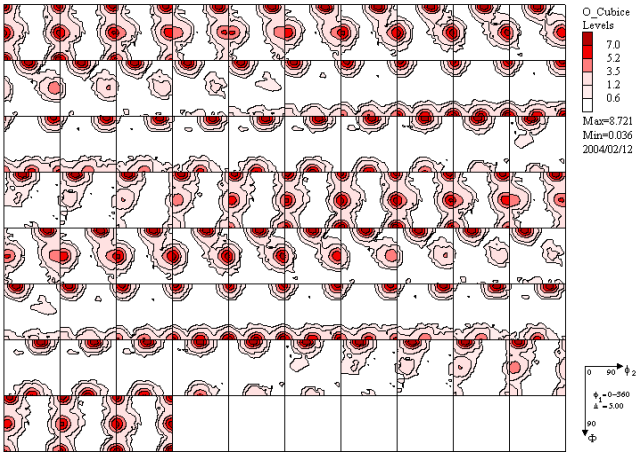


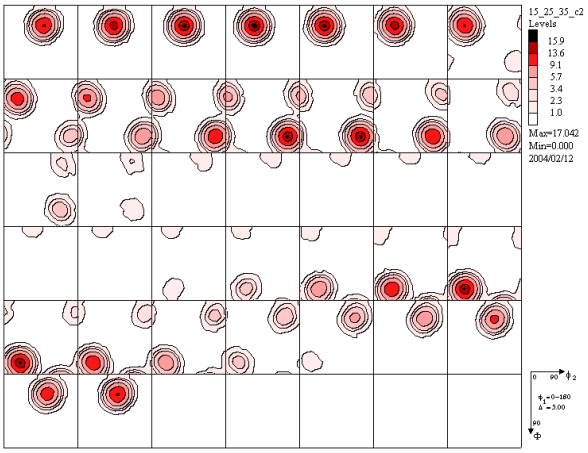
Fig. 15. Axial Sample Symmetry: $\beta = 0^0$ or $\beta = 0^0$ to X^0(Symmetry element C_∞)

If the range of β is between 0^0 and X^0 (the custom range), then the user can make the average of their result (symmetrization to the axial sample symmetry) before the ODF calculation. High sample symmetry makes the texture analysis easier because the range of the β angle is equivalent to the range of the Euler φ_1 angle on the ODF. Below, you can see examples of the ODF (cubic c.s., φ_1=const. projection) for different sample symmetries:

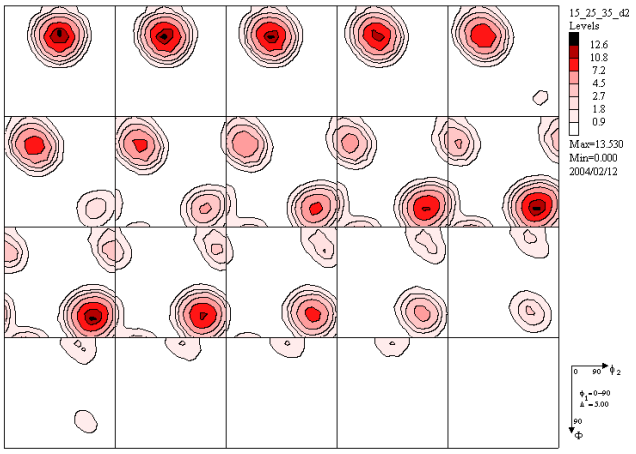
Triclinic sample symmetry



Monclinic sample symmetry



Orthorhombic sample symmetry



Axial sample symmetry

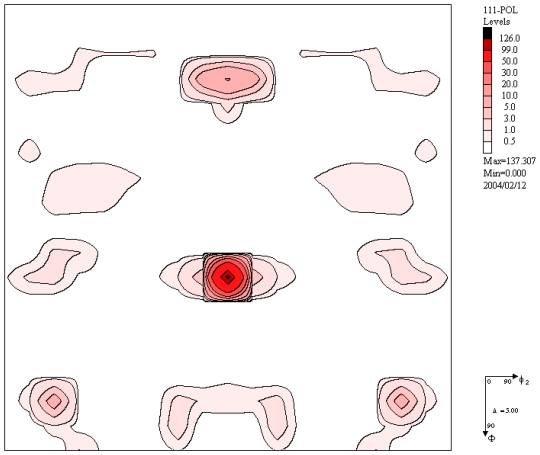


Fig. 16. E*xamples of ODF for different sample symmetries* (cubic crystal symmetry, projections : φ_1=const.)

If, after you have made the measurement, the pole figures for your sample show a higher sample symmetry than you have assumed, then you can make an 'average' of your pole figures to a higher symmetry. This process is called symmetrization. In LaboTex, you can make a symmetrization of pole figures, as well as of the ODF. You may make a symmetrization of pole figures before the ODF calculation. For example, if you have made a measurement of the pole figure in the full range of the azimuthal angle β= 0 to 360 deg. and your pole figure shows the axial sample symmetry,

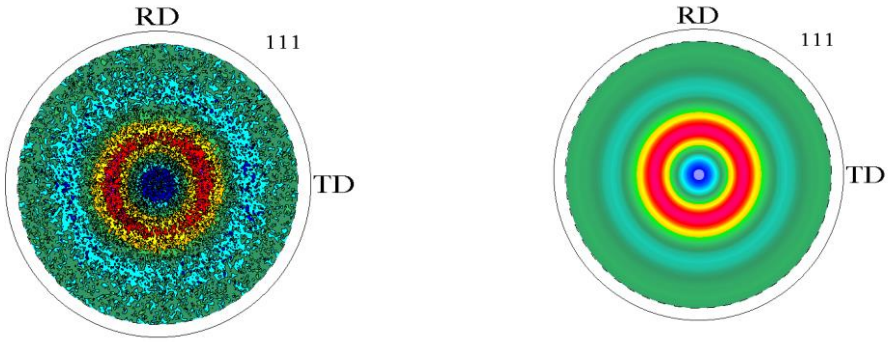


Fig. 17. (Left)- pole figure measured in the full range of the azimuthal angle and (right) - the same pole figure after the symmetrization to the axial sample symmetry.

then you should make a symmetrization to the axial sample symmetry.

As you can see in Figures 18 and 19, in LaboTex, you can make a symmetrization very simply. You can see the pole figures after the symmetrization on the screen, hence you can compare the different types of symmetrization and see the differences between them. Just looking at the pictures might give you an idea of how to make or not to make a symmetrization.

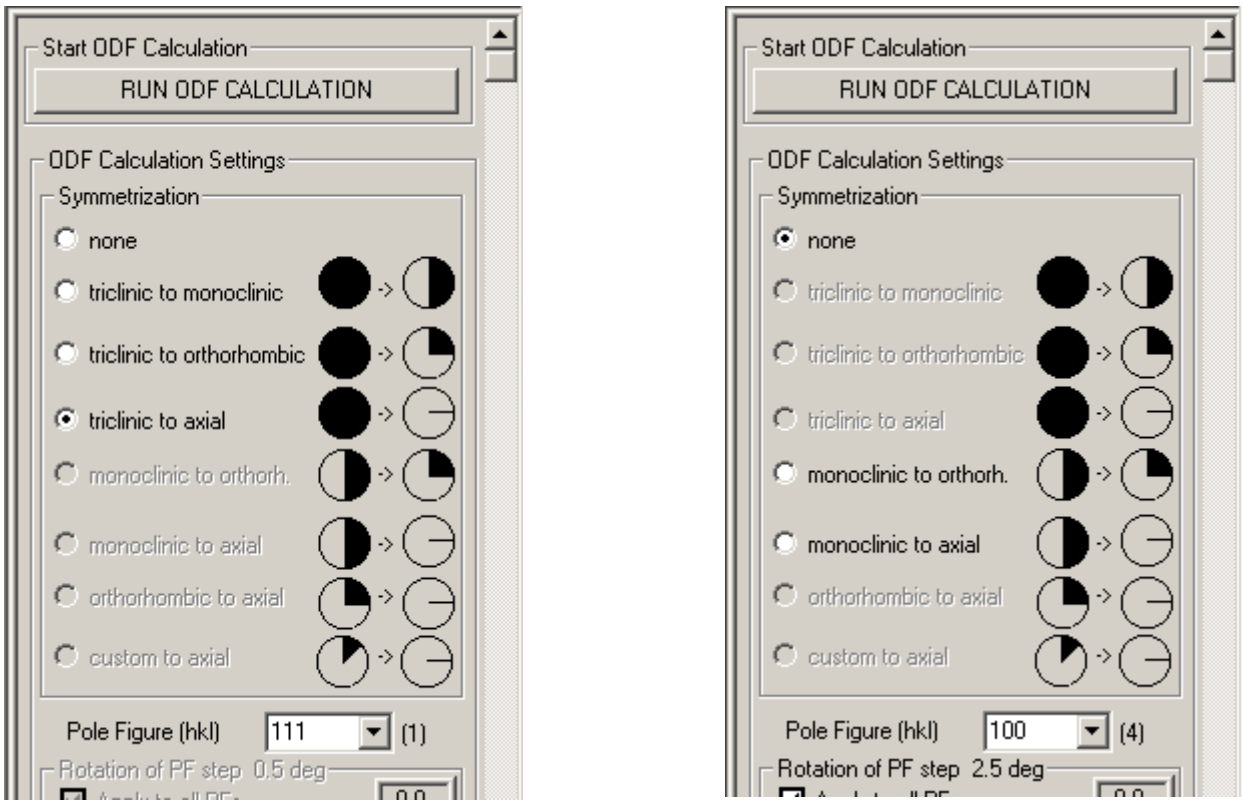


Fig. 18. Types of symmetrization for pole figures measured in the full azimuthal range i.e. such as for the triclinic sample symmetry (left) and for the pole figure measured in the half azimuthal range such as for the monoclinic sample symmetry (right).

The ODF calculations are done from several pole figures. Before the beginning of the ODF calculation, the user can exclude from it one or more bad quality pole figures, as well as only bad fragments of the pole figure (such as deformed ones, as shown in Figure 10). The user can also make a rotation of the pole figure (e.g. by eliminating the error connected with a bad mounting of the sample in the goniometer). In some XRDs, the goniometer's continuous scan of the azimuthal angle shifts the initial value of the β angle from 0 to +β/2 or -β/2 (integration effect). A correction of the above effects is very simple in LaboTex. For details, please see the report "Determination of Volume Fraction of Texture Components".

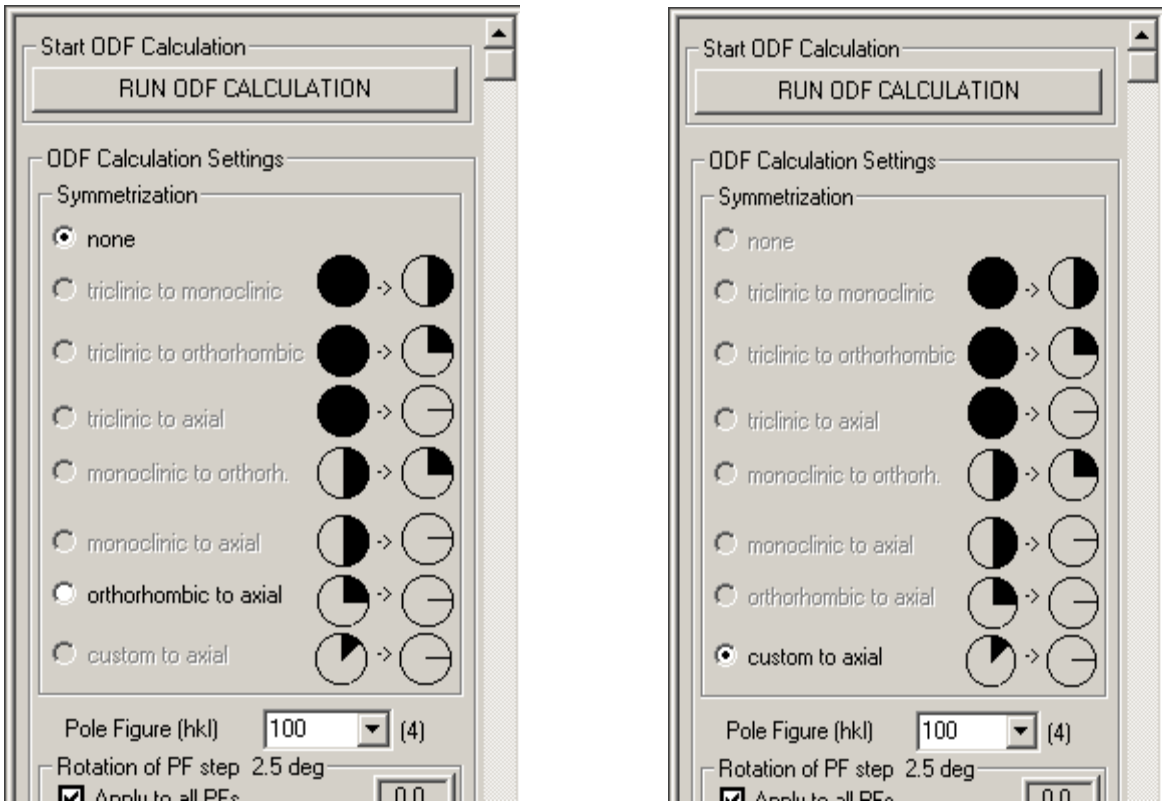


Fig. 19. Types of symmetrization for pole figures measured for a quarter of the azimuthal range i.e. such as for the orthorhombic sample symmetry (left) and for the pole figure measured for the custom azimuthal range (right).

4. Pole Figure: Correction and Normalization

Pole figures should show the statistical distribution of the normal to the given {hkl} plane, hence the intensity data should be corrected for background, defocused and next normalized.

4.1. Background Correction

The intensity values of the background should be independent of the azimuthal angle, hence one or several measurements of the background for the constant radial angle should be sufficient for a good background correction. In LaboTex, you can input the background values from the "left background" (i.e. for values of 2θ lower than 2θ for the {hkl} peak) and from the "right background" (i.e. for values of 2θ higher than 2θ for {hkl} peak). You can also make a correction using only the "left background" or the "right background", as well as input data after the background correction.

If LaboTex finds more than one value of the background for the given radial angle, then it will calculate the average of the background values. Similarly, if LaboTex finds the values for the "right background" and simultaneously for the "left background", it will calculate the average of the "left" and "right" background. In the file with the pole figure you have to set the parameter "Type of Data" to "0" for the background data and "1" for the pole figure data. A detailed description of the format of the pole figure(s) data as well of the background pole figure(s) data can be found in the report "LaboTex Formats" (http://labotex.com/format.pdf). There are also non-LaboTex formats, which can contain information about the background data: NJA (left and right background), DAT, RAW-DFB (popLA), RW1 (COR-->BGR), BKG (PFG), ASC (low and high), UXD (left and right). For details see http://labotex.com/format.htm or contact with LaboSoft.

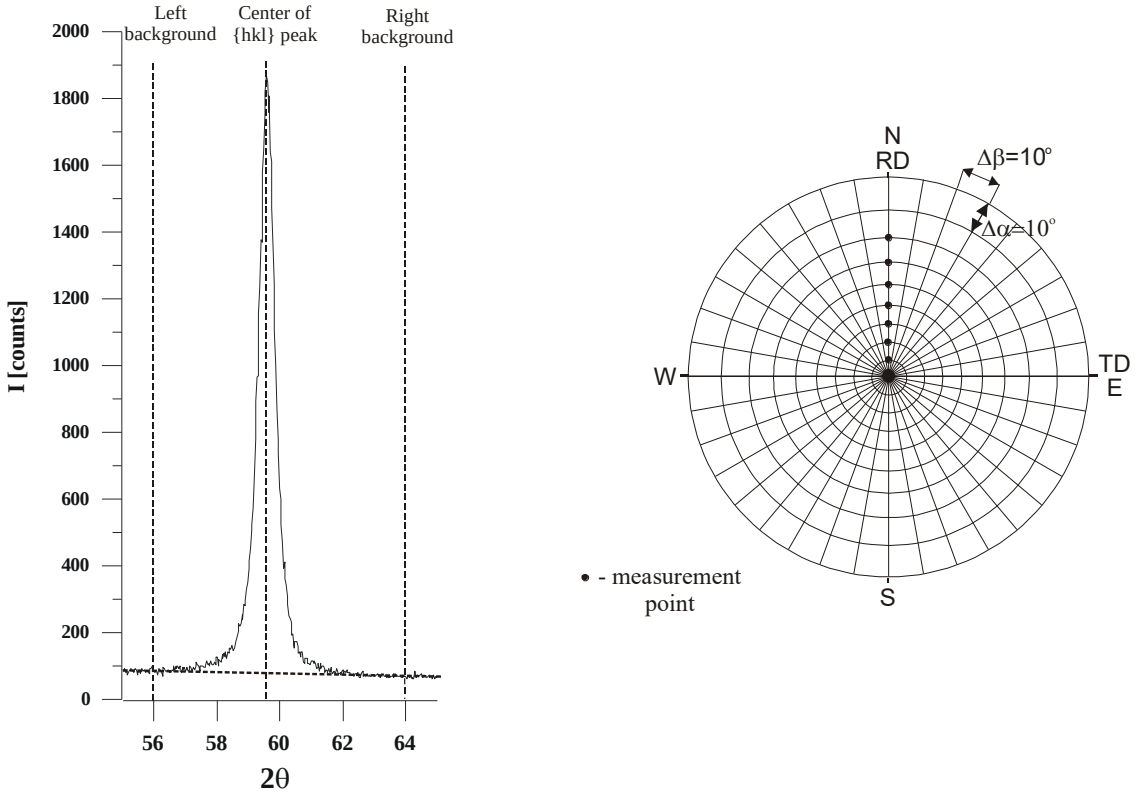
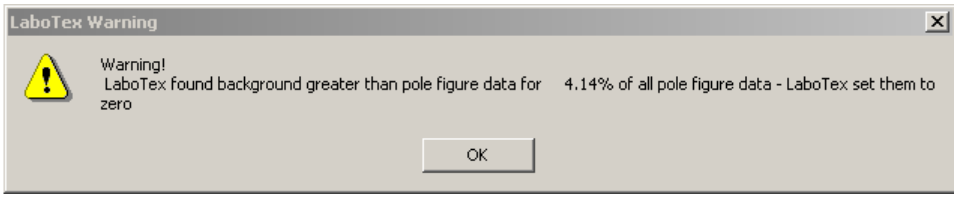


Fig. 20. (left) - {hkl} diffraction peak with background (constant azimuthal and radial angle). (right) - Example of measurement grid for background.

LaboTex informs the user when it finds data for which the background data are greater than the pole figure data and it displays the percent of these data:



When the background data of the pole figure is greater than the pole figure data, LaboTex can:

a) replace the negative values of the pole figure by zero;
b) add to all the pole figure data the lowest value of the pole figure, which, after the correction of the background, makes it posssible to obtain all the non-negative values of the pole figure (LaboTex makes all the data positive).

The user may choose option a) or b) in the menu "**Edit**" → "**LaboTex Options**" → "**Data Formats**" (see Figure 21). The default option is a).

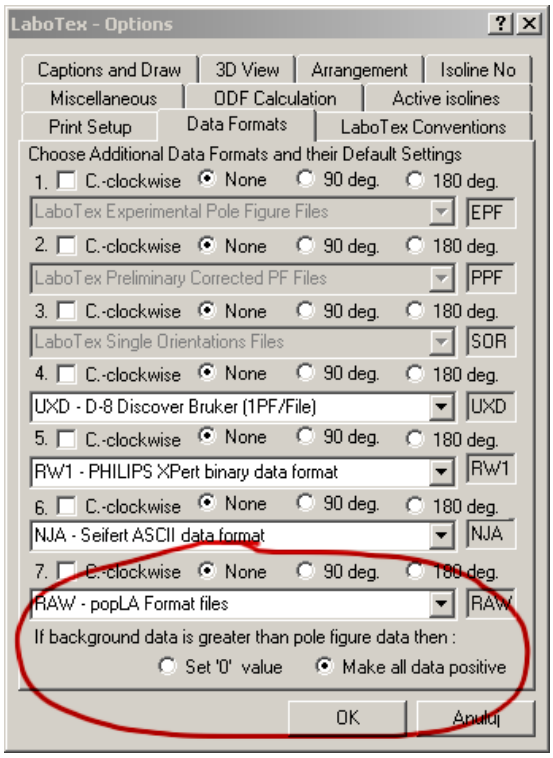


Fig. 21. Choice of the option for the background of a pole figure.

4.2. Defocusing Correction

When the radial angle (α) increases, the way of the beam in the sample for the same thickness is longer (see Figure 22A), hence different effects are observed: the absorption is greater, the peaks in the diffraction pattern are broadened, the maximum of the peaks can be shifted from 2θ (see Figure 22B). These effects (defocusing, absorption) are generally referred to as the "defocusing effect".

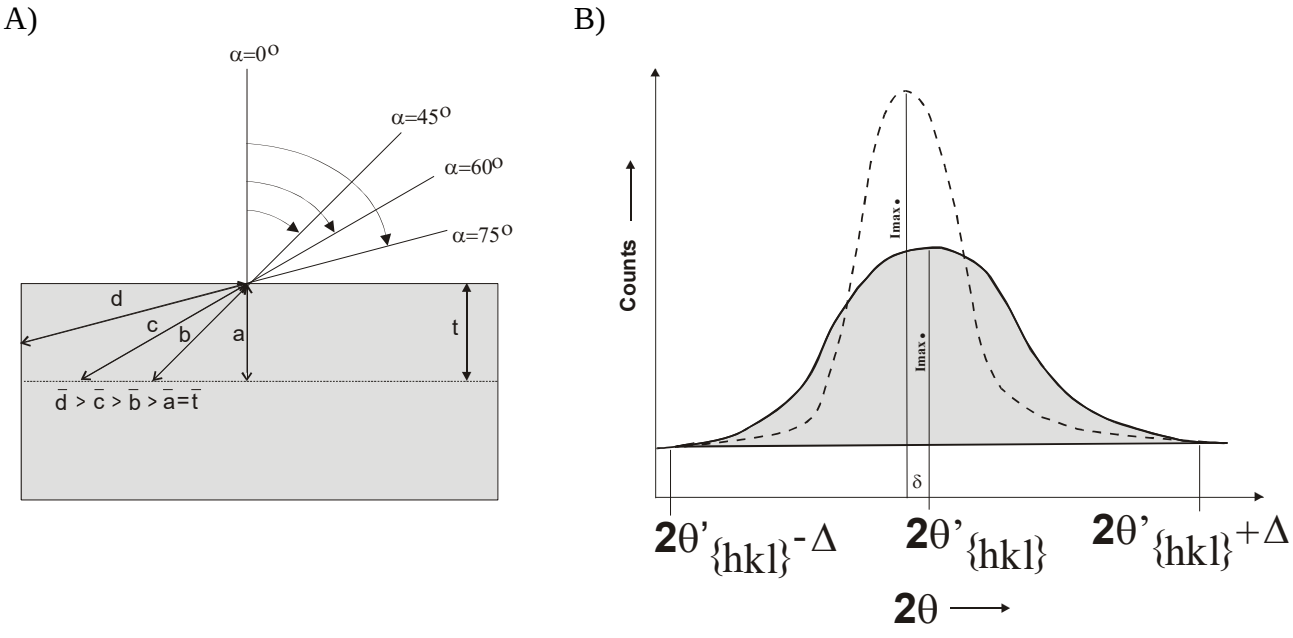


Fig. 22 Defocusing effect

The defocusing effect can be corrected in several ways:

- by measuring the pole figure on an isotropic sample (texture-free, e.g. a properly prepared powder sample) made from the material with the same composition as the main sample. In LaboTex, the pole figures for an isotropic sample (powder sample) are input simultaneously with the main pole figures, but from another list (the list is marked with a black line in Figure 23). The extension of the LaboTex file with pole figures is POW. The format of this file is described in the report "LaboTex Formats"

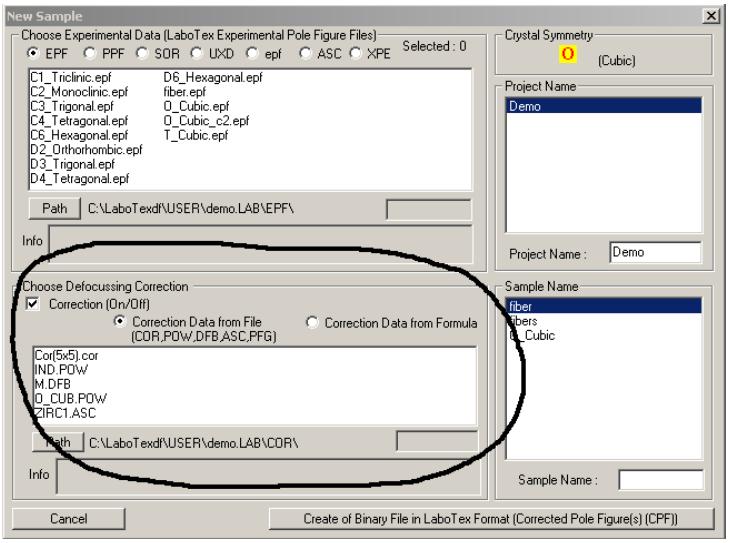


Fig. 23. Input of the file for the defocusing correction.

(http://www.labotex.com/format.pdf). There are also non-LaboTex formats available in LaboTex (DFG,ASC,PFG,NJA,DAT). The current list of these formats can be found at: http://www.labotex.com/format.htm. The ideal pole figures, without a defocusing error, for an isotropic sample, have all the values of counts the same. LaboTex calculates the correction defocusing coefficients from the pole figures for an isotropic sample in two stages:

1. In the first stage, LaboTex calculates the average values of the counts for each circle (α=constant) with the background correction;
2. In the second stage, LaboTex calculates the correction coefficients for each α by dividing the average value of the counts for α=0 by the average value of the counts for a given α.

In Labotex, you can input a set of defocusing correction coefficients which has been calculated earlier (the file with the extension COR).
For details see http://www.labotex.com/format.pdf

- by measuring the pole figure not for one value of $2\theta_{\{hkl\}}$, but in the full range of the {hkl} peak i.e. from $2\theta_{\{hkl\}}-\Delta$ to $2\theta_{\{hkl\}}+\Delta$ (see Figure 21B – the grey area). This method (called the integration method) corrects the errors connected with the broadening and the shift of the maximum of the peaks from 2θ in the diffraction pattern. The position sensitive and the area detectors are very useful in this method.
- by an estimation from the theoretical equations. Some software from your XRD can also make a defocusing and background correction from different equations. You can input the corrected data directly to LaboTex. You can also use the correction from the formula. LaboTex enables making corrections by using the Schulz formula (J.Appl. Phys., 20, 1033, 1949) for the reflection technique:

$$\frac{I_{\alpha=0}}{I_{\alpha}} = \frac{1-\exp\left(-\frac{2\mu t}{\sin\theta}\right)}{1-\exp\left(-\frac{2\mu t}{\sin\theta\cdot\sin(90-\alpha)}\right)}$$

where,

μ - absorption coefficient [1/cm]

t - penetration depth [cm]

Figure 24 shows the changes of the correction coefficients for defocusing, calculated from the Schulz formula for different parameters 2θ and μ·t

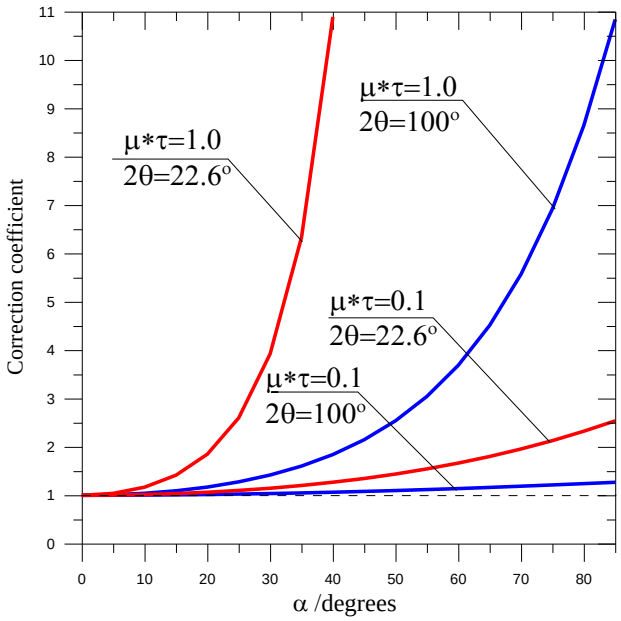


Fig. 24. Correction coefficients for defocusing calculated from the Schulz formula for different parameters 2θ and μ·t

When you would like to make a correction from the Schulz formula, please select the option "Correction Data from Formula" in the "New Sample" dialog (see Figure 25).

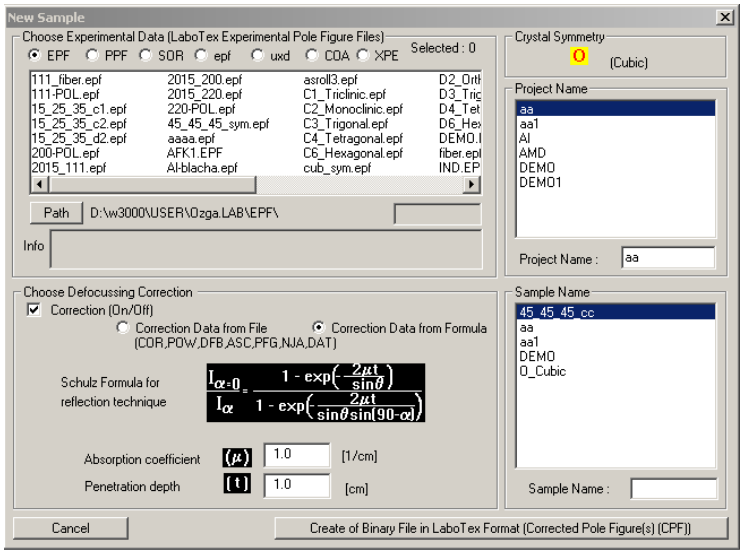


Fig. 25. Option for defocusing correction data from the Schulz formula in LaboTex

Next, you input the values of the absorption coefficient and the penetration depth for your sample. If you would like to find the file with the calculated correction coefficient, you should look for it in the LaboTex user's temporary directory (file 'COR'). You may use the defocusing correction coefficient calculated from another formula. In this case, you should use the file with the extension "COR". For details see http://www.labotex.com/format.pdf .

You can directly observe the defocusing error on 'random' samples, for which all the pole figure values should be the same. The pictures below (Fig. 25a) show examples of the experimental pole figures {110}(left) and {211} (right) of a 'random' sample made with the powder of Ferritic Stainless Steel (reflection technique, axial symmetrization):

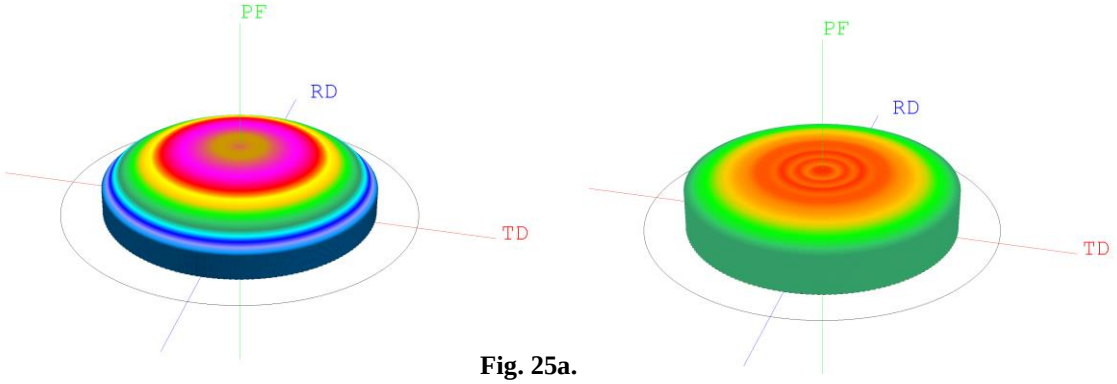


Fig. 25a.

As you can see, the defocusing effect is greater for the {110} pole figure than for the {211} pole figure. The Schulz formula for the reflection technique may, to some extent, explain these effects: the defocusing effect is greater for the pole figures with a lower 2θ, hence the pole figure {110} (2θ=52.3°) is more deformed than the pole figure {211} (2θ=99.5°)

The results of the defocusing effect (the shift and lowering of the maximum, the broadness of the diffraction peaks in 2θ when the radial angle increases) can also lead to a bad correction of the background (see Figure 25b).

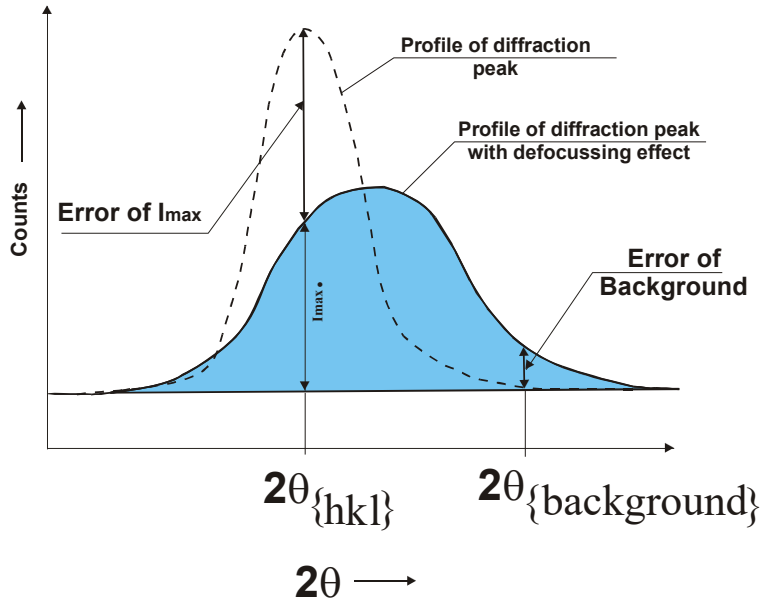


Fig. 25b. Defocusing effect: Errors in the determination of parameters of the diffraction peak.

LaboTex (version 2.1.015E) informs the user when it finds data for which the background data are greater than the pole figure data. LaboTex also displays the percent of these data.

Example:

The pole figure deformed by the defocusing effect (left) and a well corrected complete pole figure (right) obtained for the same sample (the intensity of the pole figure for the radial angle greater than 65 degrees is strongly lowered on the pole figure on the left. The intensity in the center of this pole figure is increased).

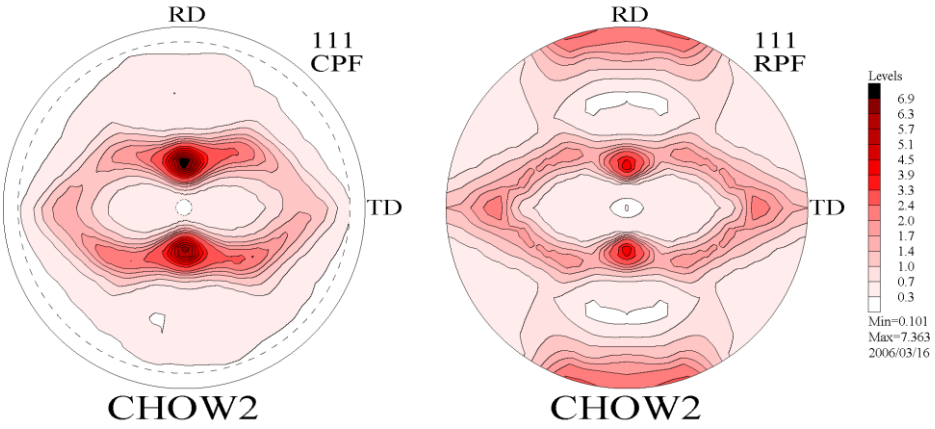


Fig. 25c. Pole figures deformed (left) and undeformed (right) by defocusing.

Warning:

1) The calculation of the ODF from deformed (not corrected) pole figures leads to a divergence in

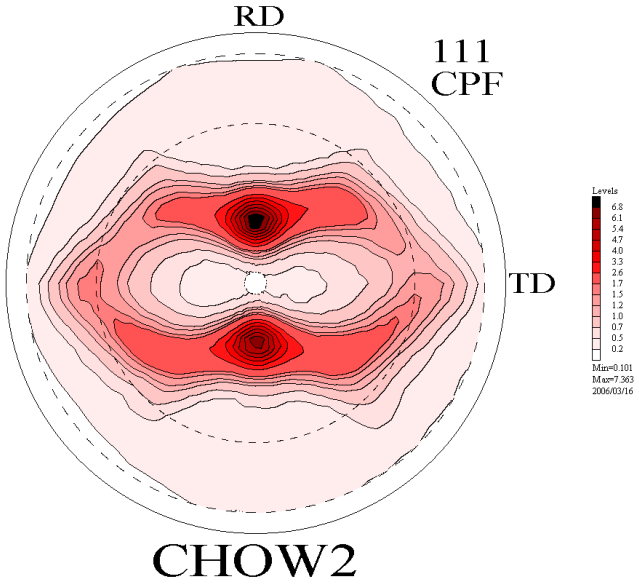


Fig. 25d. An undeformed fragment of a pole figure (the fragment between the dotted line in the center and the next dotted line), “cut out“ into the ODF calculation

the ODF calculation. You can cut out the undeformed fragments of a pole figure into the ODF calculation using sliders. A too small fragment of a pole figure can make the ODF calculation poor or impossible. You can also correct the faults in the mounting of the sample in the goniometer by rotating the pole figure by means of an appropriate slider :

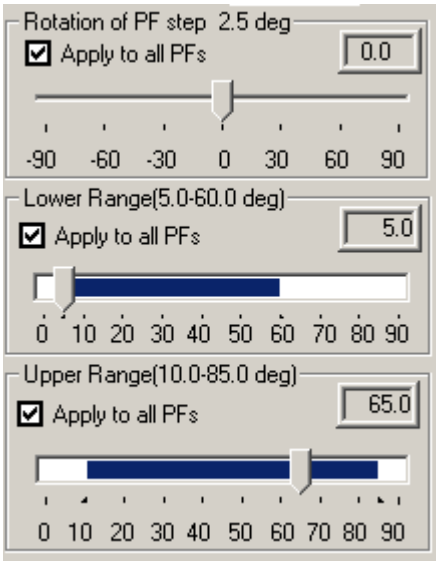


Fig 25e. Sliders for the rotation of a pole figures and for "cutting out" the undeformed fragments of pole figures into the ODF calculation.

2) LaboTex uses the defocusing correction coefficient. If you have a set of defocusing coefficients, then you have to recalculate them to the defocusing correction coefficient:

defocusing correction coefficient = 1/defocusing coefficient

3) LaboSoft s.c. offers several Texture Standards and "Random" (powder) samples for different materials (Cu-Al, Al, Ti, steel-austenitic, steel-ferritic) and for different sample symmetries (triclinic, orthorhombic). The texture index for "Random" reference samples is lower than 1.1. You can make measurements on your XRD and next, you may compare your results with the results from the Accredited Testing Laboratory (two correction methods for defocusing). You can also check the plot and registration conventions. For details see http://labotex.com/texture standard.htm . The PIM and IM methods are also described.

These methods assure obtaining reliable **"device-independent"** pole figures for the quantitative texture analysis. See also: "Texture Standard. **'Device-independent'** pole figures for the quantitative texture analysis. The **P**eak **I**ntensity **M**ethod (**PIM**) and the **I**ntegrating **M**ethod (**IM**) - basic information":

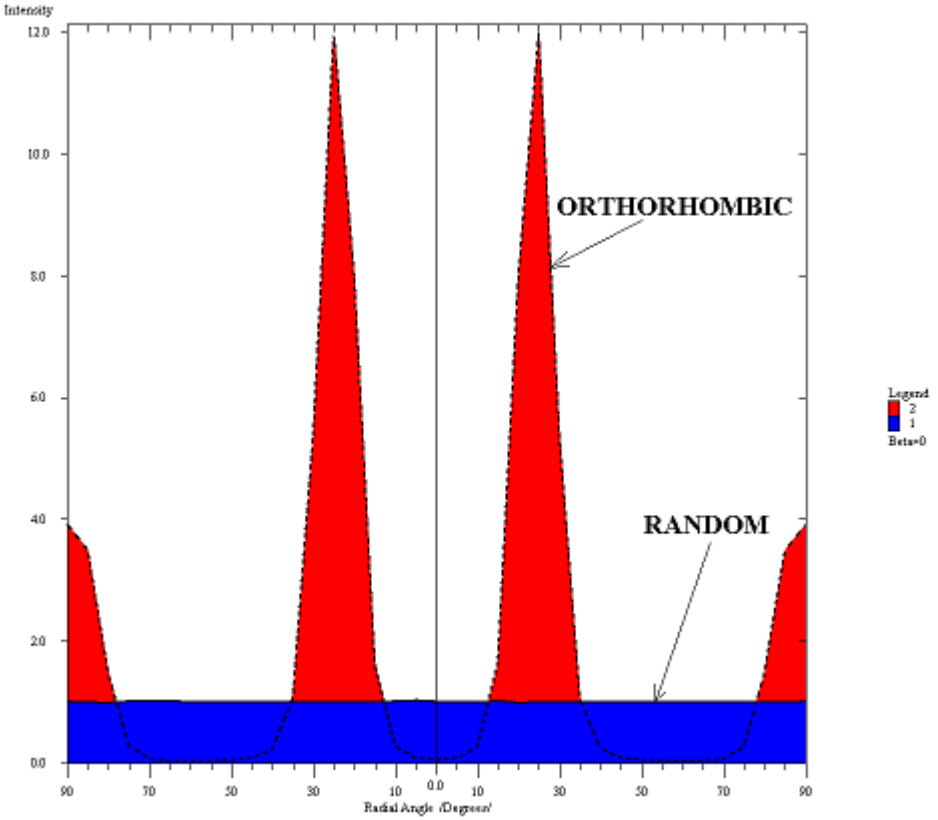


Fig. 25f. Example: Sections of pole figures for azimuthal angle=0.0: Aluminium reference samples.

- red - texturized with orthorhombic sample symmetry,
- blue - powder sample ("random" - texture free) sample.

Examples:

Pole Figures (sections) for a powder iron sample with the background correction.

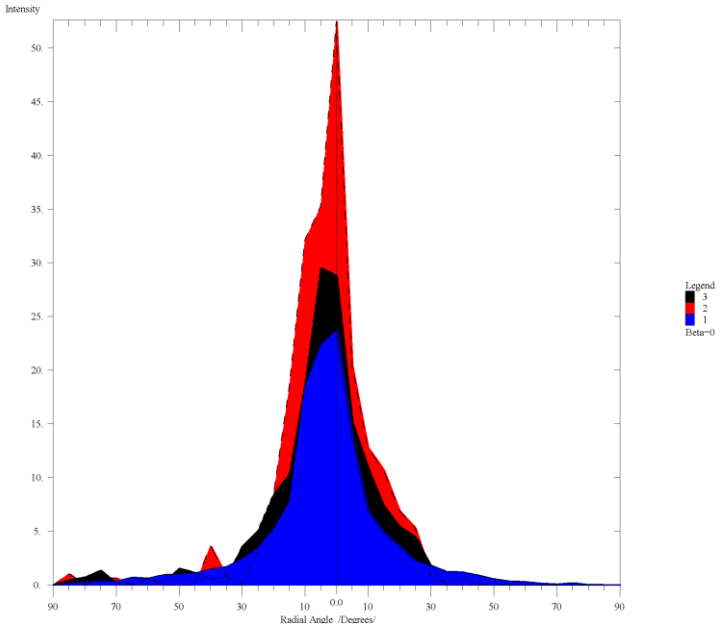


Fig. 25g. Pole Figures (sections) for a powder iron sample with a bad background correction. Measeurement with a point detector in the usual mode.

The shift of the diffraction peaks with the increase of the radial angle (Fig. 25h) causes a sharp decrease of the intensity (the initial 2Θ is not in the maximum of the peak for a greater radial angle). For this sample, LaboTex also shows that more than 40% of the background values are greater than the pole figure values. This indicates that the shift of the diffraction peak causes also a bad background correction. The below image (Fig. 25i) shows the sections of pole figures for the same sample, but with no background correction. The maximal value of the pole figure decreases from about 50 (in the case with the background correction) to 11 (in the case with no background correction).

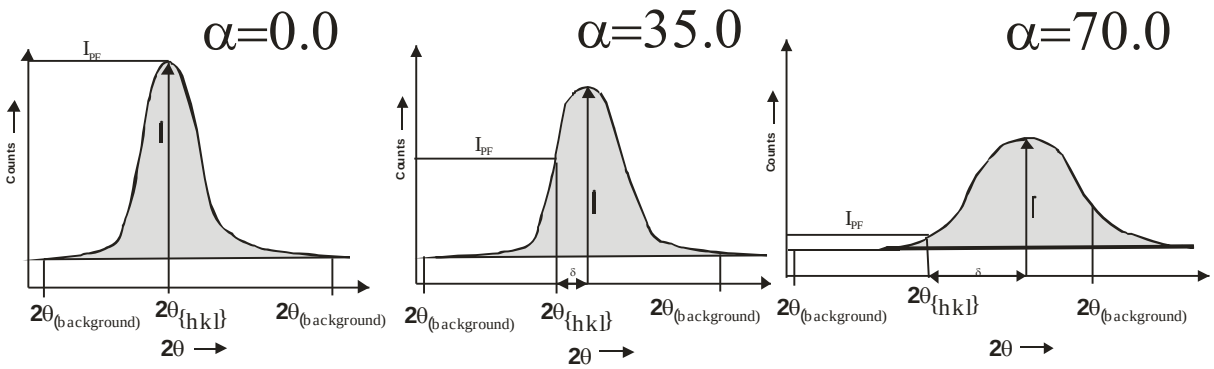


Fig. 25h. Defocusing effect. Measurement of the pole figure intensity in point (α,β) with a point detector in the usual mode. The background intensity can be greater than the PF value in some cases

.

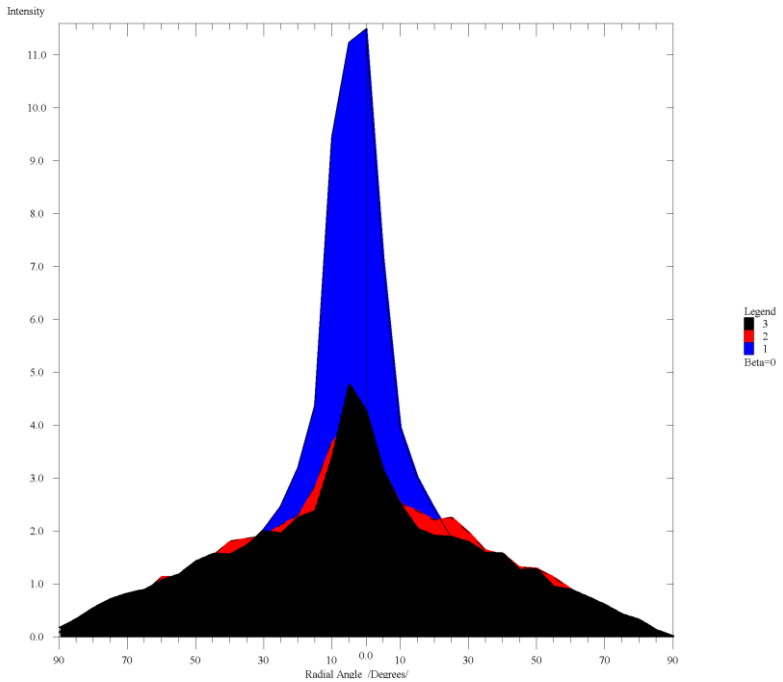


Fig. 25i. Pole Figures (sections) for a powder iron sample with no background correction. Measurement with a point detector in the usual mode.

As you can see in Figures 25g and 25i, when you are using a point detector in the usual mode, then the defocusing correction needs great correction coefficients (even about 100). This can be a source of considerable errors. The changes of the intensity of the radial angle are smaller for the integrating method when the PSD or pseudo-PSD techniques of measurement are used (see Figure 25j). In this case, the correction coefficients are lower than 2.0, within the range of the radial angle from 0.0 to 75.0 degrees. The deformation of the pole figure after such correction is small and the pole figures are of good quality

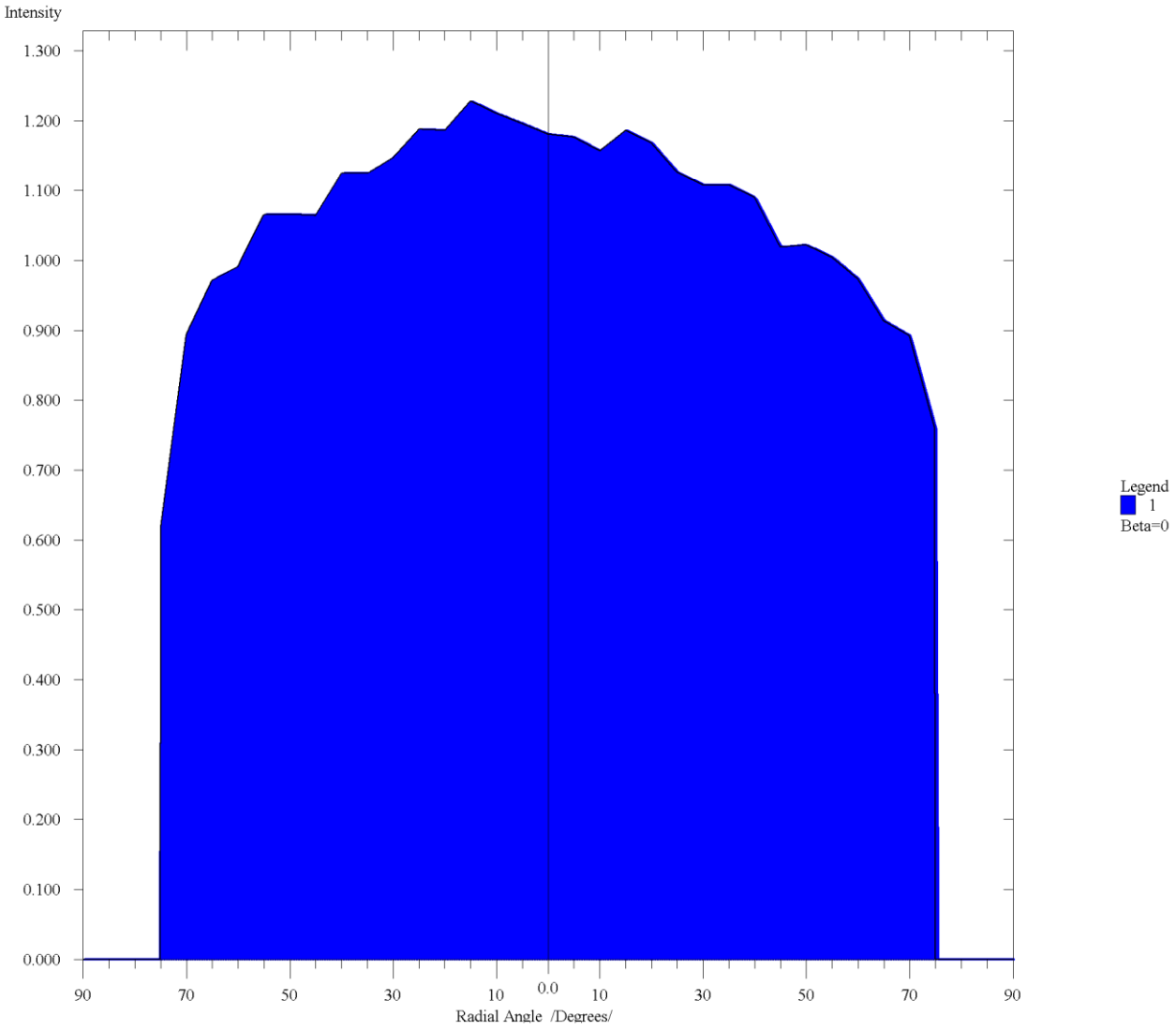


Fig. 25j Pole Figure (section) for a powder iron sample. Measurement with a point detector in a pseudo PSD mode. The Integrating Method (IM) for each point (α,β) of the pole figure.

4.3. Normalization

LaboTex inputs the data for pole figures, backgrounds, defocusing correction coefficients and next, it makes a correction:

corrected PF value (α,β)= (measured PF value (α,β)-background(α))·defocusing correction coefficients (α)

Finally, the corrected PF values are normalized with respect to the condition that the uniform values of the pole figure equalling 1.0 describe a random distribution of the lattice orientations, hence the equation for a normalized pole figure intensity $f_N(\alpha,\beta)$ (where α is the radial angle and β is the azimuthal angle) gives the area of hemisphere (2π):

$$\int_{\alpha=0}^{\alpha=\frac{\pi}{2}}\int_{\beta=0}^{\beta=2\pi} f_N(\alpha,\beta)\cdot\sin(\alpha)\cdot d\alpha\cdot d\beta = 2\pi$$

and

$$\frac{1}{2\pi}\int_{\alpha=0}^{\alpha=\frac{\pi}{2}}\int_{\beta=0}^{\beta=2\pi} f_N(\alpha,\beta)\cdot\sin(\alpha)\cdot d\alpha\cdot d\beta = 1$$

hence, for an un-normalized intensity $\boldsymbol{f_U}$:

$$\frac{1}{2\pi}\int_{\alpha=0}^{\alpha=\frac{\pi}{2}}\int_{\beta=0}^{\beta=2\pi} f_U(\alpha,\beta)\cdot\sin(\alpha)\cdot d\alpha\cdot d\beta = N_f$$

and

$$\frac{f_U(\alpha,\beta)}{N_f} = f_N(\alpha,\beta)$$

where N_f is the normalized factor.
In the case of a random sample:

$$\frac{f_U(\alpha,\beta)}{N_f} = f_N(\alpha,\beta) = 1.0$$

hence

$$\int_{\alpha=0}^{\alpha=\frac{\pi}{2}}\sin(\alpha)\cdot d\alpha\int_{\beta=0}^{\beta=2\pi} d\beta = 1.0\cdot 2\pi = 2\pi$$

As in both pole figure measurement techniques (reflection and transmission) we get incomplete pole figures, it is not possible to make a proper normalization in this stage. Instead, LaboTex **makes only a preliminary normalization** of the pole figures with respect

to incomplete α and β ranges. Next, LaboTex creates pole figures called CPF (**C**orrected and preliminary normalized **P**ole **F**igures). From these pole figures, the user can calculate the ODF. Simultaneously with the ODF, **LaboTex creates properly normalized experimental pole figures with a normalized factor calculated from the ODF.** These pole figures are denoted as NPFs (**N**ormalized **P**ole **F**igures). Different types of pole figure objects occurring in LaboTex are described in the report: "Introduction to LaboTex". **Only properly normalized pole figures should be used in the texture analysis (NPF,RPF,APF).**

4.4. Merge of pole figures

In LaboTex's pole figure data formats - EPF and PPF - you can prepare all the pole figures in a single EPF or PPF file. An EPF file can also contain the pole figures' background data. You can prepare the data in a different PPF or EPF file and merge it in LaboTex. If you would like to input several files referring to one sample, click on all the file names and simultaneously hold pressed the CTRL (control) key.

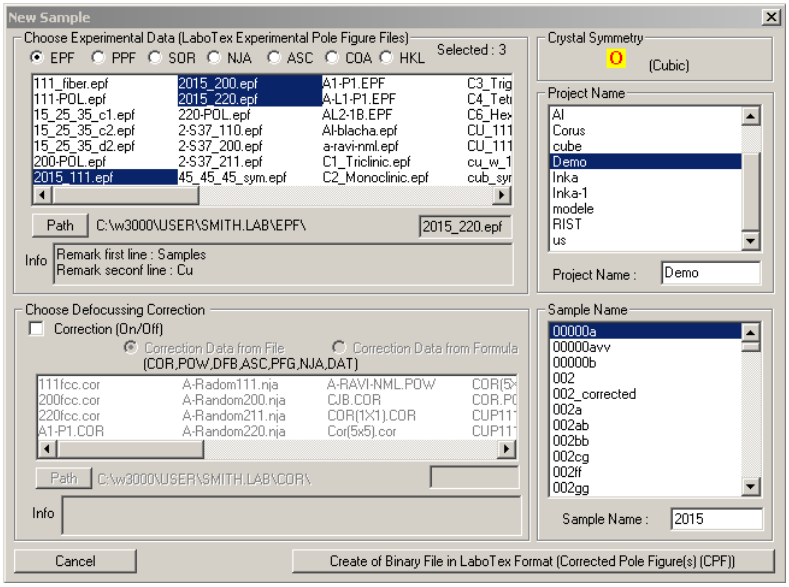


Fig. 26. Input several files with pole figures to LaboTex.

Similarly, you can merge pole figures for the defocusing correction (files in the POW format) or pole figures with the defocusing correction coefficients (files in the COR format).

As you can see in Figure 27, there are only 7 different file formats available simultanously in LaboTex, when you open the dialog "**New Sample**". The LaboTex formats are in positions 1-3. These formats are permanent. You are free to choose the data formats 4 - 7 in the

"**LaboTex Options**" from among about 30 different formats (you can find the current number of the data formats available in LaboTex at http://www.labotex.com/format.htm).

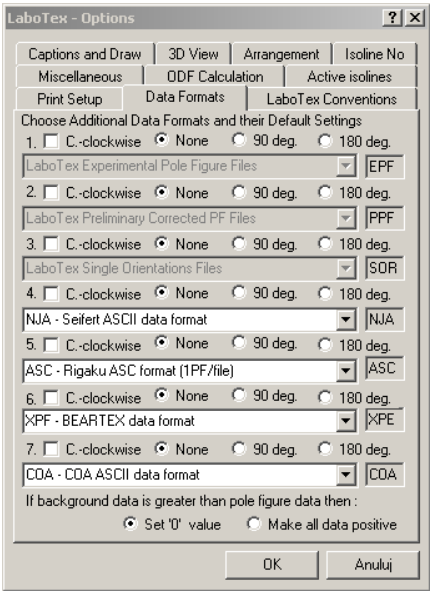


Fig. 27. Choice of additional formats in LaboTex.

The files with pole figures data in non-LaboTex formats don't contain the information about the crystal symmetry, hence if you click on the file in a non-LaboTex format, you have to select the crystal symmetry of your sample (see Figure 28). The default is set at the O – the cubic crystal symmetry.

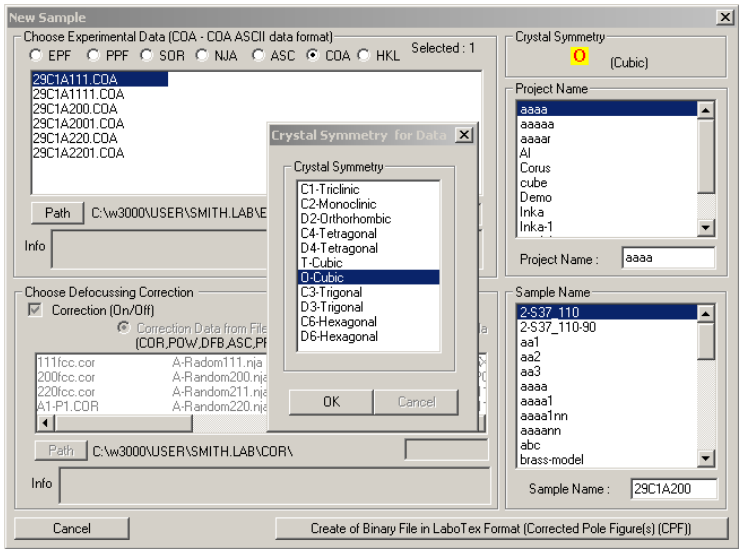


Fig. 28. Choice of the crystal symmetry of a sample

Next, you can make a multiselection for all the files with the pole figure data referring to your sample (see Figure 29). If the data format (similarly to the "COA" format) contains the

corrected pole figure data, then the lower list (the list of files for the defocusing correction) is greyed.

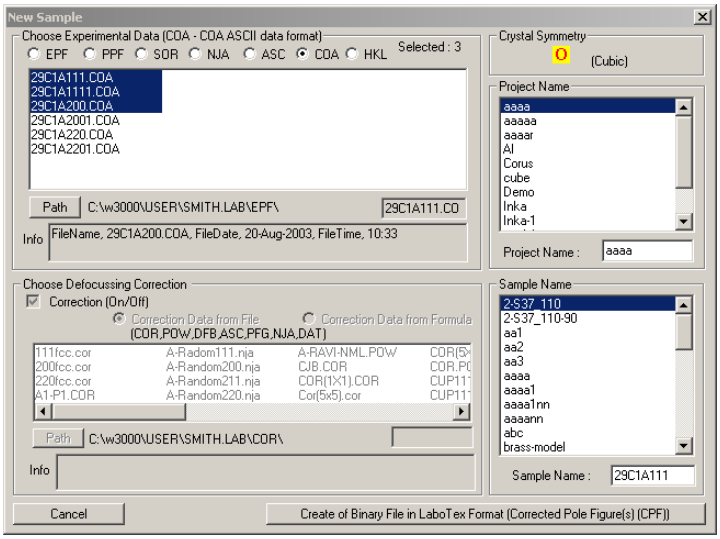


Fig. 29. Multiselection for input of several files with pole figures in a non-LaboTex format.

Files with pole figures data in non-LaboTex formats don't contain information about the cell parameters. For lower symmetry than the cubic crystal symmetry, this data are necessary for the ODF calculation. LaboTex accepts relative cell parameters. The order of the cell parameters is important for a proper ODF calculation.

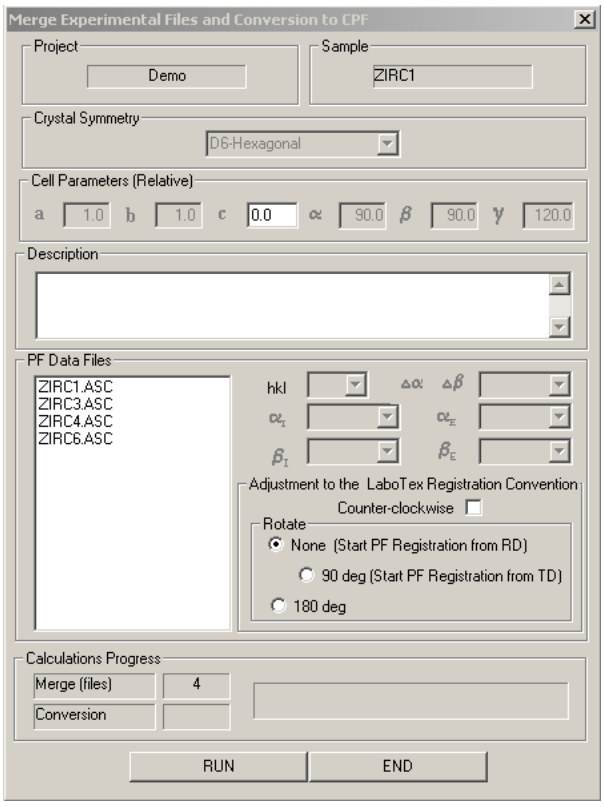


Fig. 30. Completed of cell parameter(s) for a sample in the case of a lower symmetry than the crystal symmetry.

5. Convention of cell parameters

For a lower symmetry than the cubic crystal symmetry, you have to input the cell parameters of your samples into LaboTex. In LaboTex, we use the most popular Matthies convention (see the table at the following page). LaboTex does not permit the input of the parameters of the cell in any other order.

Warning: A bad order of the cell parameters can change the results of the texture analysis.

Example:

In the case of the pole figures:

{020},{110},{200},{201},{310}

for a sample with the orthorhombic crystal symmetry, the cell parameters

a=0.741nm; b=0.495nm, and c=0.255nm

are in an incorrect order. According to the Matthies convention, the order should be:

a=0.255nm b=0.495nm c=0.741nm

or, in relative units:

a=1. b=1.94 c=2.91

(the angles are the same: 90,90,90), hence the pole figures hkl should be input in the way shown in the second column below:

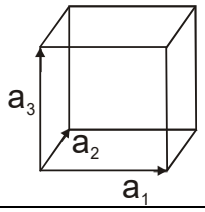
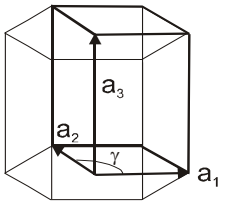
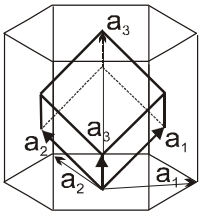
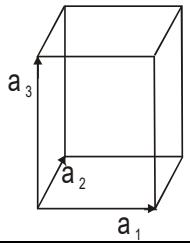
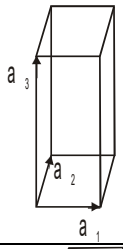
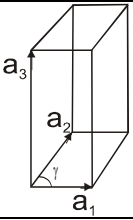
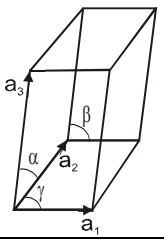
020 ---> 020

110 ---> 011

200 ---> 002

201 ---> 102

310 ---> 013

Crystal System	Crystal Class		basic vectors*		Figure
			$\|a_1\|$ $\|a_2\|$ $\|a_3\|$	α_{23} α_{13} α_{12}	
			a b c	α β γ	
Cubic	**O**	**O_h,O**	a = a = a	90° 90° 90°	
	T	**T_d,T_h,T**			
Hexagonal	**D_6**	**D_{6h}, D_6**	a = a c	90° *90°* γ = 120°	
	C_6	**C_{6h}, C_{6v}, C_6**			
	D_3	**D_{3h}**			
	C_3	**D_{3h}**			
Trigonal	**D_3**	**$D_{3d.}$, D_3**	a = a = a	$\alpha = \beta = \gamma < 120°$	
	C_3	**C_{6v}, S_6, C_3**			
Tetragonal	**D_4**	**D_{4h}, D_4**	a = a c	90° 90° 90°	
	C_4	**C_{6h}, C_{6v}, C_6**			
	D_2	**D_{2d}**			
	C_2	**S_4**			
Orthorhombic	**D_2**	**D_{2h},D_2**	a < b < c	90° 90° 90°	
	C_2	**C_{2v}**			
Monoclinic	**C_2**	**C_{2h},C_2**	a < b c	90° 90° γ < 90°	
	C_1	**C_1**			
Triclinic	**C_1**	**C_1**	a < b < c	α β γ < 90°	

* a, b, c, α, β, γ: the denotations of the cell parameters used in LaboTex

Example:

Sample:
component: cubic {100}<001>
crystal symmetry : *cubic*
sample symmetry: *orthorhombic*
cell parameters: 4,4,4, 90,90,90

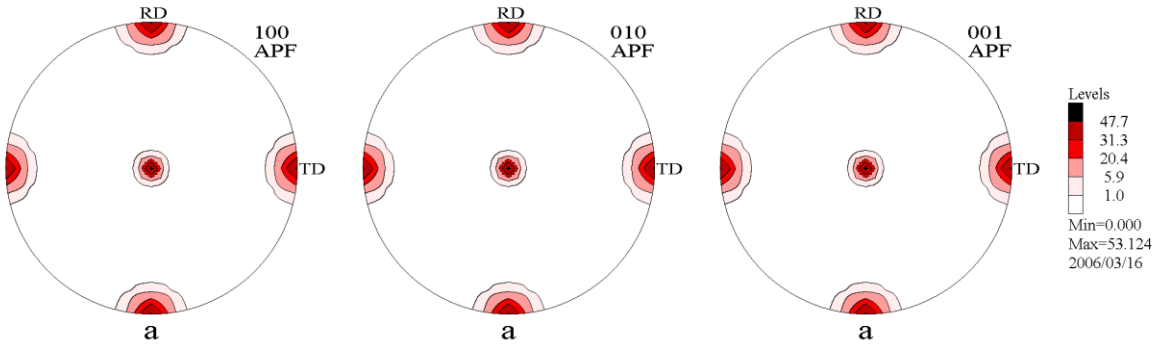


Fig. 30a. Pole figures {100},{010} and {001} for cubic crystal symmetry.

Sample:
component: cubic {100}<001>
crystal symmetry : *tetragonal*
sample symmetry: *orthorhombic*
cell parameters: 4,4,8, 90,90,90

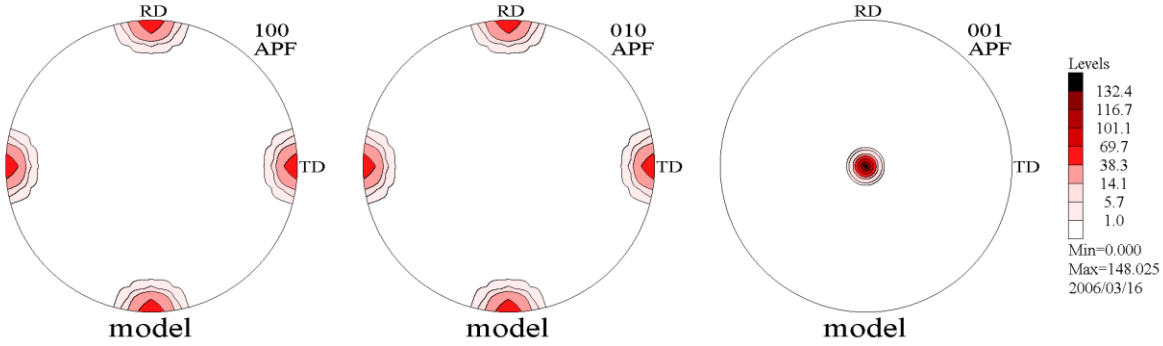


Fig. 30b. Pole figures {100},{010} and {001} for the tetragonal crystal symmetry (lack of the pole in the center of {100} and {010} pole figures, as the "c" cell parameter is different than the "a" cell parameter).

Sample:
component: cubic {100}<001>
crystal symmetry : *tetragonal*
sample symmetry: *orthorhombic*
cell angles: 90,90,90
relative cell parameters :

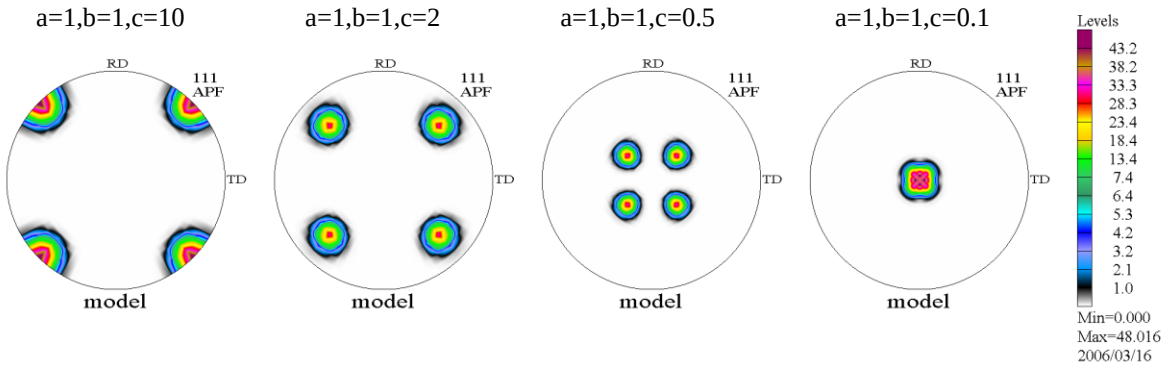


Fig. 30c. Pole figure {111} for different c/a in tetragonal crystal symmetry.

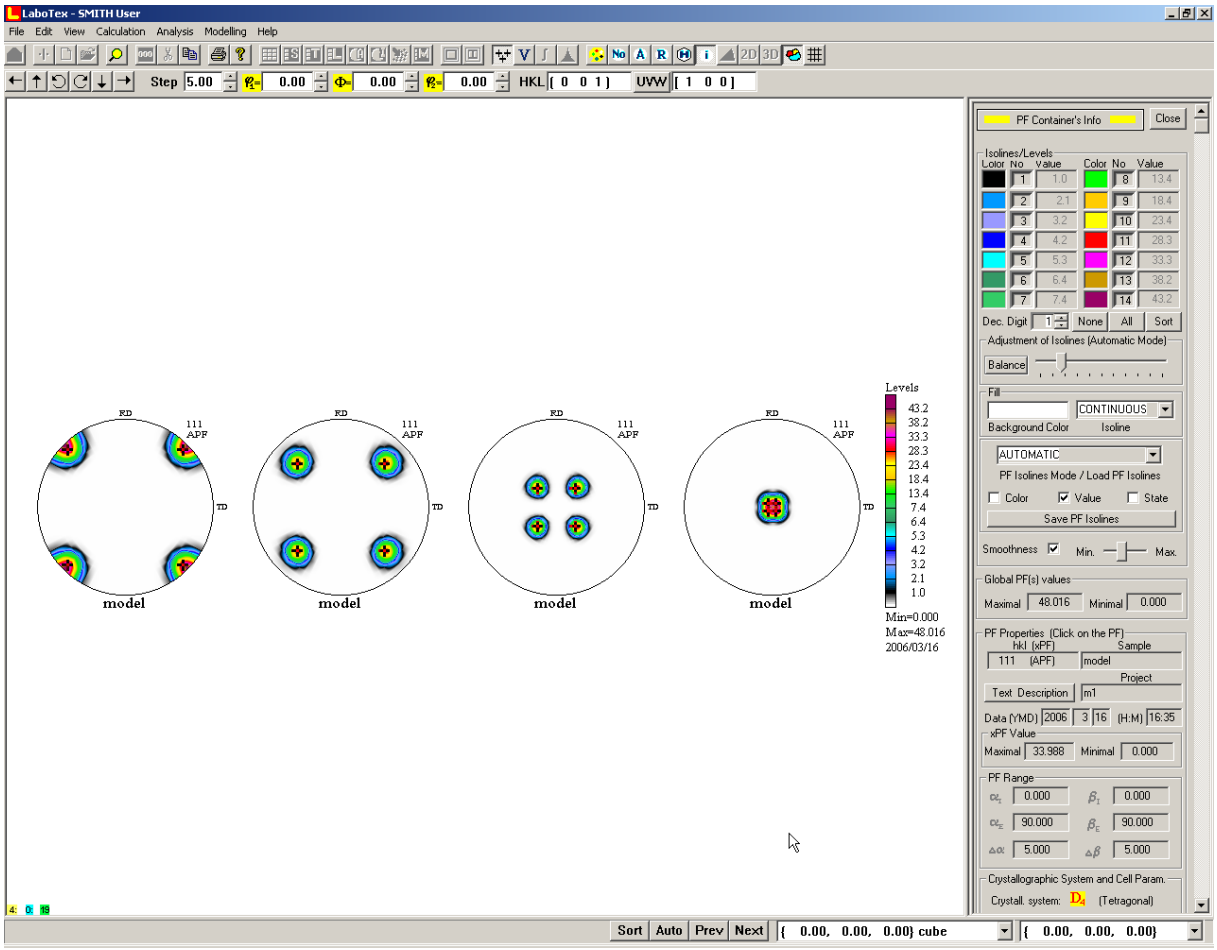


Fig. 30d. LaboTex orientation analysis. LaboTex shows poles (cross marks) of {001}<100> orientation in different (but proper) places in the pole figure
(the position of the poles depends on the c/a ratio for samples with tetragonal crystal symmetry).

6. Pole Figure - Registration Convention

A sample have to be physically marked in the texture measurement. An axis system can be connected to the sample, as it is shown in Figure 31. For a rolled sample, for example, the sample face RD-TD is usually the rolling plane and the preferential direction of the sample is the rolling direction (RD). There are different ways of pole figure registration depending on the type of the motion of the texture goniometer and the start point of the pole figure registration:

(1) a clockwise rotation from the rolling direction (RD) of the sample (or from another preferred direction of the sample);

(2) a counter-clockwise rotation from the rolling direction (RD);

(3) a clockwise rotation from the transverse direction (TD);

(4) a counter-clockwise rotation from the transverse direction (TD).

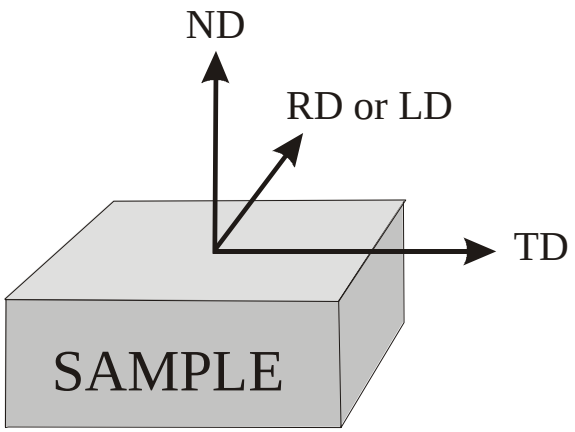


Fig. 31. Sample axis definition

LaboTex uses convention (1).

It is possible to adjust the pole figure data to the LaboTex registration convention using the tools available in LaboTex:

- the replacement of "clockwise" by "counter-clockwise" is possible during the creation of CPF. The user should only mark the suitable option (see Figure 32);
- the replacement of the start point of the pole figure registration, i.e. the direction from RD to TD and vice versa is also possible during the creation of CPF. The user should select and mark the suitable option (see Figure 33). The upturned figures will be shown as CPF objects;

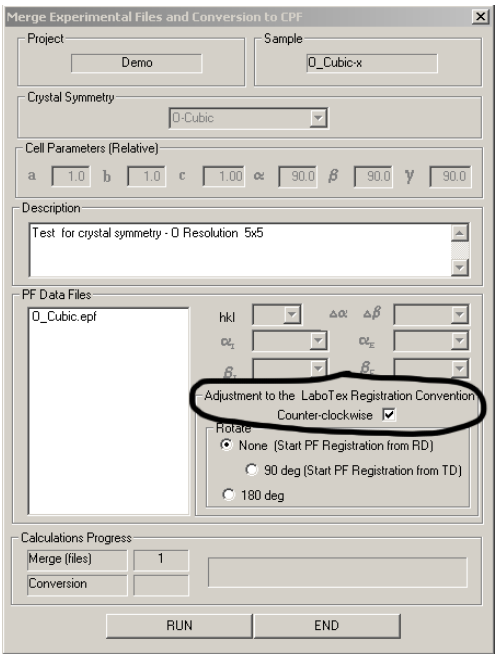


Fig. 32 The replacement of "clockwise" (default) by "counter-clockwise"

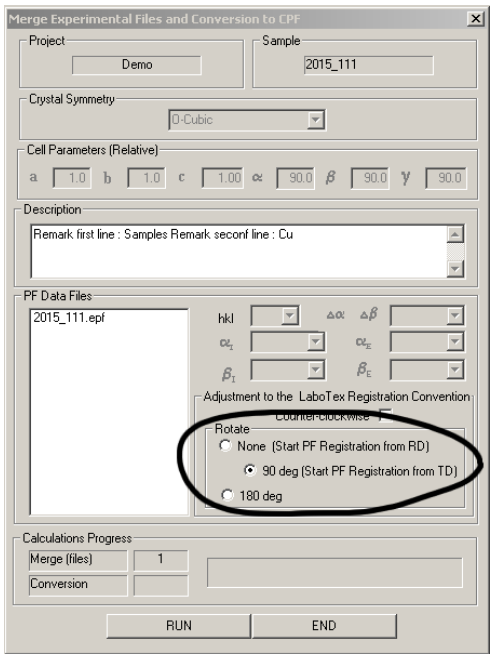


Fig. 33 The change of the start point of the pole figure registration

- the replacement of the start point of the pole figure registration is also possible before the calculation of the ODF (after selecting the "**PF→ODF**" menu command).

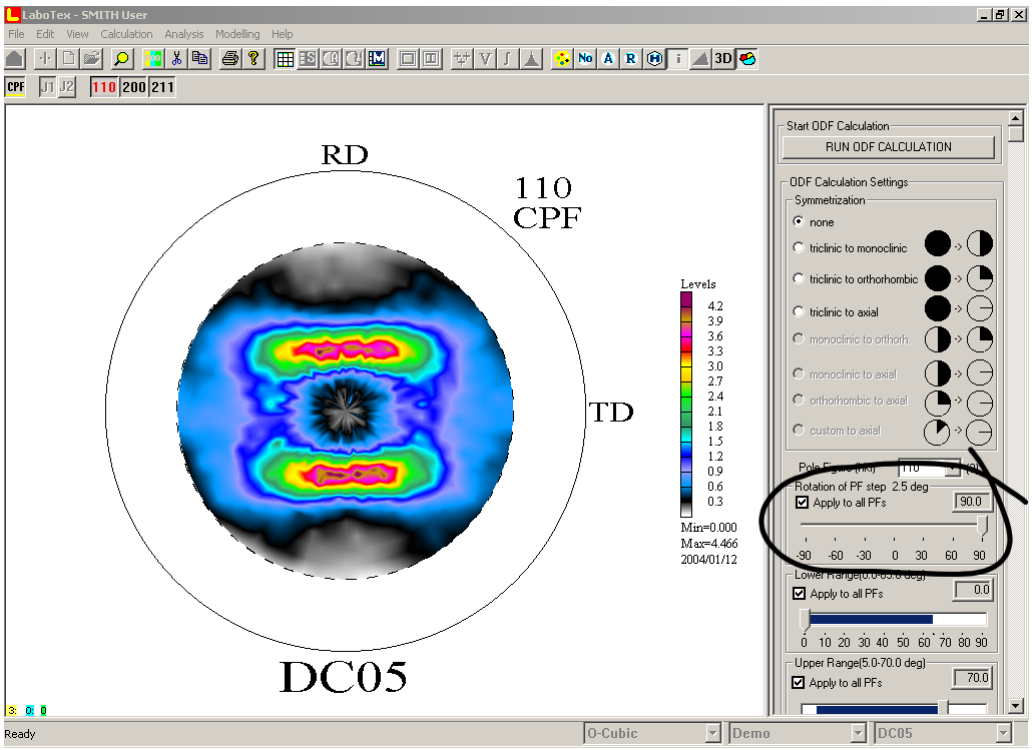


Fig. 34. The change of the start point of the pole figure registration before the calculation of the ODF

The user should rotate the pole figure (CPF) with -90 or +90 degrees (select the option "**Rotation of PF**" and mark the suitable angle -90 or +90 degrees with the slider (see Figure 34)). The upturned figures will be shown as NPF objects after the ODF calculation (in this case, the CPF figures will not be upturned).

You can also adjust the pole figure data with a rotation of about 180 deg (Figure 33).

7. Pole Figure - Plot Convention

If your registration convention is the same as the LaboTex registration convention, but the pole figures from your XRD software are different than those from LaboTex, then your XRD software can use a convention for the plotting of pole figures other than LaboTex. There are different ways of pole figure plot convention, depending on the start point of the pole figure plot. The most common use is:

(1) a clockwise rotation from the N direction;

(2) a counter-clockwise rotation from the N direction;

(3) a clockwise rotation from the E direction;

(4) a counter-clockwise rotation from the E direction.

LaboTex plots the pole figures as in point (1) (see Figures 35).

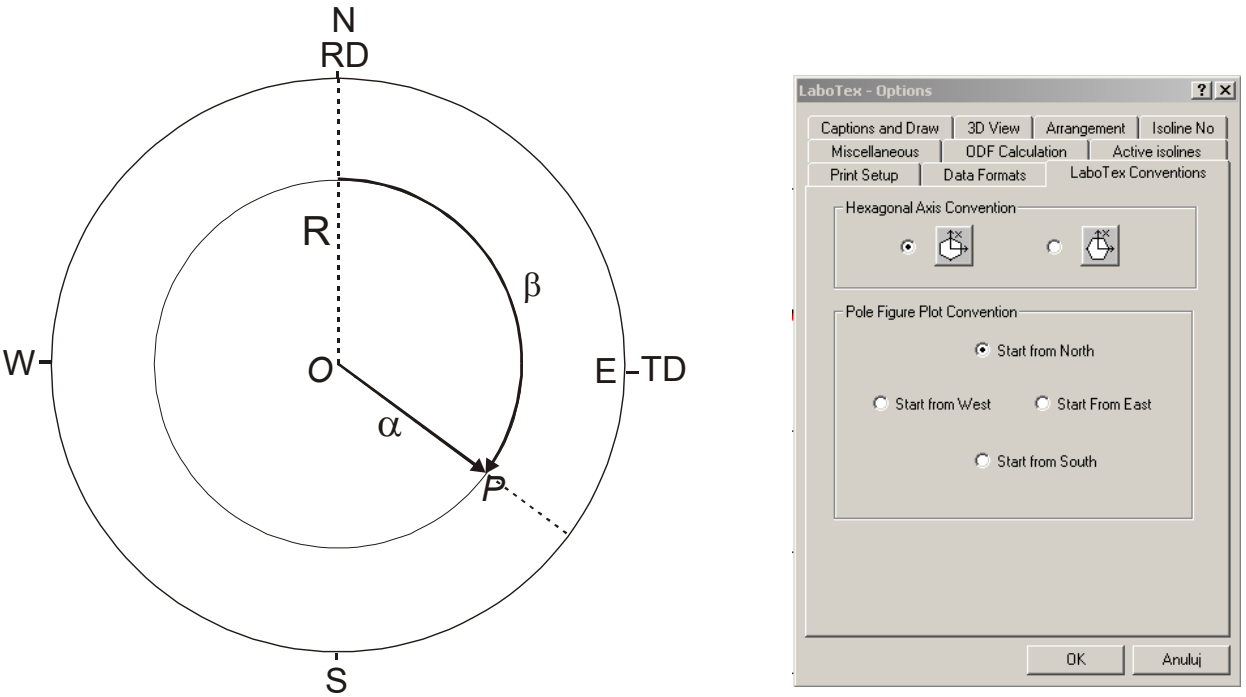


Fig. 35. Default plot convention in LaboTex: clockwise rotation, North – the start point of the pole figure plot

You can change the default for the plot convention (Fig. 35) in the menu "**Edit**"→"**LaboTex Options**"→ "**LaboTex Conventions**". For example, if you would like to set the RD in the East position, as on the plot in Figure 36, then you should first change the option in "**LaboTex Options**" to "**Start from East**" (Figure 36 - left side).

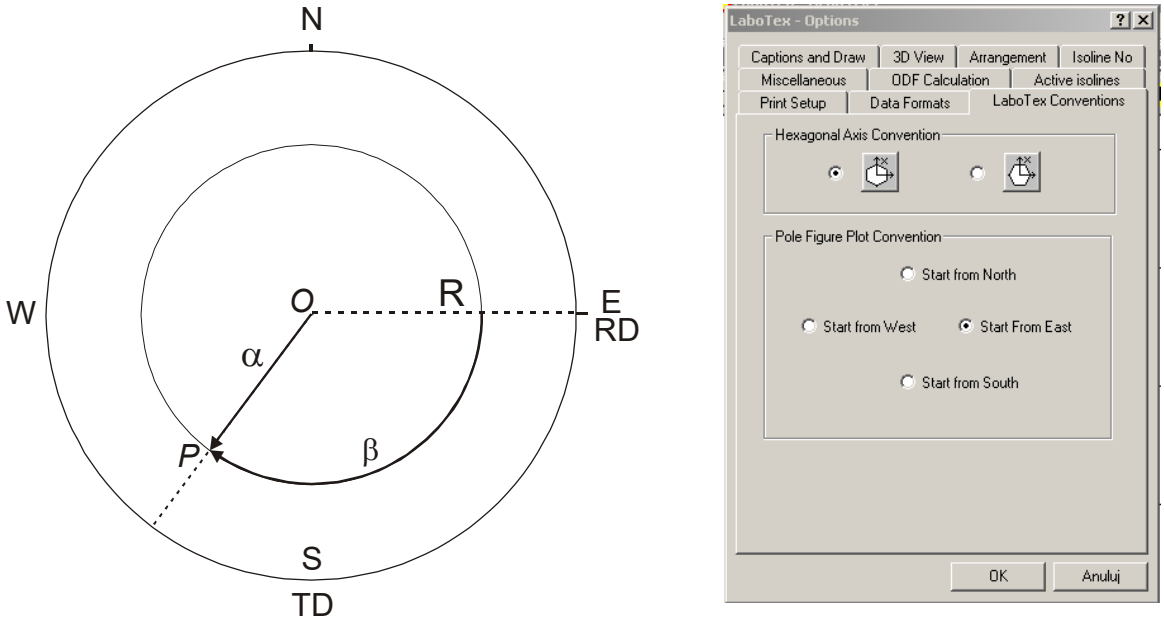


Fig. 36. Pole figure plot convention: clockwise rotation, East –the start point of the pole figure plot.

If the pole figure was registered from the RD direction (default LaboTex registration convention) then you should change the default axis description, as it is shown in Figure 37. In the menu "**Edit**"→"**LaboTex Options**"→ "**Captions and Draw**" you can adjust the axis description to a new plot convention.

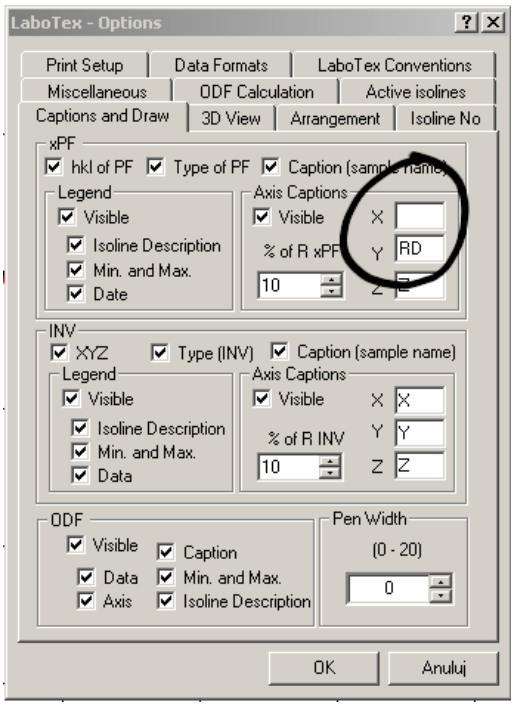


Fig. 37. Pole figure plot convention: adjustment of the axis description to a new plot convention

A) **B)**

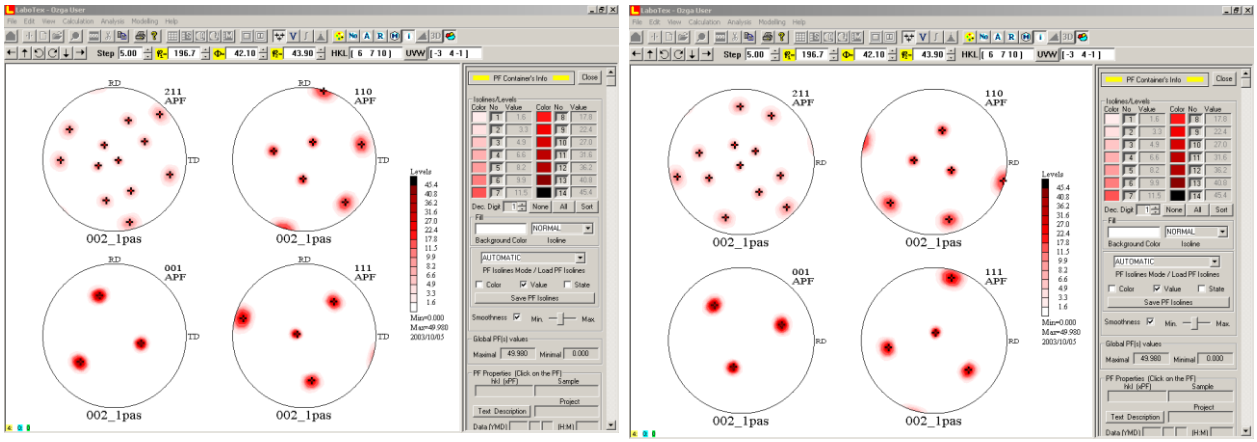


Fig. 38 Visualization of a pole figure in different plot conventions: (left) - default LaboTex plot convention; (right) - pole figure plot convention: clockwise rotation, East – the start point of the pole figure plot.

In Figure 38, you can see that LaboTex has also adjusted the visualization of orientation (the cross marks denote poles), the Euler angles and the Miller indices to a new plot convention. For the visualization of a pole figure we often use the following convention:

- a counter-clockwise rotation,
- East – the start point of the pole figure plot for a pole figure registered from the RD direction.

This plot convention is shown in Figure 39. If your pole figures are registered in accordance with LaboTex's default convention, then for an adjustment of this convention to LaboTex, you should set the start point of the pole figure plot to East (as in Figure 39) and next, you should also change the option to "counter-clockwise" while inputting the pole figure(s) (as in Figure 32).

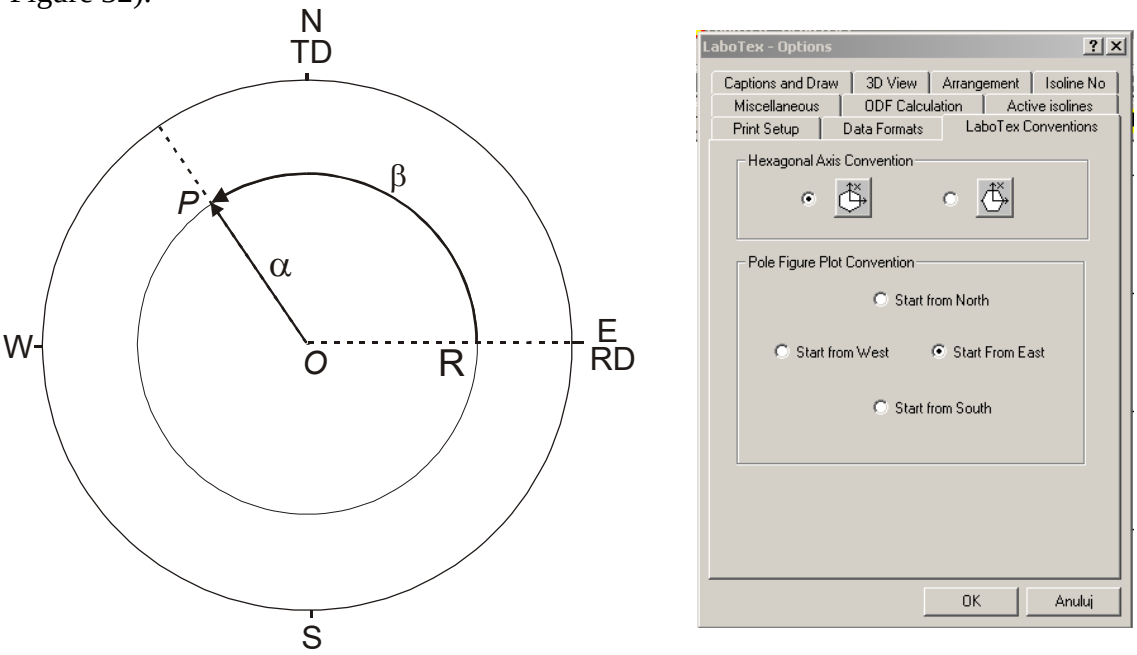


Fig. 39. Pole figure plot convention: counter-clockwise rotation, East – the start point of the pole figure plot.

Warning: The change of the plot convention is global. All your pole figures will plot in the new convention.

8. Pole Figure - Registration Convention - Permanent Settings

In LaboTex, there is also a possibility of an adjustment of the registration convention to the current data format. This adjustment can be made in the menu "**Edit**"→"**LaboTex Options**"→ "**LaboTex Data Formats**" (see Figure 40). These settings are permanent, but you can always change them, while inputting the pole figure data, as is shown in Figures 32 and 33.

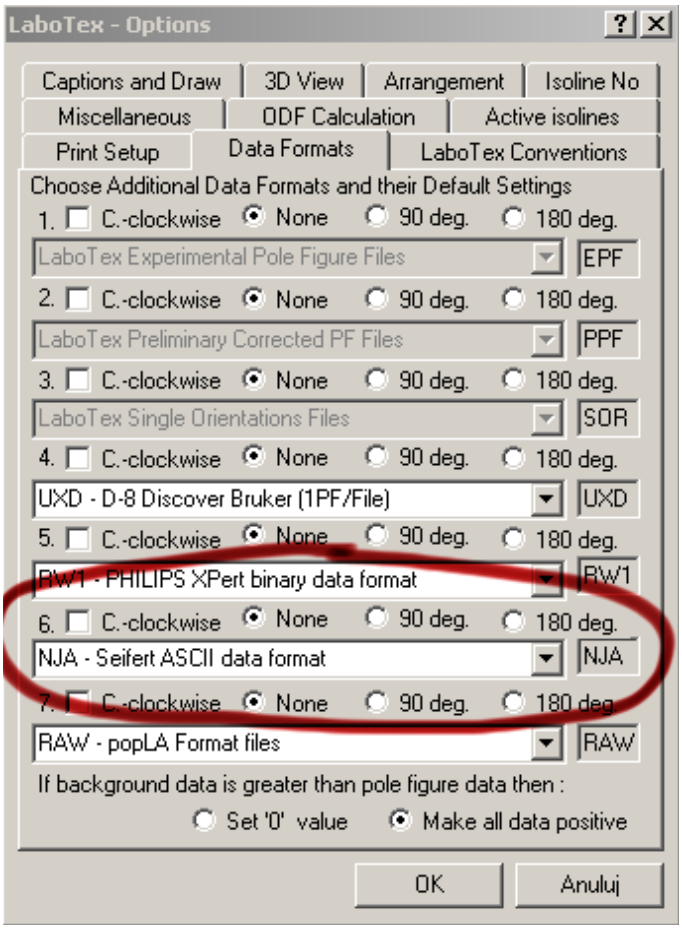


Fig. 40 Adjustment of the registration convention to the data format

9. Rotation of pole figures

Rotation of pole figures is useful in many cases. The simplest case is when we want to rotate the pole figures around the ND direction. We can find this case when we inaccurately install a sample in the goniometer, as in Figure 40a.

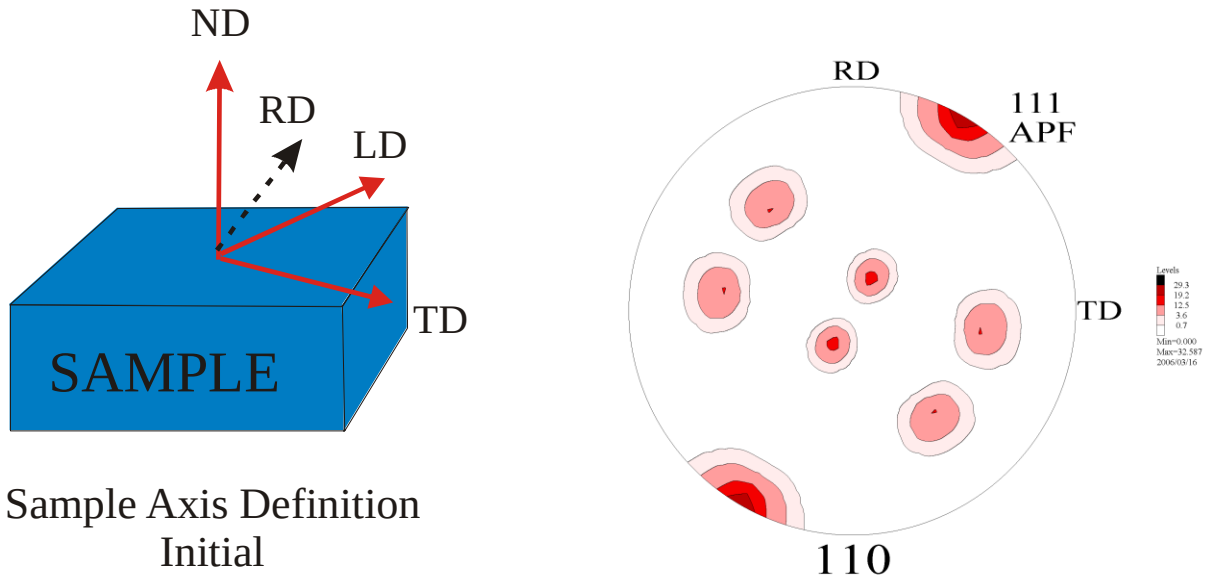
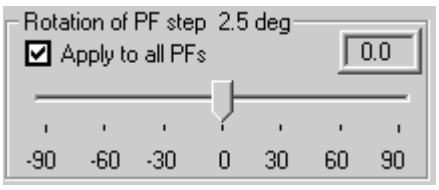


Fig. 40a. Pole figure for inaccurately install a sample in the goniometer.

It is due to the difficulty in the positioning of the sample in the goniometer. We can make a pole figure rotation around the ND direction using the slider, as in the image below, which is available for the user before the ODF calculation:



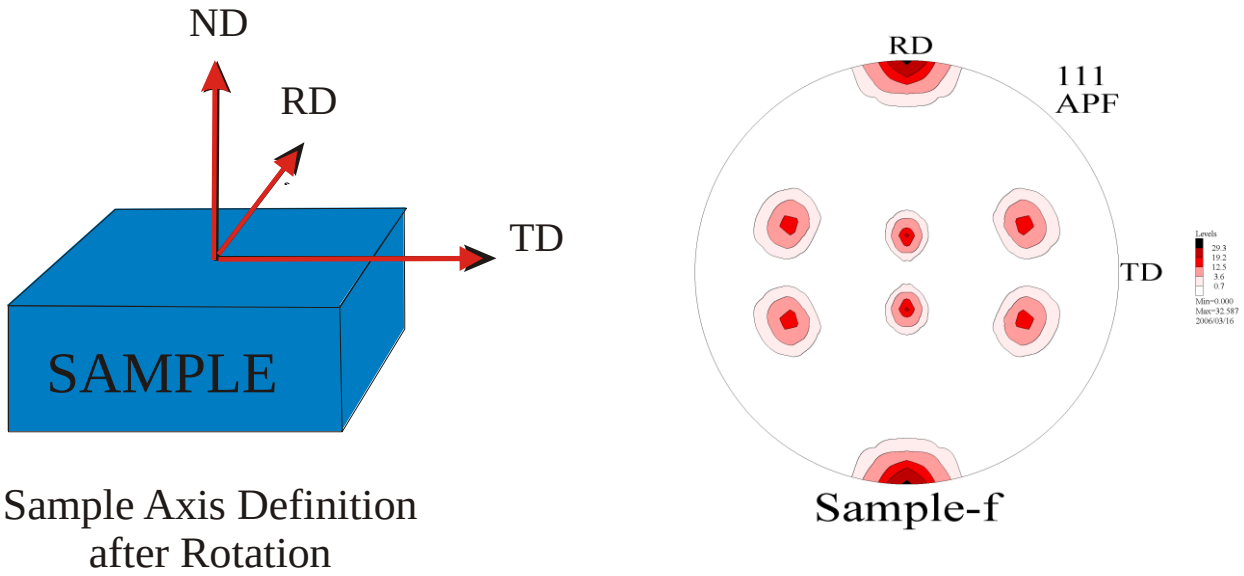


Fig. 40b. Pole figure for inaccurately install a sample in the goniometer – after software correction.

You can make more complex pole figures rotations using ODF transformations. LaboTex can calculate a new ODF, which is the result transformation of the initial ODF. The new ODF is created in a new "*job*" for the same "*sample*" as the initial ODF. Next, you can make a calculation of the new pole figures (the pole figures after rotations) using the APF calculation. There are two kinds of transformations:

- Sample Frame Rotation;
- Crystallites/Planes Rotations.

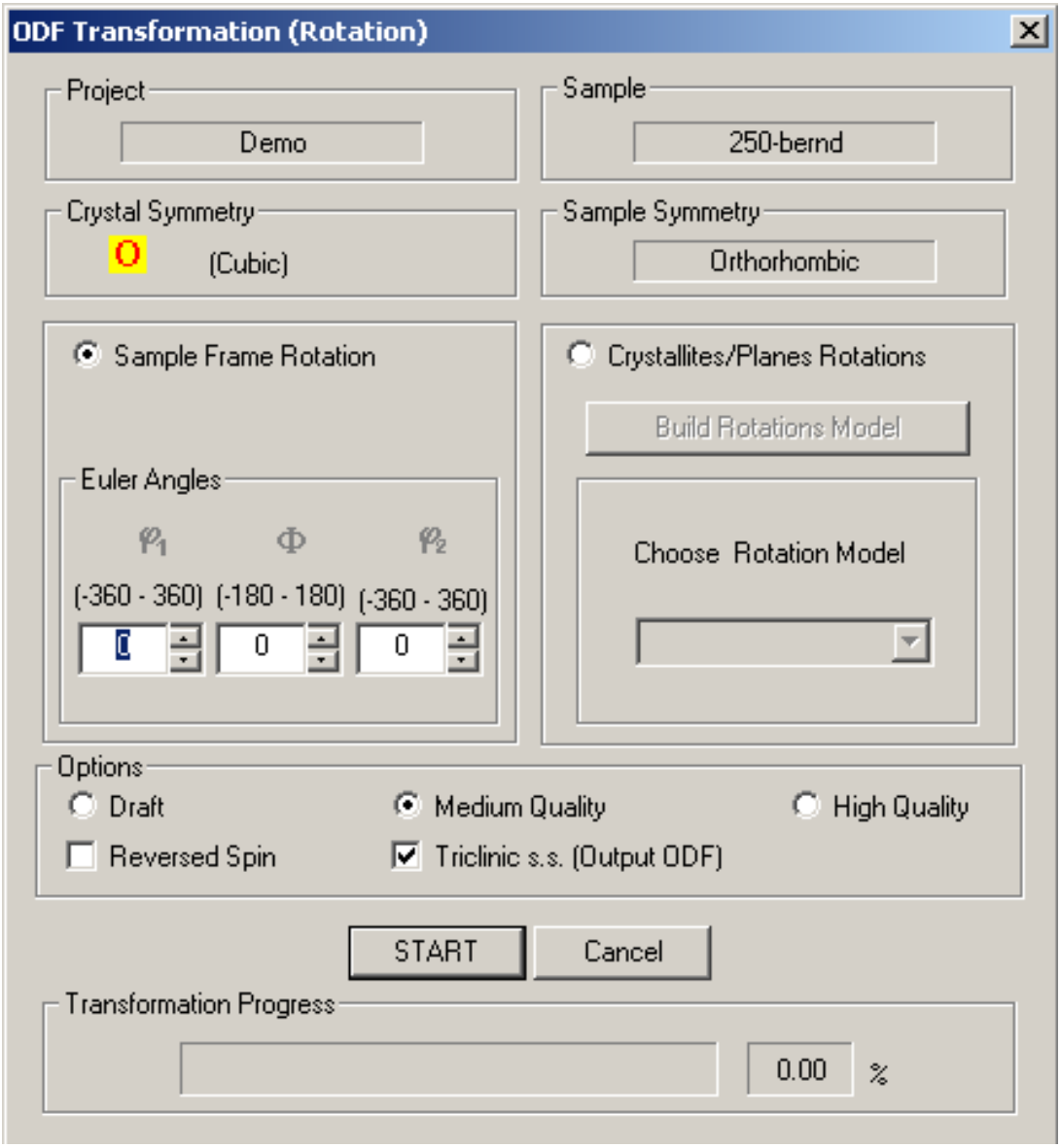


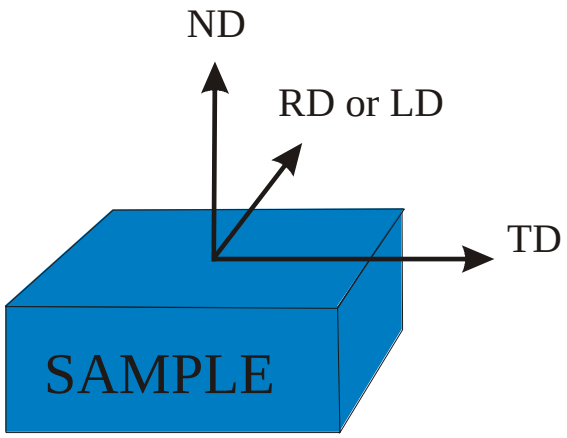
Fig. 41.

9.1. Sample Frame Rotations

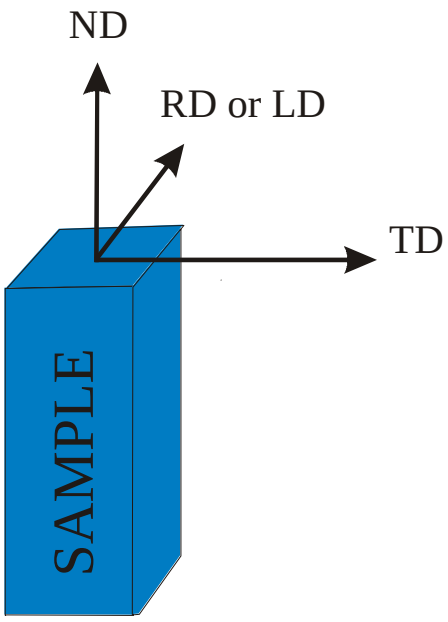
By using the dialog “Sample Frame Rotations”, the user can rotate the sample frame. This option is very important if the user would like to see the pole figures for another (different) sample position. The user can also change the sample symmetry for the transformed ODF.

Example 1:

You want to see the pole figures for the perpendicular surface in relation to the surface which was measured:



Sample Axis Definition
Initial



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

Figure 42.

Fig 43. ODF for the initial axis definition. Sample: Ferrite – triclinic sample symmetry

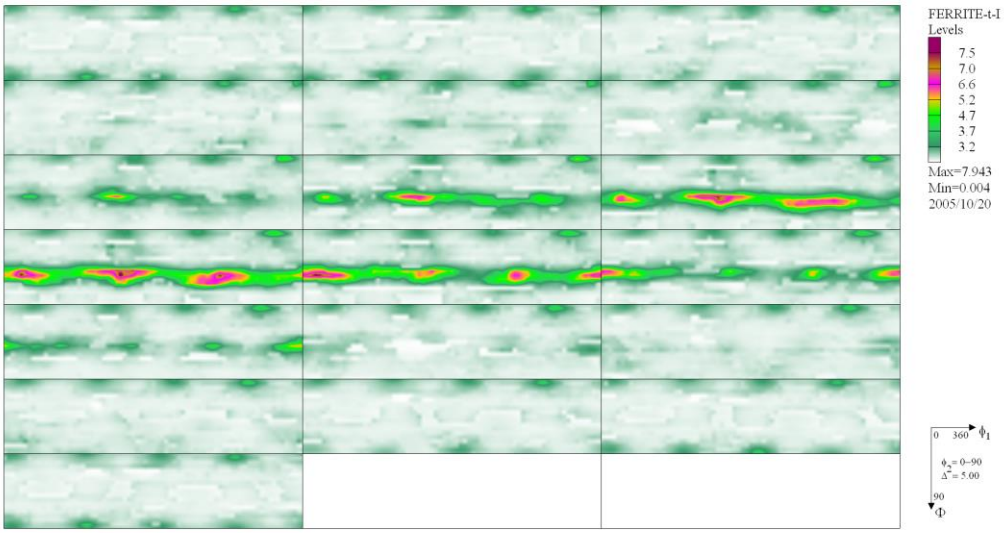


Fig. 44. ODF after frame rotation : (0,90,0). Sample: Ferrite – triclinic sample symmetry

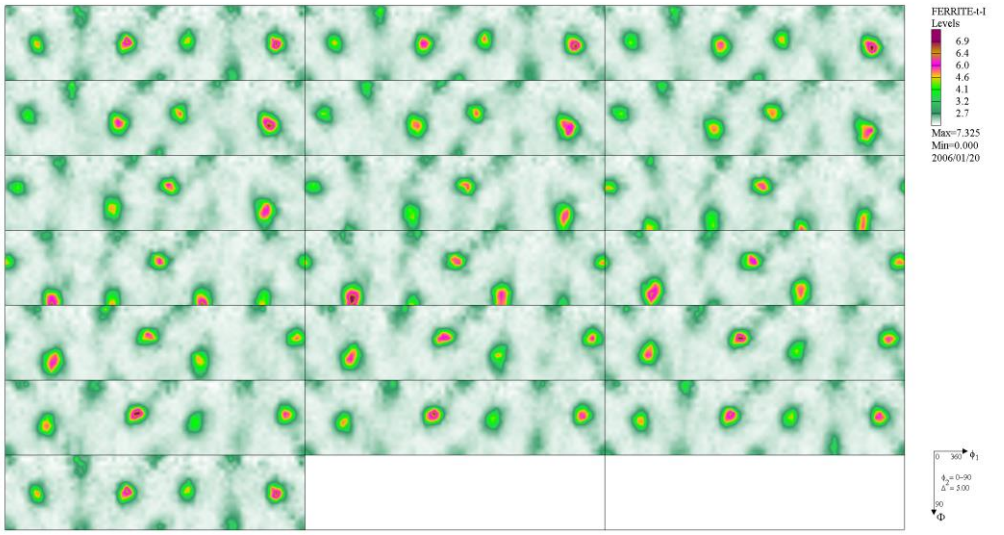
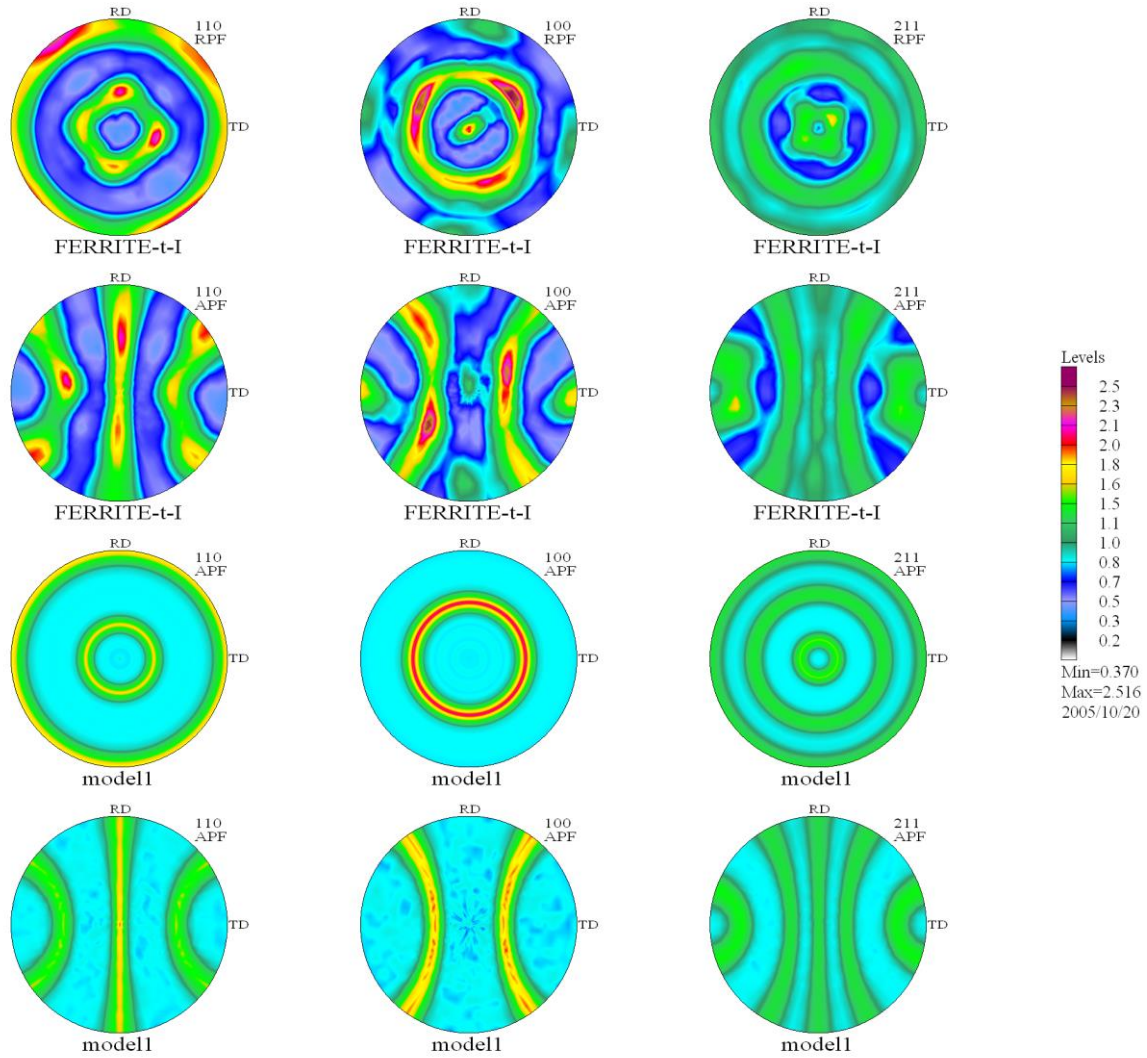


Figure 45.

Pole figures:

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



Example 2

:

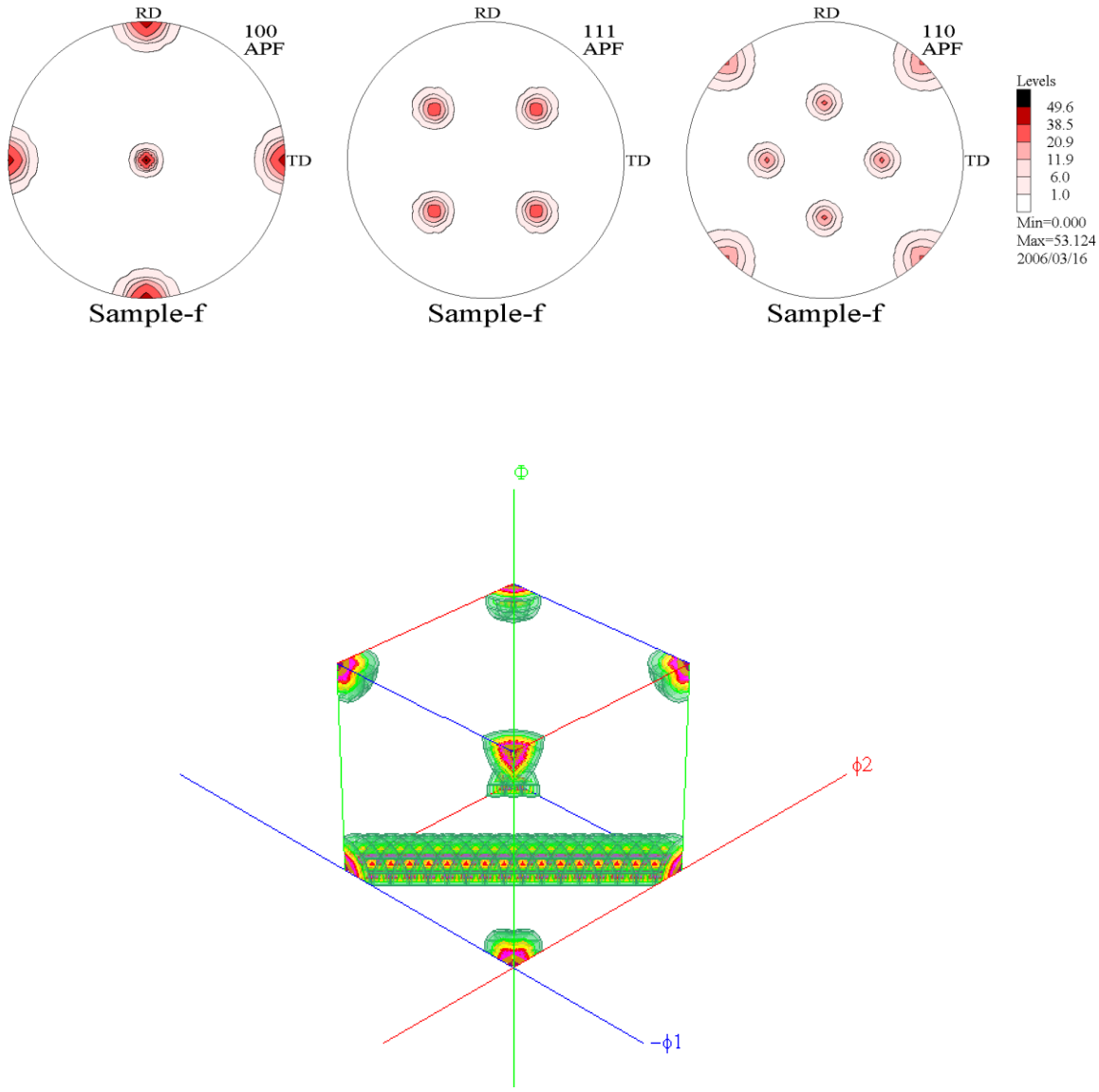


Fig. 46. Initial Pole Figures and ODF – Cubic component.

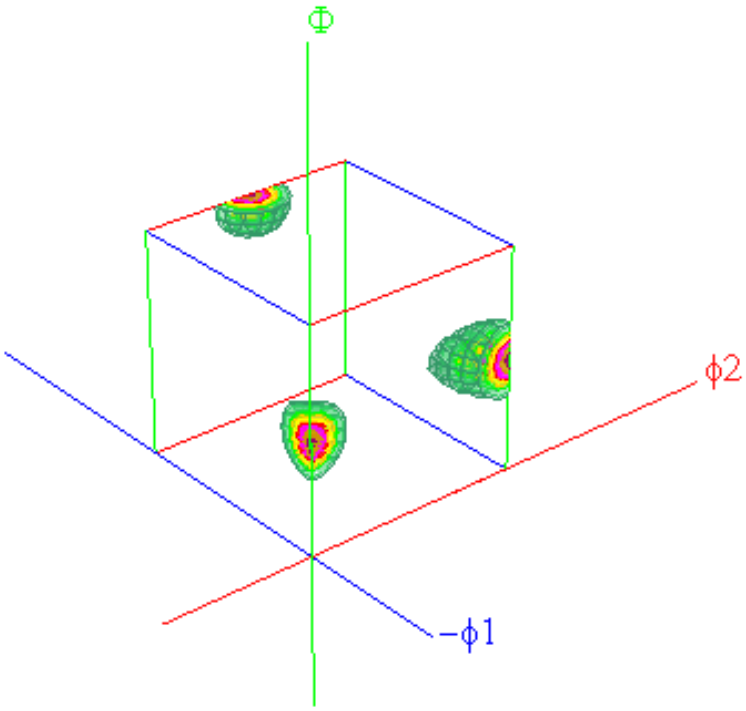


Fig. 47. ODF and pole figures after the transformation of the frame (45 degrees, Phi axis) - pole figures and ODF with Goss Component.

9.2. Crystalites /Planes rotations.

If you would like to make a rotation of some crystallites in the sample and observe the change of the pole figures and the ODF, then you should make this transformation in three steps:

1) A preparation and creation of a model for the crystallites rotations.
2) A transformation of the current ODF using the model for the crystallites rotations.
3) A calculation of the pole figures from the new (transformated) ODF using the option **"APF Calculation".**

For the preparation of the model for the crystallites rotations you should:

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

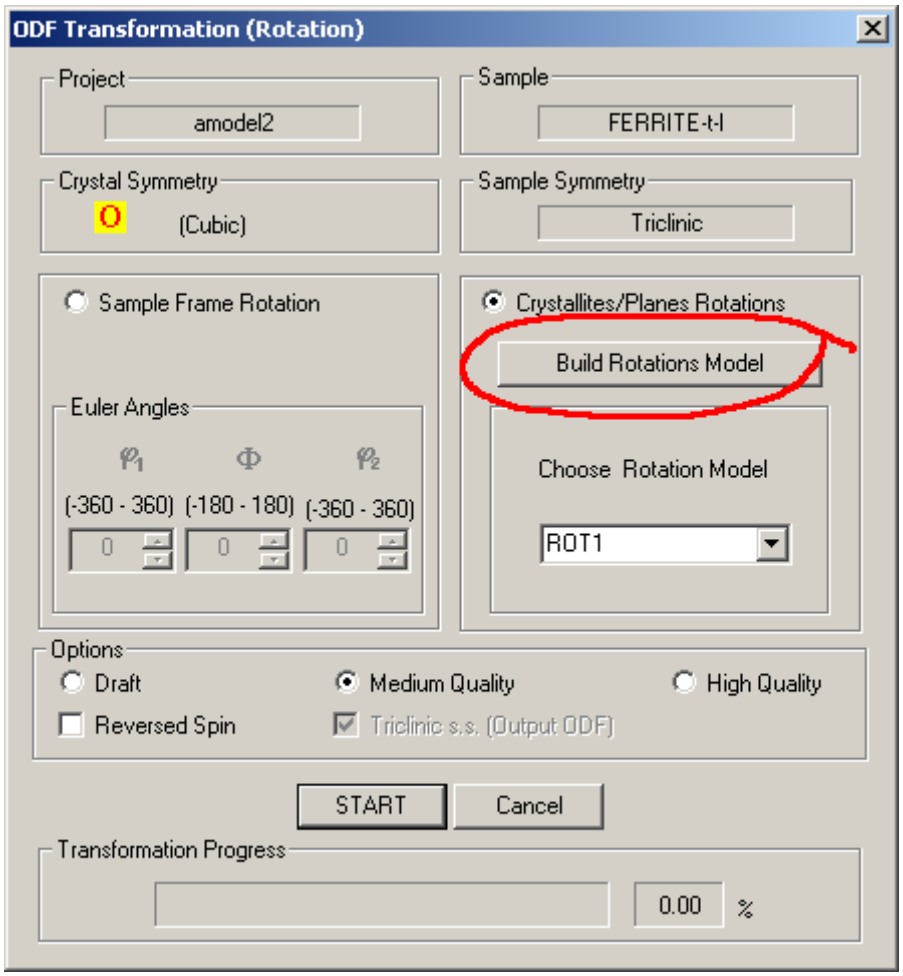


Fig. 48. Crystalites /Planes rotations – dialog window.

In the rotation model, you can select from up to 10 texture components, for which you set:

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

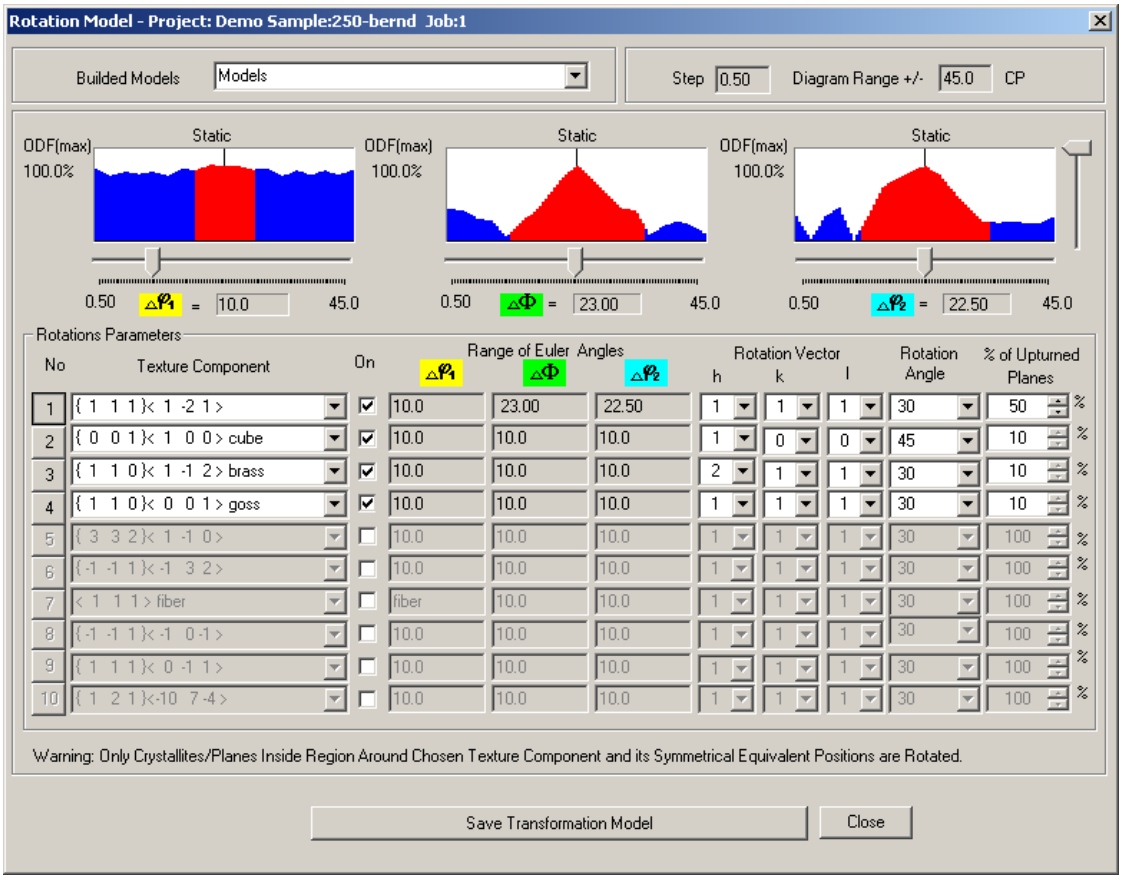


Fig. 49. Rotations model – dialog window.

When you select all the parameters of your rotation models, then click on the button **"Save Transformation Model".** You can define any name for your model.

In the second step, you should select the rotation model from the **"Choose Rotation Model"** combo box.

Next, you can select the quality of the calculated ODF:

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

You can also change the spin of the rotations.

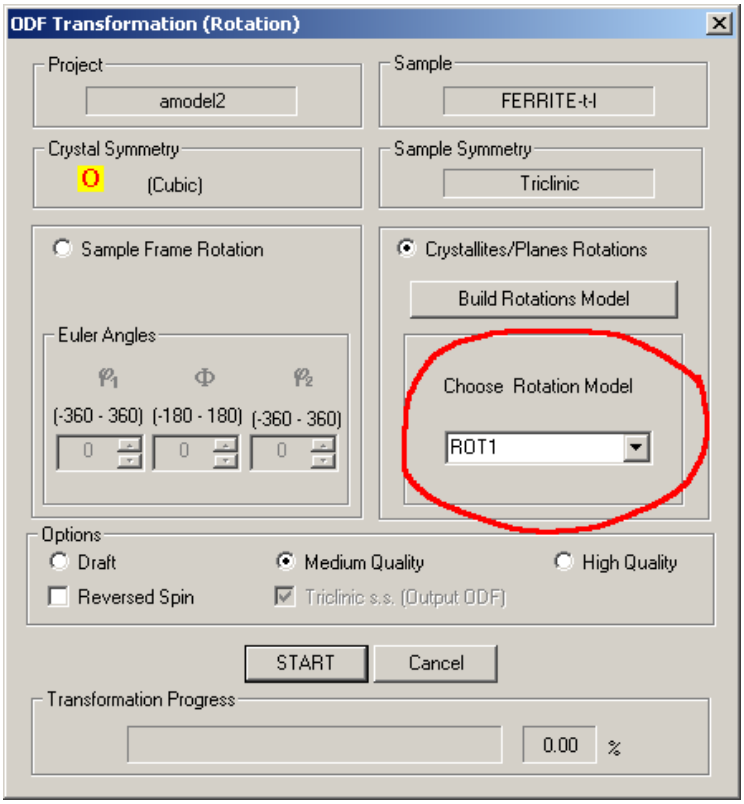


Fig. 50. The choice of rotations model

In the last step, you start the transformation calculation by clicking on the **"START"** button.

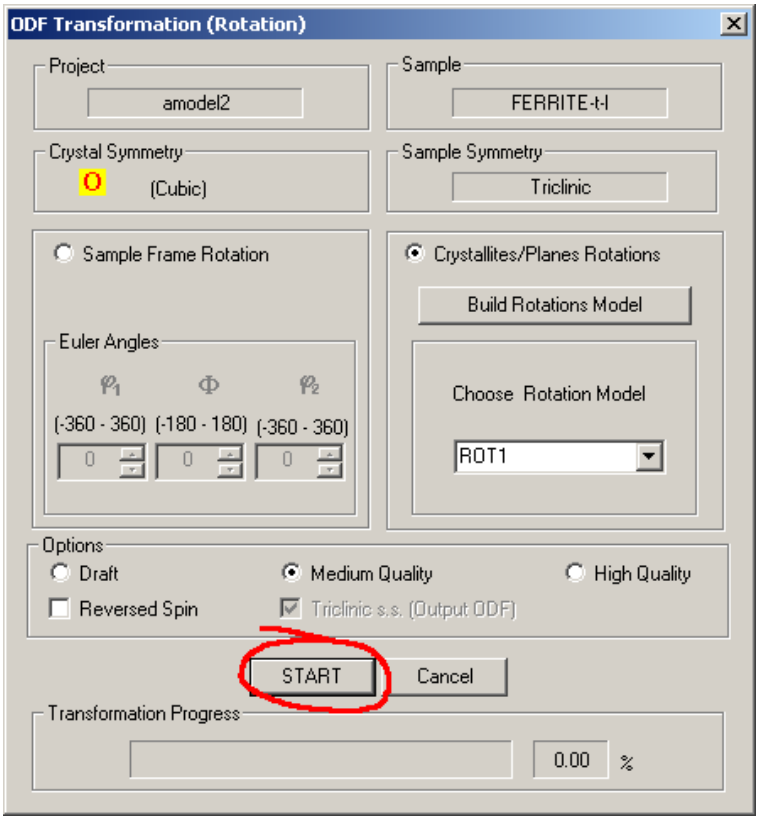


Fig. 51. The ODF transformation calculation – start calculation

Example:

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

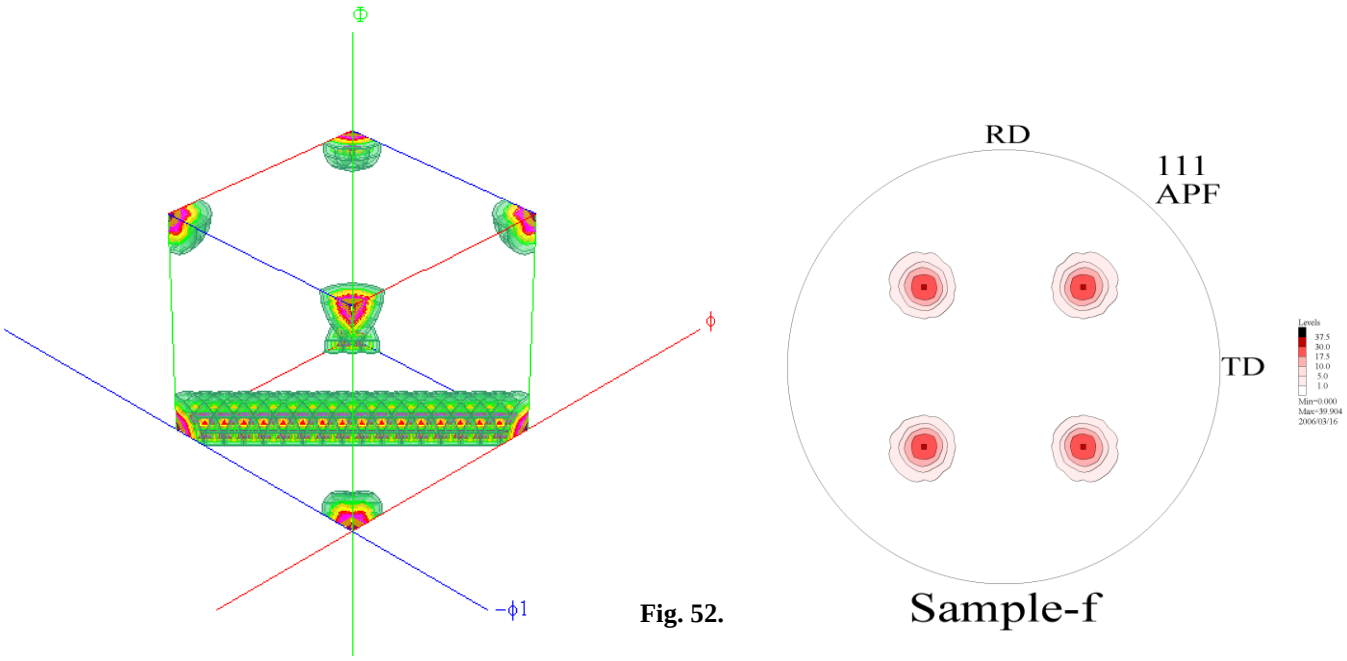


Fig. 52.

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

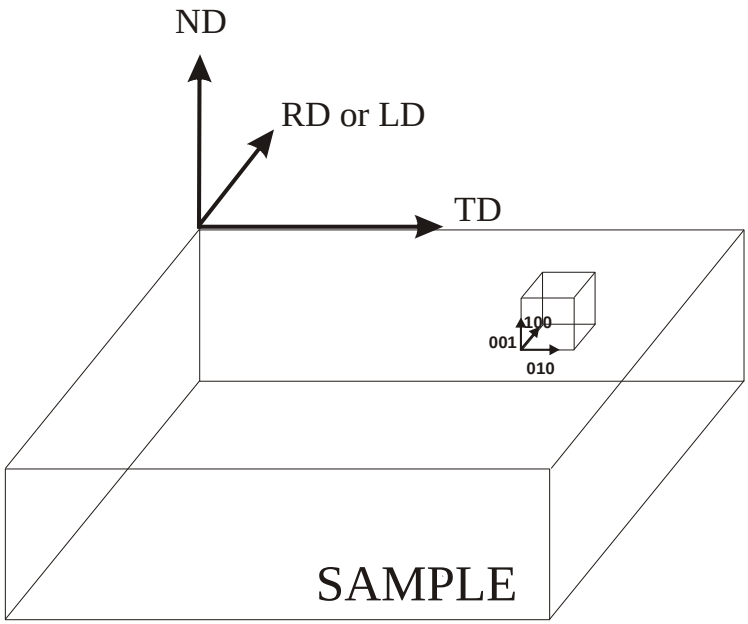


Fig. 53.

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

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

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

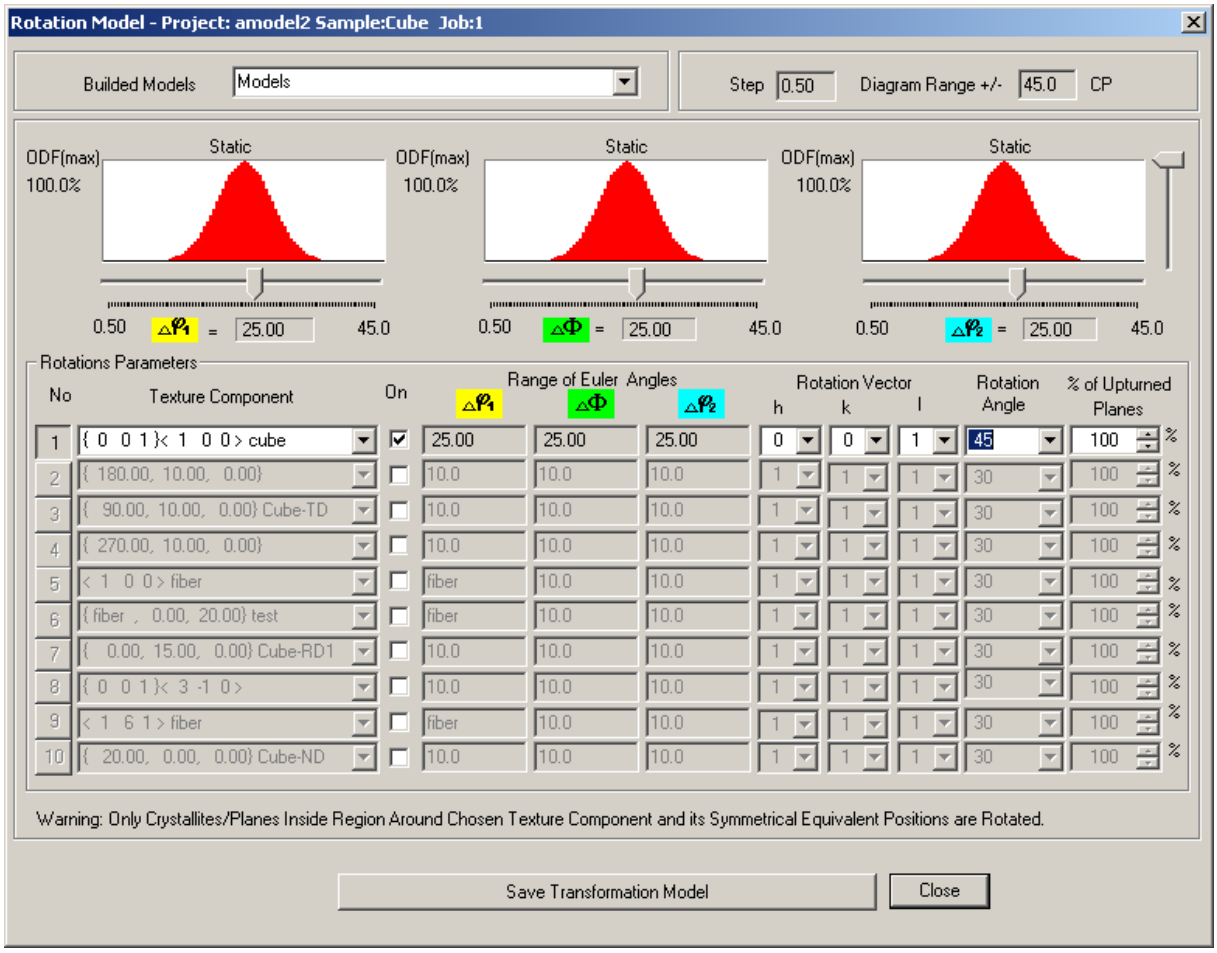


Fig. 54. Rotations model – dialog window.

We can thus show the same crystallite after the model rotation <001>45°:

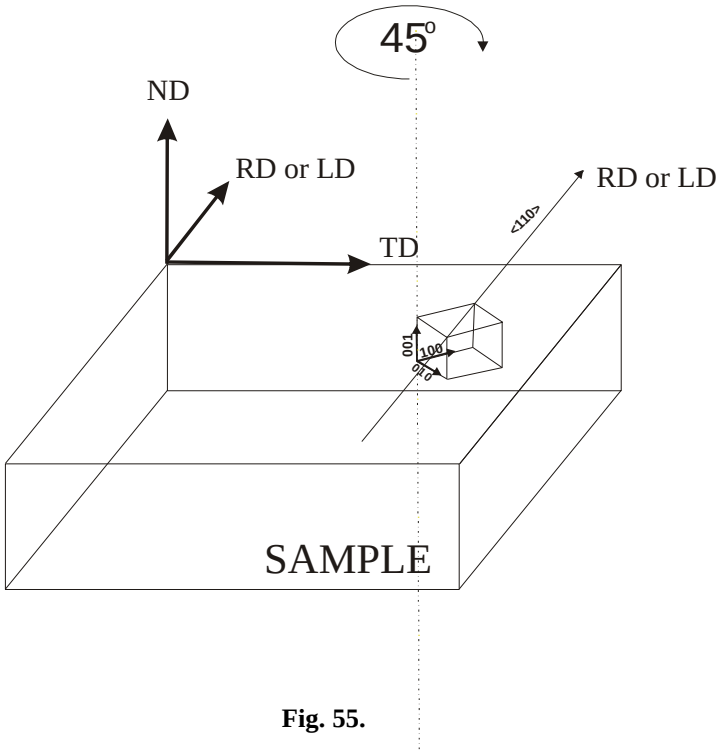


Fig. 55.

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

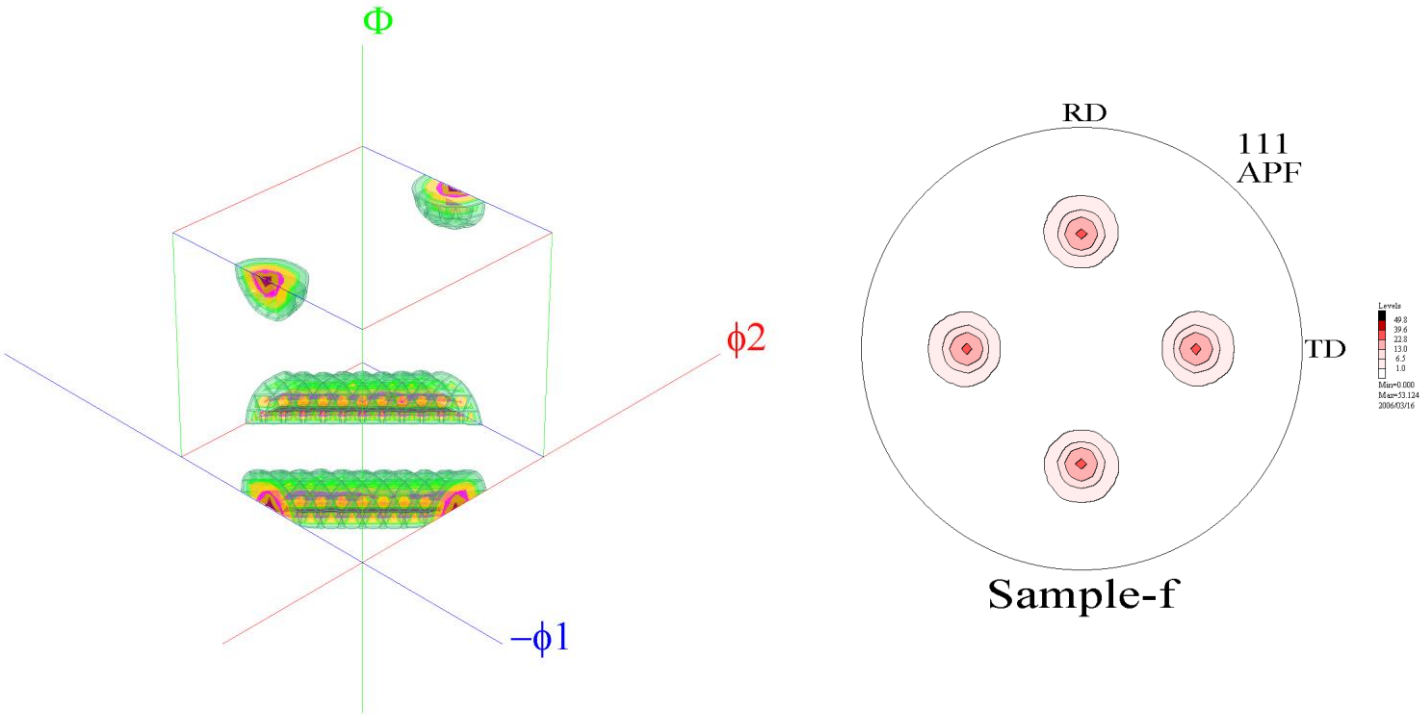


Fig. 56. ODF and pole figure {111} after a model transformation: <001>45^0. The main component in the transformed ODF is {001}<110>

In this example, we can show the same crystallite as in Figure 53 after the model rotation <111>30°:

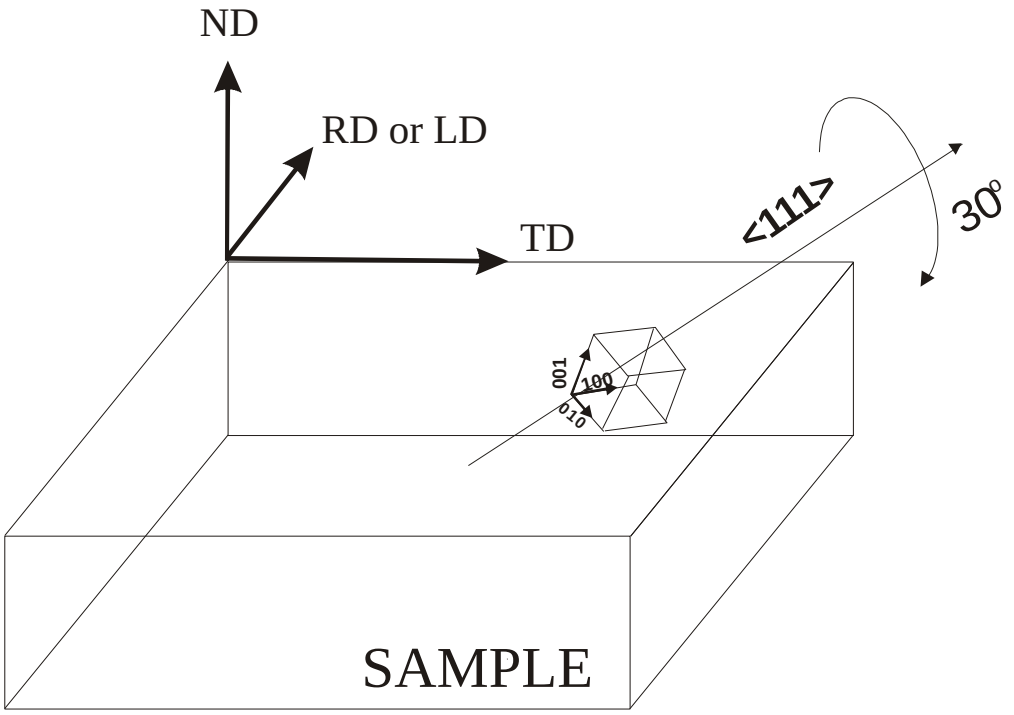


Fig. 57.

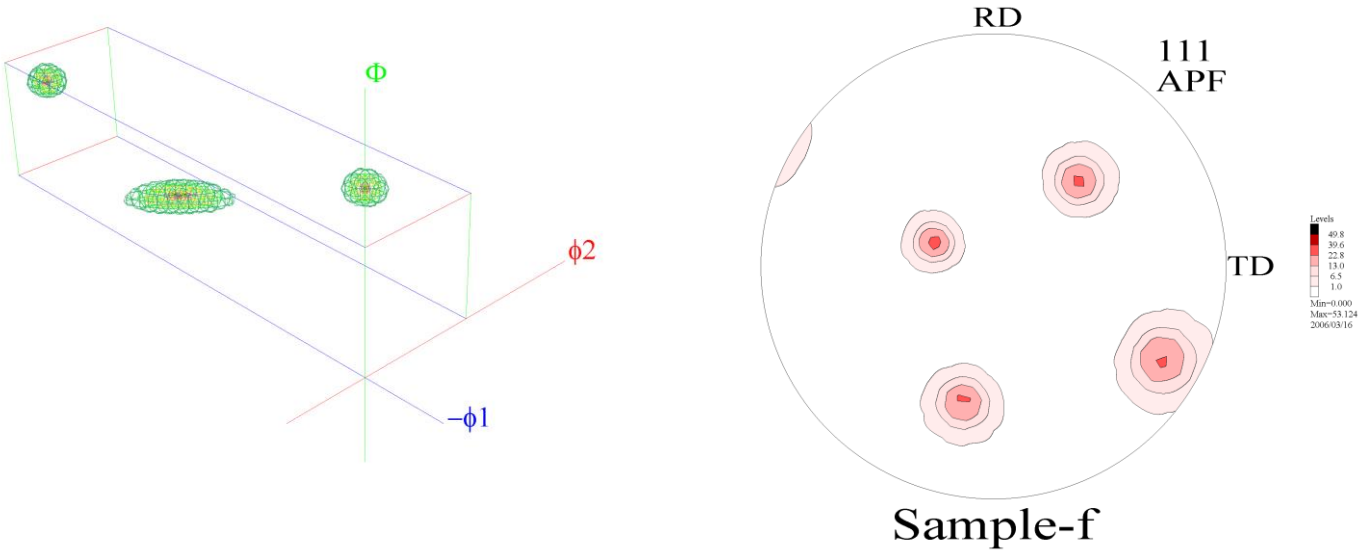


Fig. 58. ODF (not symmetrical) and pole figure {111} after the model transformation: <111>30^0

Example transformation: <111>45° for a lower symmetry than the cubic symmetry.

Sample:
component: cubic {100}<001>
crystal symmetry : *tetragonal*
sample symmetry: *orthorhombic*
cell angles: *90,90,90*
relative cell parameters :

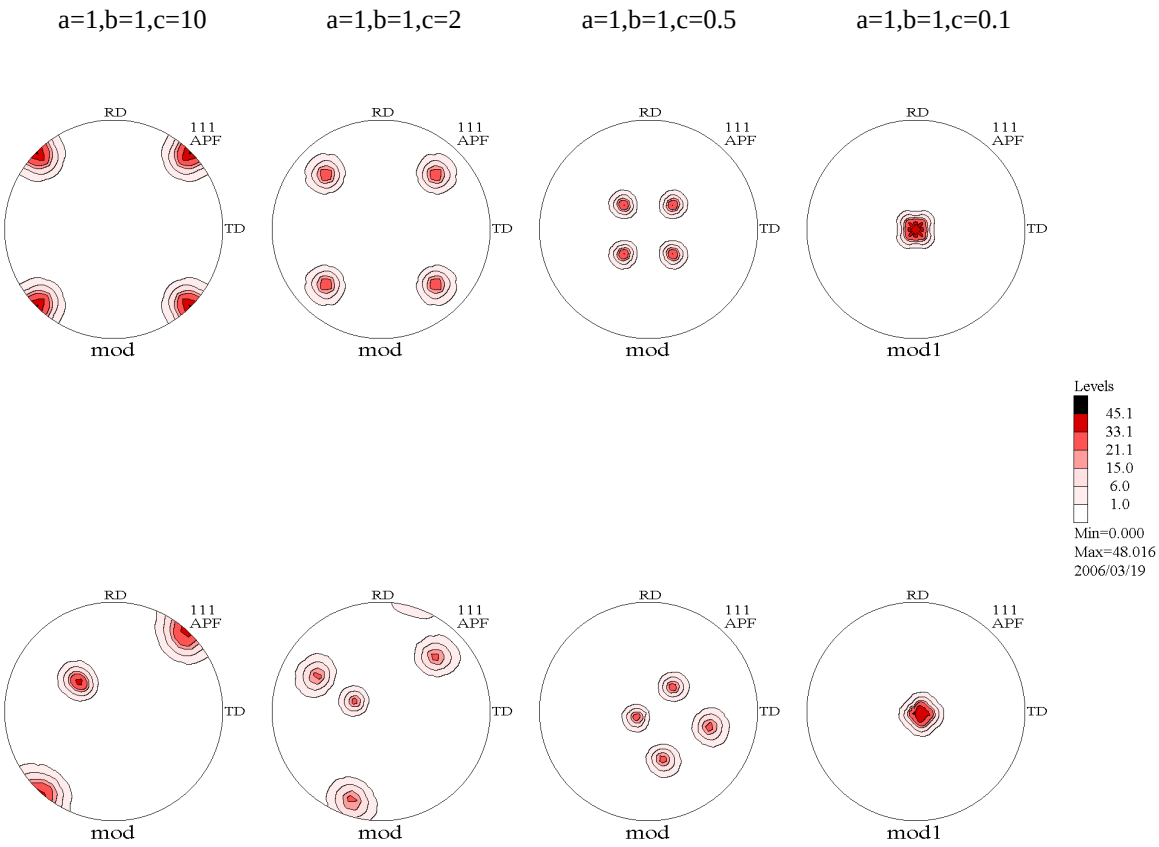
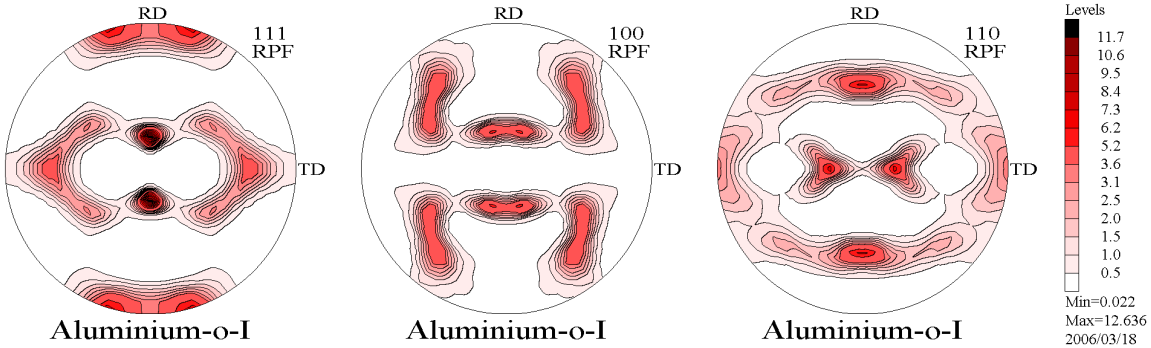


Fig. 58b. Tetragonal crystal symmetry. {001}<100> component for different c/a ratios (first row) and after a model transformation: <111>45° (second row)

-

10. Pole figures – texture component model

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



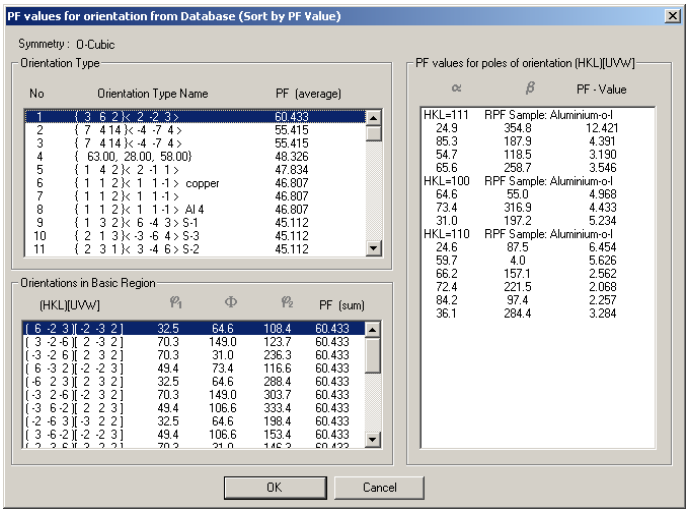
In the first step, we have to find the main texture components. For this purpose, we use the orientation analysis:

We can use both methods : automatic and manual.

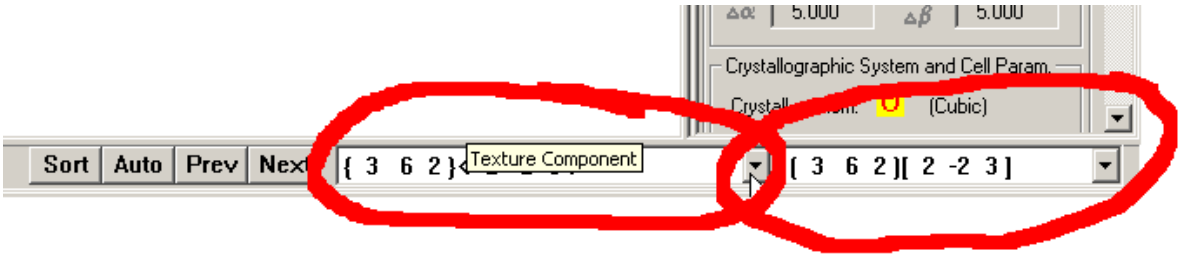
Automatic method (SORT)

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

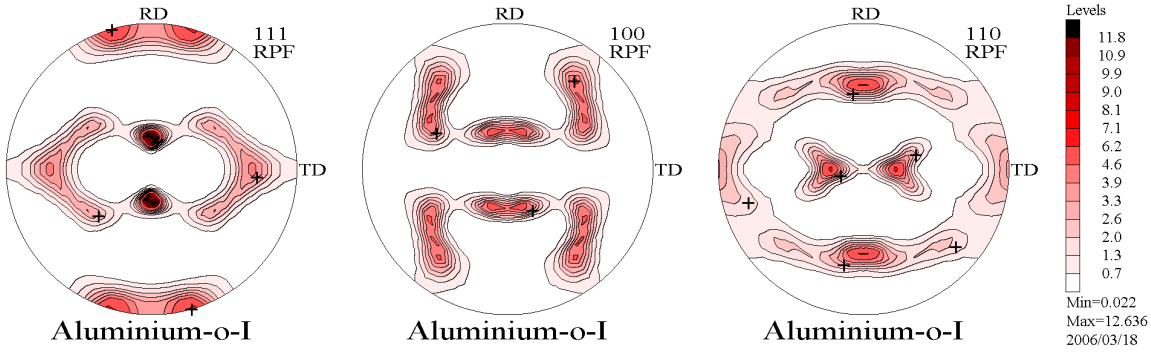
then you can see all the components from the database and their average pole figue values.



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



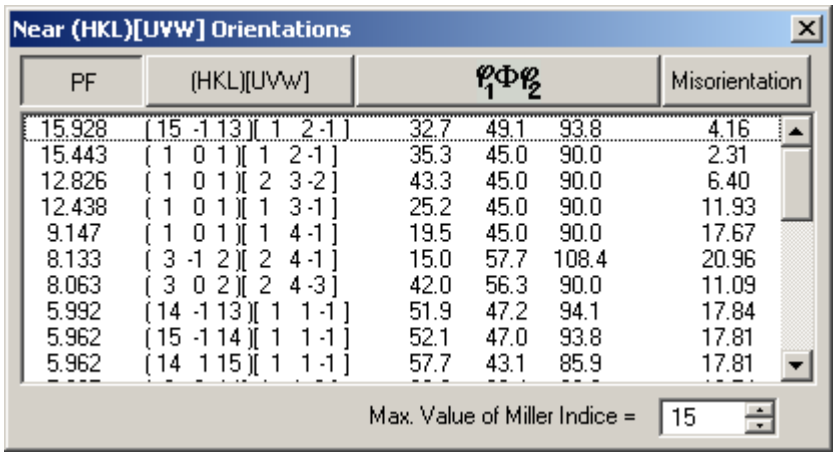
LaboTex displays a cross mark (+) in the place where the poles for a selected orientation of the active component lie ({132}<6-43> in the case below):



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

Manual method

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



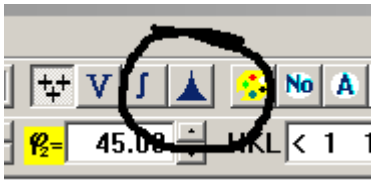
LaboTex displays the near orientations sorted by the average value of intensity of the pole figures, the miller indices or the misorientation. You can change the type of sort by clicking on the appropriate button.

First approximation

After step 1, we have found that we can describe the maximas of the analyzed pole figures using the 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 >

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



The dialog window helps you with the least-squares' fitting of the model functions into your ODF and with the creations of the model ODF nearest to the experimental ODF. In the calculation, LaboTex automatically uses the following parameters from the analyzed experimental ODF:

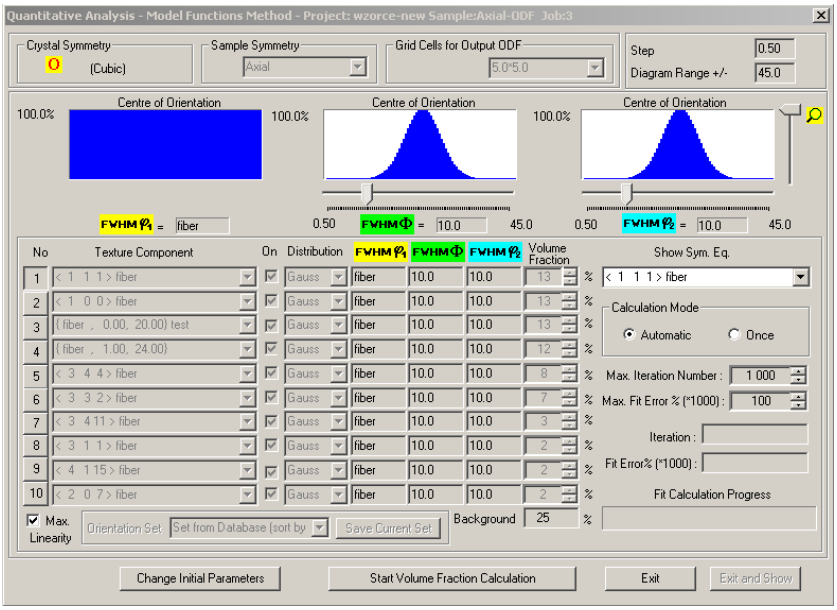
- crystal symmetry;
- sample symmetry;
- cell parameters;

- grid cell.

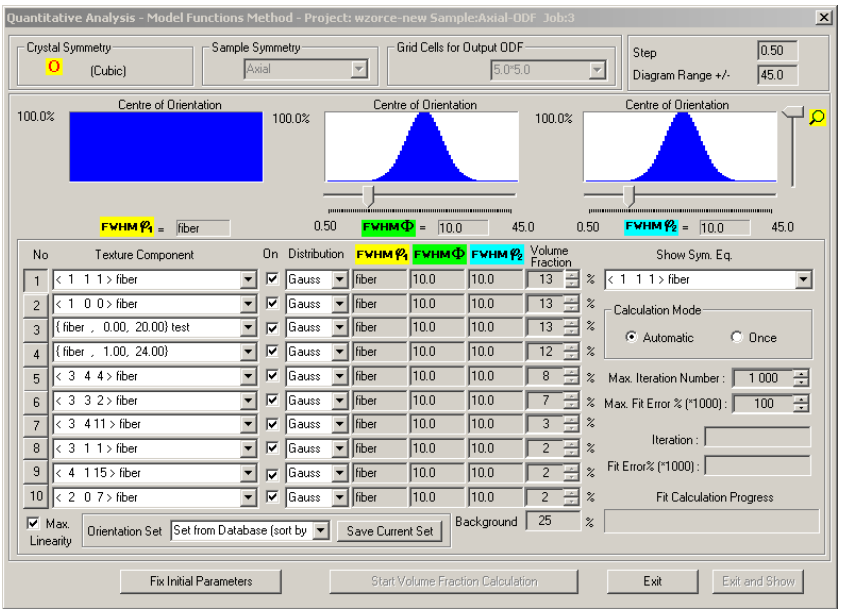
These parameters are greyed and the user can't change them.When you start the dialog window, LaboTex calculates the average ODF values for the components and sorts the components using the average ODF values. Hence the component No. 1 is the component which has the greatest average ODF value. LaboTex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

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

You can start the calculations or you can change the initial parameters.



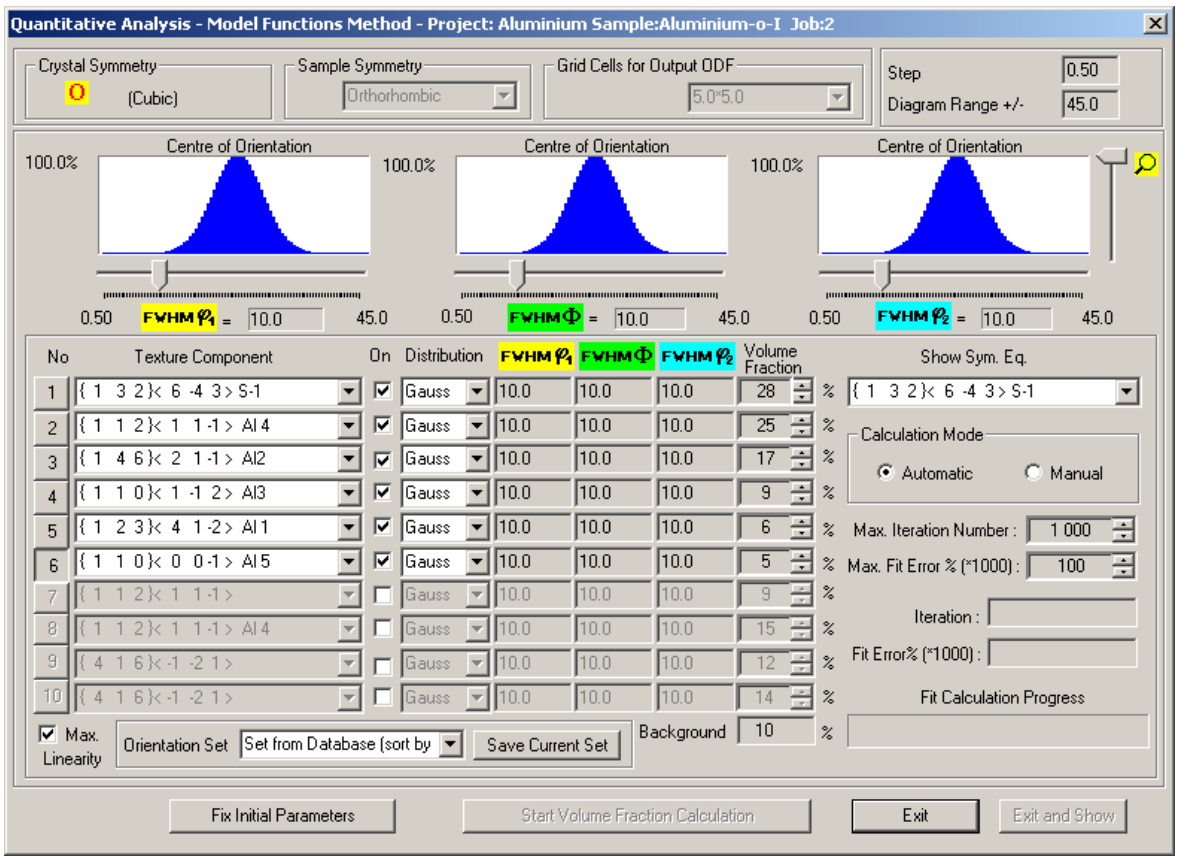
When you clic on '*Change Initial Parameters*', then new options are available.



You can:

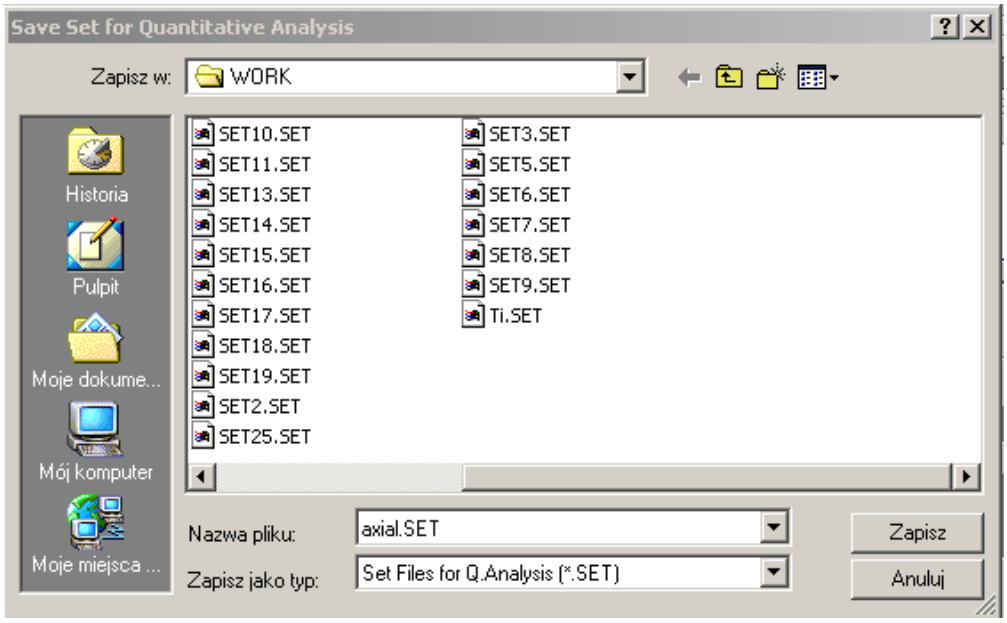
- change the texture component (using the suitable Combobox);
- turn on/off the component from the calculations (using the suitable Checkbox);
- set the kind of distribution (Gauss or Lorentz);
- set the initial FWHM for each Euler angle;
- set the initial volume fraction of the component.

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



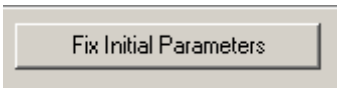
You can save the current set of components by clicking on the "*Save Current Set*" button:

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



LaboTex remembers this set and you can input it by the selection from the list of Combobox: The default set (the set proposed by LaboTex when the dialog starts) is a set built on the basis of the database sorted by the ODF value:

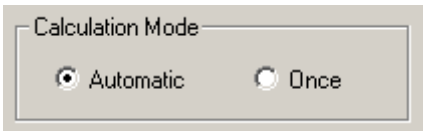
When you have finished the setting up of the initial parameters, you should click on the "*Fix Initial Parameters*" button :



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

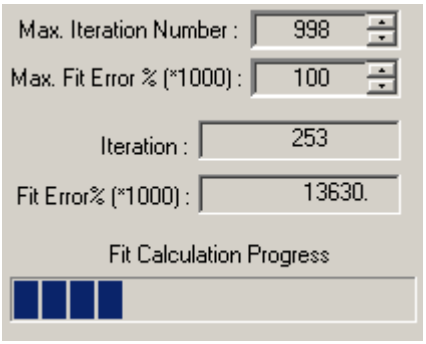
- the Maximal Number of Iteration (default is 1000);
- the Maximal Fit Error in percent (where the fit error is the relative error between the model and the experimental ODF). You should input the value of the error multiplied by 1000 into LaboTex (the default is 100 => 0.1%).

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



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

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



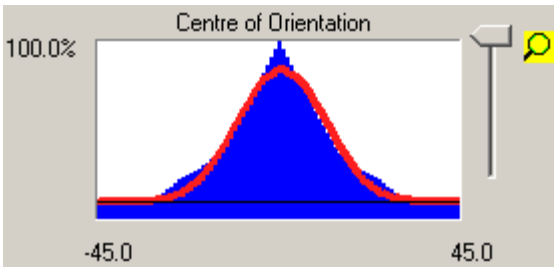
Click on the "Calculation Break" button to break the calculation at any time:

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

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

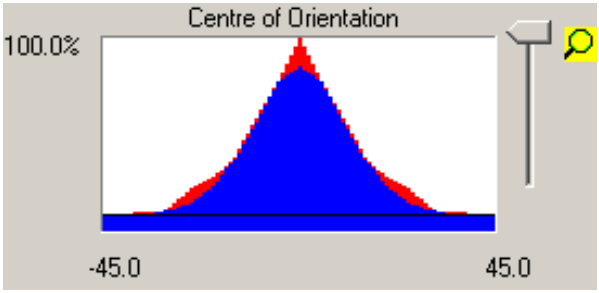
You can change the mode by clicking on the button *'Norm.'* or *'Diff.'*.
In the '*Norm.*' mode, LaboTex displays the diagrams using the following colours:

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

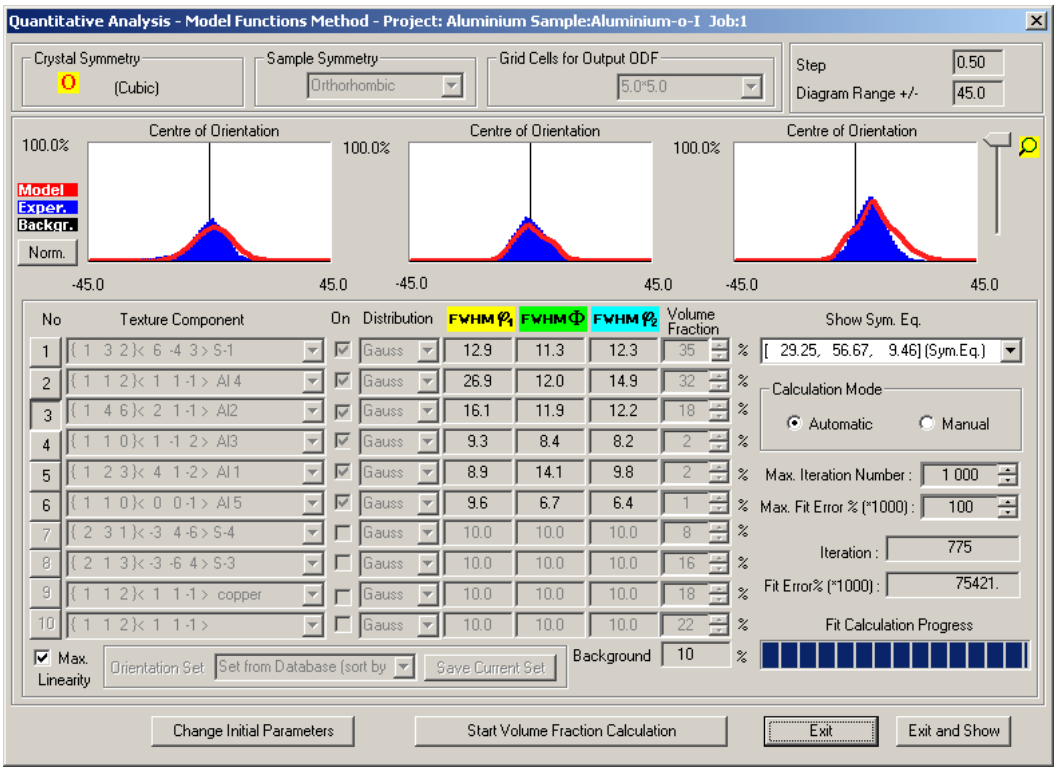


In the 'Diff.' mode, LaboTex displays the diagrams using the following colours:

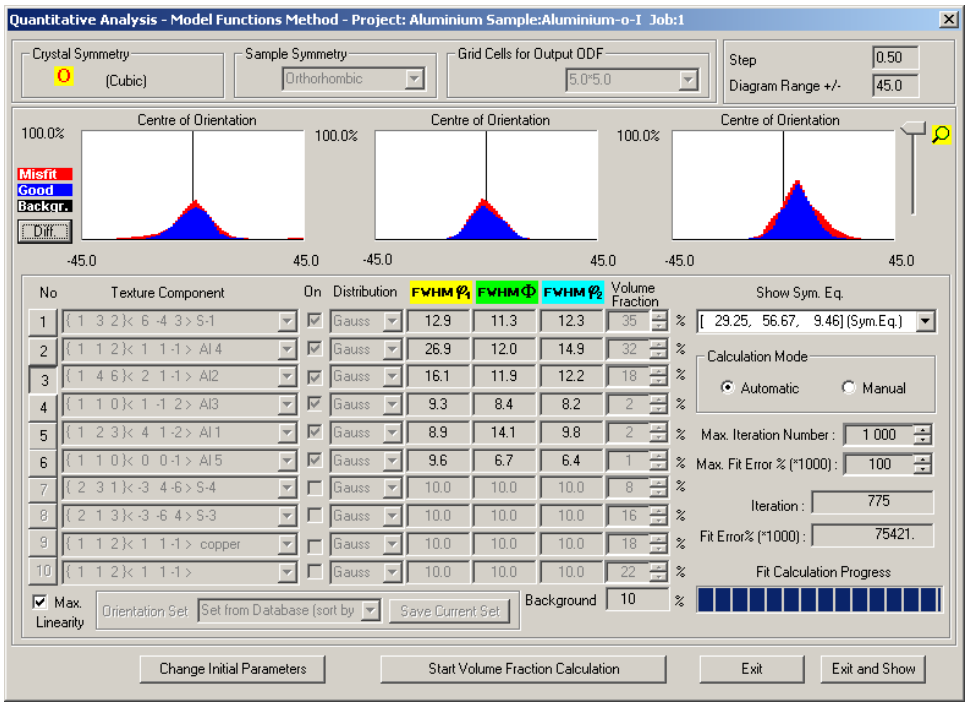
- blue (blue area) - for the common area of the experimental and the model ODF;
- red (red line) - for the non-common area of the experimental and the model ODF;
- black (black line) - for the background of the model ODF.
-



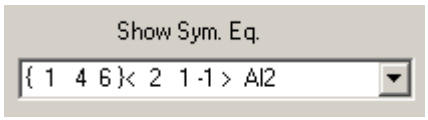
The Figure below shows the complete dialog window with the diagrams for the {1 4 6}<2 1 -1> component in the 'Norm.' mode.



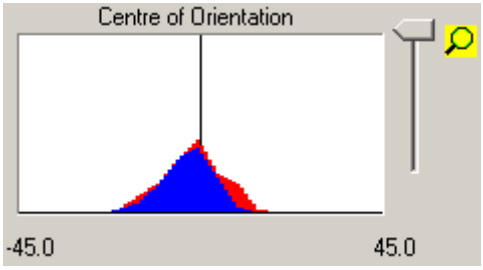
The Figure below shows the complete dialog window with the diagrams for the {1 4 6}<2 1 -1> component in the 'Diff.' mode.



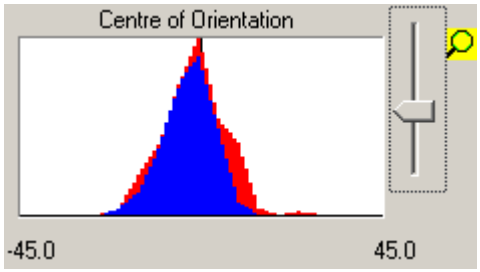
You can select any symmetrically equivalent orientation from the "*Show Sym. Eq.*" Combobox, to display the comparison diagrams:



The component {1 4 6}<2 1 -1> is weak, hence the quality of the diagrams is poor.



You can change the magnification of the component plot using the slider. The value in the left corner of the diagram shows the percent of the maximal ODF value.



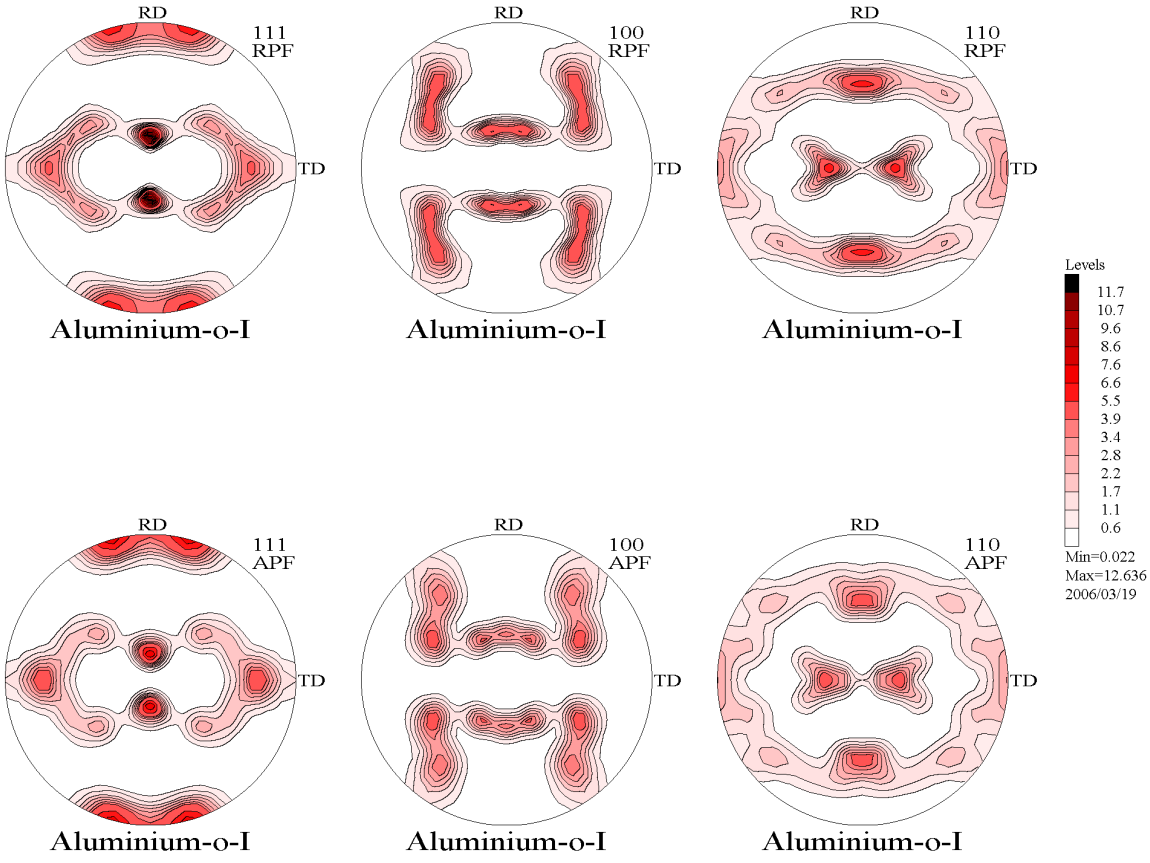
The comparison between the 'experimental' and the calculated ODF for the {1 4 6}<2 1 -1> component exhibits a greater complication of the experimental ODF. In the following approximation of the ODF, we can correct this difference.
Finally, we receive the results of the calculation:

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

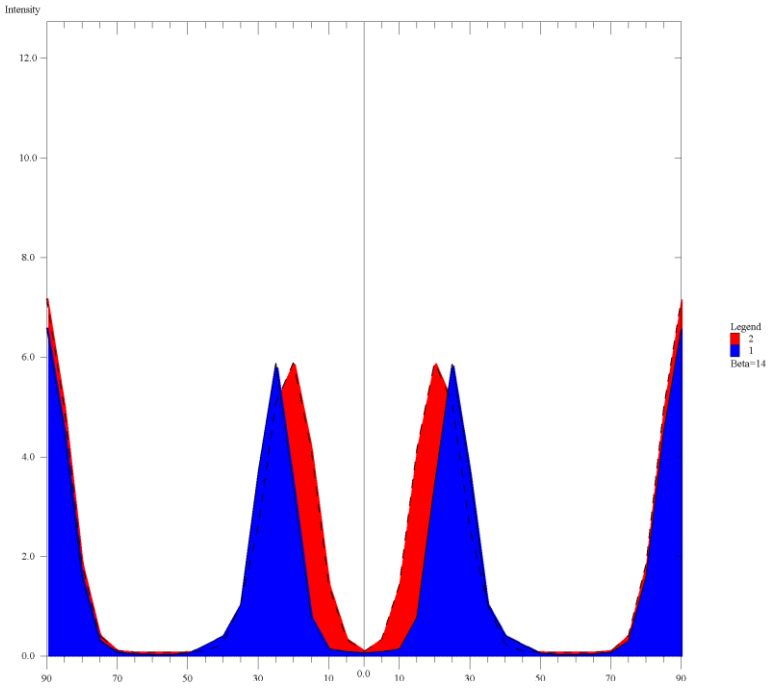
Volume Fraction	FWHM Phi1	FWHM Phi	FWHM Phi2	Orientation
Component No 1 - Distribution :Gauss				
37.4	12.6	12.0	12.5	{ 1 3 2 }< 6 -4 3 > S-1
Component No 2 - Distribution :Gauss				
34.5	29.7	11.9	15.7	{ 1 1 2 }< 1 1 -1 > Al 4
Component No 3 - Distribution :Gauss				
18.2	19.0	12.2	13.6	{ 1 4 6 }< 2 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

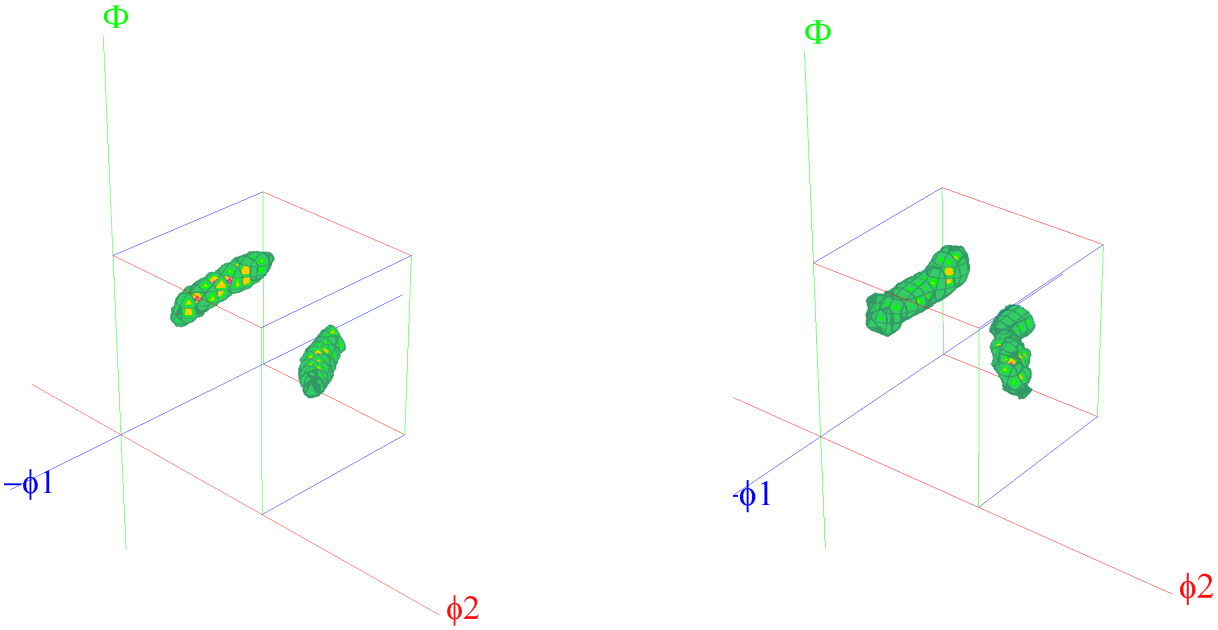
Next, we can make the pole figure calculation from the model ODF and make a comparison between the experimental (first row) and the model (second row) pole figures.



We can also make a comparison between the sections of the pole figures as in the example below, for the (111) pole:



.
"Experimental" (left) and model ODF (right):

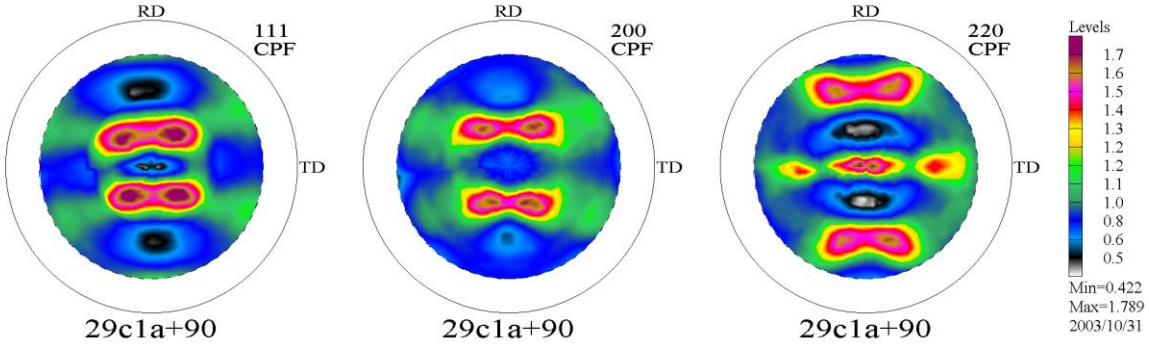


You can add new components (or replace one component by two components) and build a more complicated model, on the basis of the differences between the calculated and the 'experimental' pole figures or the ODFs from the previous step.

11. Pole figure conventions and errors in determining the orientation

Selecting the plot convention of the pole figures does not change the calculated ODF, while the selection of the registration convention can lead to changes in the ODF and errors in determining the orientation. The images below show two sets of pole figures which are rotated about 90 degrees between themselves, analogically to the case with the wrong choice of the registration convention (the start from '**RD**', instead of the start from '**TD**')

A)



B)

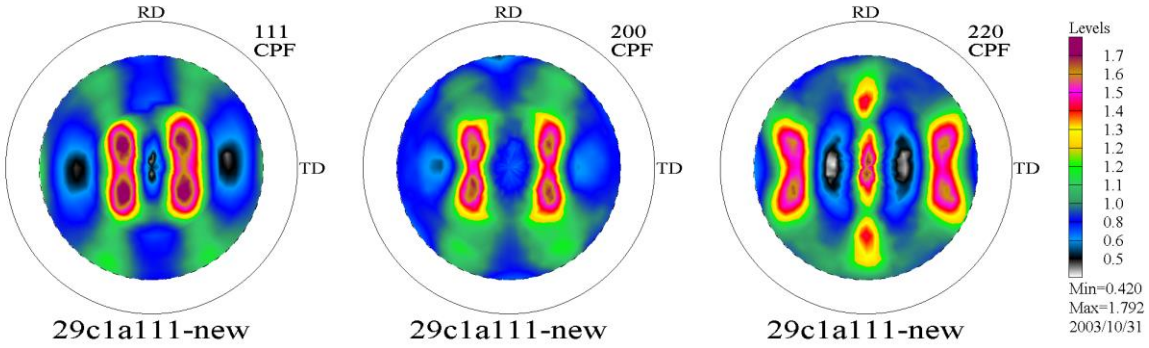
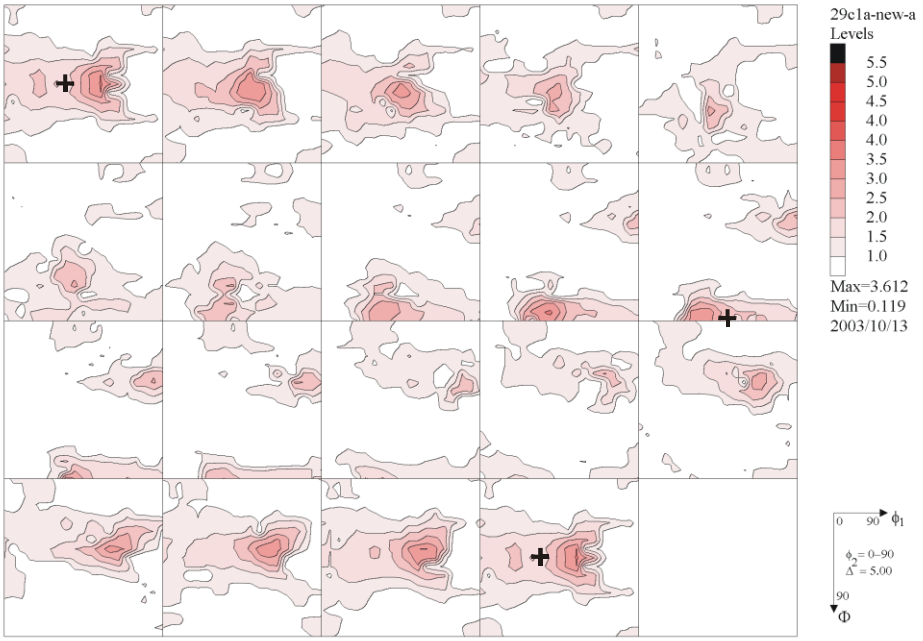


Fig. 59 Two sets of pole figures differing in rotation, analogically to the case with the wrong choice of the registration convention (rotation about 90 degrees)

The plots of the ϕ_2 projection of the ODF calculated on the basis of each set of pole figures are shown in Figures 60A and 60B. As you can see, in Figure 60A, the maximal values of the ODF are for a different component than in Figure 60B. In the first case, you can find the component (110)<1-12> (Brass) in the maximum of the ODF, while in the second case, you can find the component: (101)<-1-11>. The cross marks on both images indicate all the symmetrically equivalent orientations of the (101)<-1-11> component. The measurements of the Texture Standards from LaboSoft s.c. with the triclinic sample symmetry can be very helpful in adjusting the pole figures convention. It is very important for the exclusion of serious errors.

A)



B)

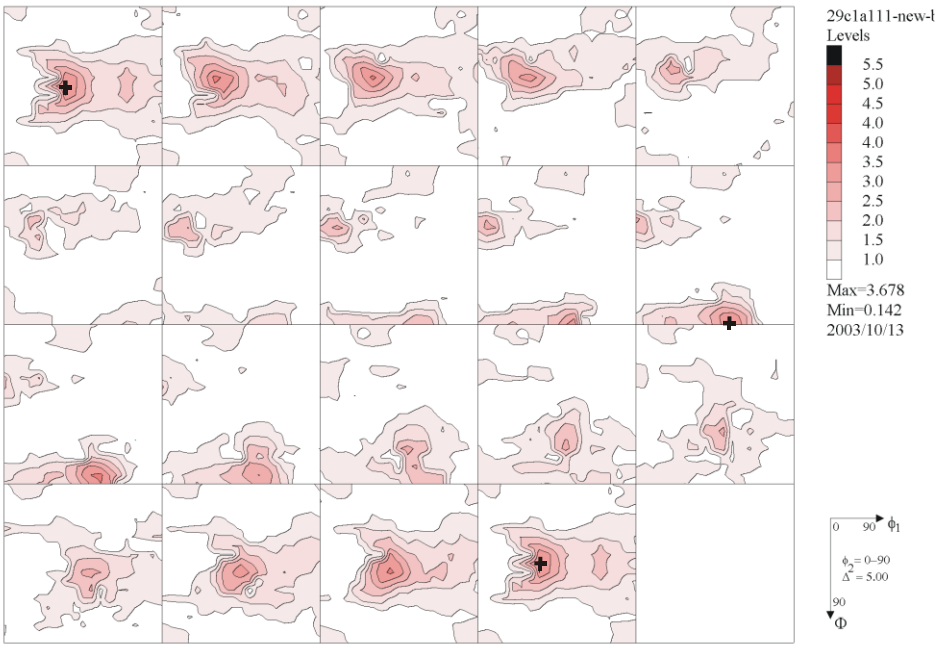


Fig. 60. ODFs calculated from two sets of pole figures differing in rotation, analogically to the case with the wrong choice of the registration convention (rotation about 90 degrees)