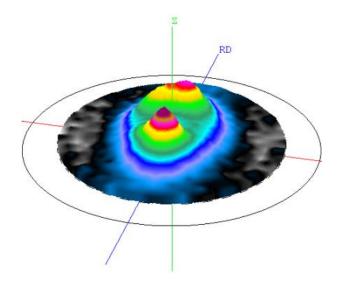


LaboTex

Version 3.0

Texture Analysis Software for Windows



Introduction to LaboTex

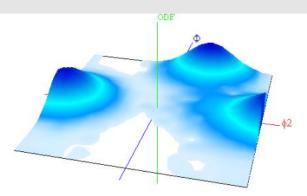
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1. Introduction



1.1. Main Program Features

LaboTex software is a Windows 2000/XP/2003 tool for complex and detailed analysis of crystallographic textures. This user-friendly program enables you to conduct a variety different calculations and graphic analyses of Orientation Distribution Function (ODF), Pole Figures (PFs) and Inverse Pole Figures (IPFs). The main LaboTex features include:

- ODF calculation by ADC method with the ghost correction;
- ODF free from truncation errors of the series;
- ODF calculation using both types of experimental data: pole figures and sets of individual orientations;
- ODF, PF and IPF data measured, calculated and presented in a wide range of grid cells from radial angle 1.0 to 10 degrees with a background and defocusing correction;
- texture analysis of all types of sample symmetry;
- a fiber texture analysis;
- a texture analysis for materials of all types of the crystal lattice symmetry;
- 2D and 3D graphic presentation of ODFs, PFs and IPFs;
- simple on-line identification of the orientations, giving its parameters in Euler angles and Miller indices;
- creation of additional pole figures and inverse pole figures;
- creation of misorientation histograms;
- creation of model ODF on the base of model functions (Gauss, Lorentz);
- comparisons of ODFs and PFs (up to 12);
- diagrams for the skeleton lines (alpha fiber, beta fiber etc.);
- an on-line qualitative texture analysis;
- a texture database;
- a quantitative texture analysis: the volume fraction of texture components by a model function and integration in the Euler space;
- ODF transformations (frame rotations, crystallites rotation models);
- ODFs logical functions (sum, union etc.);
- transformations of ODF to a set of single orientations;
- input data in more than 30 data formats;
- rotations and symmetrizations of experimental pole figures;
- plotting graphics on mono and colour printers;

- passing graphical objects to other Windows applications via the clipboard or creating image files in the *.BMP or *.TIF format;
- exporting ODF and pole figures to the ASCII format;
- easy management of the data and results by collecting in symmetries, projects, samples and jobs.

1.2. LaboTex - Range of Applicability

LaboTex is a versatile piece of software which can be used to handle: crystallographic textures of materials such as metals and alloys, ceramics and composites, semiconductors and superconductors, polymers and rocks.

All these materials can be:

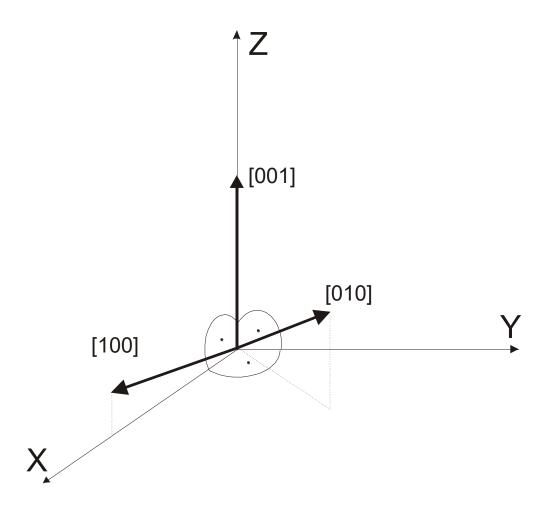
- of all types of the sample symmetry :
 - 1) orthorhombic,
 2) monoclinic,
 3) triclinic,
 4) axial,
- of all types of the crystal lattice symmetry :
 - 1) triclinic (symmetries after Schoenflies: C₁),
 - 2) monoclinic, (C_2) ,
 - 3) orthorhombic (D_2) ,
 - 4) trigonal (D_3, C_3) ,
 - 5) tetragonal (D_4, C_4) ,
 - 6) hexagonal (D_6, C_6) ,
 - 7) cubic (O, T).

1.3. Representation of Orientations by Euler Angles.

Crystal orientation is commonly described by three Euler angles. The three Euler angles $(\varphi_1, \Phi, \varphi_2)$ are defined in the space of $0 - 2\pi$ for φ_1 , $0 - \pi$ for Φ and $0 - 2\pi$ for φ_2 . The orientation is described by the rotation that transforms a sample fixed coordinate system into a crystal-fixed coordinate system of a crystallite. The orientation can be described by three counter clockwise partial rotations:

- (a) the crystal coordinate system is rotated by ϕ_1 angle around Z axis of the sample coordinate system,
- (b) then it is rotated by Φ angle around X axis (in a new position) of the crystal coordinate system,
- (c) Finally it is rotated by φ_2 angle around Z axis of the crystal coordinate system.

1.4. Crystal and sample coordinate systems: LaboTex Axis and Angles Convention.





LaboTex uses the following convention of the axis for fixing the crystal and sample coordinate system (Figure 1) :

- 1. X,Y,Z axis are perpendicular to each other.
- 2. [100] axis is in XZ plane.
- 3. Z axis is paralel to the [001] crystallographic axis.
- 4. The crystal coordinate system and the sample coordinate system should be at the same order i.e. both right-handed or both left-handed.
- 5. Bunge definition of Euler angles:

where X,Y,Z - the axis of the crystal coordinate system, [100], [010], [001] - the crystallographic axis.

The exception is the hexagonal system for which user may to choose axis convention A or B (Figure 2) :

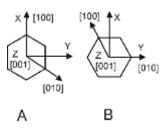


Figure 2

1.5. ODF definition

The Orientation Distribution Function (ODF) is defined as:

$$\frac{dV}{V} = f(g)dg$$

where :

f(g) - values of ODF;

 $g(\phi_1, \Phi, \phi_2)$ - orientation;

dV - the volume of crystallites with the orientation g in the element of the orientation space $dg = sin\Phi d\Phi d\phi_1 d\phi_2$ where ϕ_1, Φ, ϕ_2 are Euler angles;

V - the sample volume.

1.6. Basic ranges of ODF. LaboTex structure code.

LaboTex shows ODF in a reduced basic range. The Euler angle space can be reduced due to the crystal and sample symmetries. The boundaries of the basic range of ODF in the Euler space and symmetry structure code used in LaboTex are collected in table below:

Symmetry		Cubi	c**	Hexa	gonal	Tetra	agonal	Trig	gonal	Ortho- rhombic	Mono- clinic	Triclinic	
			0	Т	D ₆	C ₆	D ₄	C_4	D ₃	C ₃	D ₂	C_2	C1
Lab	oTex		7	6	11	10	5	4	9	8	3	2	1
stru	cture code												
	triclinic*	(C ₁)	360°	360°	360°	360°	360°	360°	360°	360°	360°	360°	360°
ϕ_1	monoclinic*	(C_2)	180°	180°	180°	180°	180°	180°	180°	180°	180°	180°	180°
·	orthorhombic	*(D ₂)	90°	90°	90°	90°	90°	90°	90°	90°	90°	90°	90°
	axial*		_***	-	-	-	-	-	-	-	-	-	-
Φ			90°	90°	90°	180°	90°	180°	90°	180°	90°	180°	180°
\$ 2			90°	180°	60°	60°	90°	90°	120°	120°	180°	180°	360°

* - sample symmetry

** - there are three non-linear basic regions inside the described region

*** - for any ϕ_1 angle

The structure code is introduced to experimental data files (EPF,POW,PPF...).

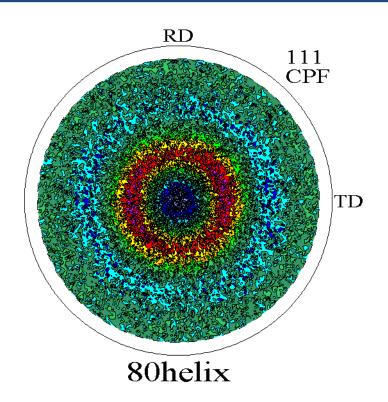
1.7. Pole Figures

The experimental pole figures are obtained via X-ray and neutron measurements. LaboTex pole figures processing comprises of the correction of the pole figures on account of their defocusing and background, as well as the preliminary normalization and the possibility of different kinds of symmetrization. ODF calculation from the pole figures is one of the main areas of applications of LaboTex. Experimental pole figures are unnormalised i.e. the measured intensities depend on the type of X-ray or neutron source, on the type of a counter, the collimating system, the absorption properties of measured material and so on. Therefore experimental pole figures cannot be compared with each other. Pole figures can be correctly normalized only in the ODF calculation process. There are three types of pole figures, from point of view of normalization, used in LaboTex:

- i unnormalized
- ii approximately normalised
- iii precisely normalised.

Pole figures (also max. intensities) from the experimental pole figures (i and ii) usually have different intensities than type iii pole figures. All comparisons between pole figures should be conducted inside type iii pole figures. Quantitative analysis can be done using **only normalised** pole figures.

You can find more details in the LaboTex manual: **"Pole Figures: Registration and Plot Conventions"** available from our websites: <u>www.labosoft.com.pl</u> or <u>www.labotex.com</u>



1.8. The ODF Calculation

The orientation distribution functions determined using LaboTex are ghost corrected. In comparison with the method of the ODF reproduction based on Fourier series, the results obtained using LaboTex are free from truncation errors of the series. Obtaining these error-free results is of great importance when very sharp textures are analyzed. LaboTex calculates the ODF using both types of experimental data:

- ODF calculation from Pole Figures using the ADC method [1-10]. The algorithm of the ADC method used in the program has been verified using a large number of models and experimental data. The results were published in many papers and proceedings (see *ADC Method* on <u>www.labosoft.com.pl/adcmethod</u>). LaboTex reproduces the orientation distribution function with a great precision in a wide range of texture sharpness (from textures close to the random distribution to those of deformed single crystals). ODF can be calculated from complete and incomplete pole figures (measured in an arbitrary range of a radial angle).
- ODF calculation from a set of individual orientations. The number of individual orientations may be arbitrary. Individual orientations may be weighted or not. Individual orientations should be given in Euler angles (degrees or radians are valid).

1.9. Definitions of fit error in ODF calculation

The texture index and definitions of fit error RP (controlling the iteration procedure of ODF calculation) are defined as:

$$f^2 = \frac{1}{8\pi^2} \int_G f^2(g) dg$$

where :

 f^2 – texture index, f(g) – value of ODF, g – orientation, G - orientation space.

$$RP_{\{hkl\}} = \frac{1}{N} \sum_{i=1}^{N} \left| \frac{\left\{ PF_{exp.} \right\}_{i} - \left\{ PF_{calc.} \right\}_{i}}{\left\{ PF_{exp.} \right\}_{i}} \right| \cdot 100\%$$

where :

 $RP_{\{hkl\}}$ - relative error for $\{hkl\}$ pole figure,

 $\{PF_{exp.}\}_i$ - intensity of experimental (corrected and normalized) pole figure in point i,

 ${PF_{calc.}}_i$ - intensity of calculated pole figure in point i, N - number of measured points on pole figure.

$$RP = \frac{1}{M} \sum_{j=1}^{M} RP_{\{hkl\}_j}$$

dRP – absolute change of RP between successive iterations.

1.10. Qualitative Texture Analysis

The Identification of the orientation using cursors, giving their parameters in Euler angles and Miller indices, can be done on the PF and ODF. The identification of the orientation on the different types of objects (PF and ODF) is possible simultaneously in the *Compare* mode. The *Compare* mode is very important for education (the interdependence of orientations on PF and ODF). The values of PFs and ODFs are shown in the points chosen by the cursor. The orientations are optionally collected by users from the orientations data base. Users can add, edit and delete the orientations from the database. The orientations can be entered in a form of Miller indices (HKL UVW) or Euler angles (ϕ_1, Φ, ϕ_2). There is an option to write the angles or indices of the orientation directly into the text box visible in the toolbar. Users can see the value of the intensity for the selected orientation. The values of ODF or/and PF are displayed on the status bar (the sums PF value(s) or/and ODF value).

Qualitative analysis is easy and straightforward to conduct. Users select the appropriate objects and then click 'SORT'. A window with assorted orientations from database by PF or ODF will appear. Users can also analyse the near (HKL)[UVW] orientations by clicking in the selected points on the pole figure or the ODF projection. "Near orientations" can be sorted by PF or ODF values, Miller indices or distance.

1.11. Modelling of ODF, pole figures and inverse pole figures

An ODF model can be easily created using LaboTex. In order to do that, user should select only:

- Crystal Symmetry;
- Sample Symmetry:
- Grid cells for output ODF.

Then one or more components (up to 10) should be selected. For each texture component users can choose:

- volume fraction;
- FWHM for each Euler angle (phi1, phi2 and phi);
- distribution (Gauss or Lorentz).

You can find more details in the LaboTex manual: **"LaboTex: Modelling of ODF, Pole Figures and Inverse Pole Figure"** available from our website <u>www.labosoft.com.pl</u> or <u>www.labotex.com</u>

1.12. Quantitative Texture Analysis. I - Volume fraction of texture components by integration methods (IM).

LaboTex includes on-line quantitative analysis of a volume fraction of texture components. The volume fraction of each component, g, can be calculated by integrating over the appropriate subvolume in the orientation space [11] according to:

$$\frac{dv}{V} = \frac{1}{8\pi^2} \iiint f(g) dg$$

where

- dV/V is the volume fraction of grains with orientation $g(\phi_1, \Phi, \phi_2)$,
- f(g) is the value of orientation distribution function, and $dg = \sin \Phi d\Phi d\phi_1 d\phi_2$
- $-\phi_1, \Phi, \phi_2$ are Euler angles that parameterize the orientation space.

The fundamentals for calculating a volume fraction of texture components are:

- LaboTex makes the integration around the orientation in the ranges delta chosen by the user for each Euler angle:
 - $(\phi_1 \Delta \phi_1)$ to $(\phi_1 + \Delta \phi_1)$,
 - $(\Phi \Delta \Phi)$ to $(\Phi + \Delta \Phi)$,
 - $(\phi_2 \Delta \phi_2)$ to $(\phi_2 + \Delta \phi_2)$,
- In the case of exceeding the basic region of ODF space (Euler angles space) LaboTex continues the integration in the equivalent area of the basic region.

The overlapping problem

The overlapping problem appears when the integration ranges (delta) are too wide or when the orientations are closely situated in the Euler angles space. The integration area of texture components can be overlapped in two ways:

i) by overlapping of the integration ranges between symmetrically equivalent positions of the component;

ii) by overlapping of the integration ranges between the different components.

LaboTex offers three different abilities (strategies) to solve the problem of overlapping of the integration ranges between symmetrically equivalent positions of component (case i):

• "Simple Integration" – the overlapping region is multiple integrated. The integration around any single component in the full range of basic region gives (100% minus background)*number of a symmetrically equivalent position.

• "Single Counts in Overlapping Area" - the overlapping region is only single integrated for the component. The integration around any single component in a full range of the basic region gives 100% minus background.

• "Divide by Number of Symmetrically Equivalent Position" - LaboTex integrates for all symmetrically equivalent positions of the components with proper weight equal to 1/number of symmetrically equivalent positions. Integration around any single components in a full range of the basic region gives 100% minus background.

To solve the problem of overlapping of integration ranges between different components in LaboTex (case ii) users can:

• Adjust the total percent of overlapping (overlapping volume fraction) which is displayed in the *Orientations Overlap*" window. Overlapping volume fraction can be limited by diminishing integration ranges of texture components.

1. In "Simple Integration" the overlapping volume fraction refers to the sum of overlapping between different components and between symmetrically equivalent positions of all overlapped components.

2. In "Singlely Counts in Overlapping Area" the overlapping volume fraction refers to the sum overlapping between different components.

3. In "Divide by Number of Symmetrically Equivalent Position" the overlapping volume fraction refers to the excessive orientation overlap. The excessive orientation overlap area is defined in the points where the sum of weights is greater than 1. The weight is equal to 1/number of the symmetrically equivalent positions. The excessive ODF value in given point is equal to the product of the ODF value and sum of weights minus 1. The volume fraction of the excessive orientation overlap is the integral of excessive ODF values in the mentioned area.

• An overlapping volume fraction can be divided among overlapping orientations. This option causes the division of ODF values from overlap areas among overlapping orientations:

1. In "Simple Integration" and "Singlely Counts in Overlapping Area" the ODF values in the overlapping areas are divided proportionally to the number of the symmetrically equivalent overlap orientations.

2. In "Divide by Number of Symmetrically Equivalent Position" the excessive ODF values in the overlapping areas are divided among components proportionally to the weights and to the number of symmetrically equivalent overlapping orientations.

You can find more details in the LaboTex manual: **"Determination of Volume Fraction of Texture Components** Using LaboTex - Integration Method"

Available from our websites: <u>www.labosoft.com.pl</u> or <u>www.labotex.com</u>

1.13. Quantitative Texture Analysis. II - Volume fraction of texture components by Model Function Methods (MFM)

LaboTex program includes a second method for determination of the volume fraction of texture components. Users can fit a model ODF (described in point 1.11.) to a real ODF and they select only the components (up to 10 components) and the distribution (Gauss or Lorentz). LaboTex fits:

- volume fraction;
- FWHM for each Euler angle (phi1, phi2 and phi);

Users can also change the initial volume fraction and the FWHM parameters.

Crystal symmetry, sample symmetry and grid cells for an output ODF are the same as for a real ODF.

You can find more details in the LaboTex manual: **"Determination of Volume Fraction of Texture Components Using LaboTex - Model Functions Method"** Available from our websites: www.labosoft.com.pl or www.labotex.com

1.14. ODFs Comparison

LaboTex offers three methods for comparison of ODFs:

- **ODF line sections (cuts)** users define two points in Euler Space. LaboTex shows ODF intensity along the section defined on the basis of these points. Users can also choose the initial points from the orientations database (by clicking the '*Start Point*' or '*End Point*' button). It is possible to compare up to 12 ODFs.
- **Skeleton lines** users can create a number of diagrams such as alpha-fiber, beta-fiber, gamma fiber etc. Users can choose the skeleton lines on the basis of the Euler angle (Phi1, Phi or Phi2) and:
 - maximal intensity;
 - integral intensity.

Users can change the range in which LaboTex will look for the maximal ODF value or will conduct the integration (from +/-2 to +/-20 deg). Users can make comparisons of up to 12 skeleton lines.

• **Misorientation histograms.** Users define the starting point in Euler Space from which LaboTex will show the misorientation diagrams. Misorientations diagrams are calculated on the basis of ODFs within the range from 0 to 80 degrees counting from the starting point

(the starting orientation). LaboTex shows the intensity which is the relative intensity, that is the intensity which relates to the intensity of a random sample (I=I(sample)/I(random sample)) for the same range of the misorientation angle. Users can make comparisons of up to 12 misorientations histograms. Users can change the histogram step within the range from 1 to 10 degrees.

1.15. ODF Transformation

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

- **Frame rotations** users can rotate a sample frame along any Euler angle. This option is very important to see the ODF for other (different) sample position (for example, to see the ODF for the perpendicular surface with relation to the surface which was measured, you should transform the initial ODF by Phi=90deg). Users can create a changed sample symmetry for a new ODF.
- **Model rotations builder -** (crystalites/planes rotations) firstly, users should build a rotation model and save it. Secondly, you can choose up to 10 orientations of the rotation model for which you set:
 - the ranges of Euler angle around the center of the orientation (and for the symmetrically equivalent positions);
 - the vector "hkl" around which crystalites/planes will be rotated (only these crystalites/planes which are included in the chosen ranges);
 - the rotation angle;
 - the recent of the rotated crystalites/planes (from 0 to 100%).

Finally, users choose the rotation model and conduct the ODF transformation.

1.16. ODFs - logical operations

Logical operations are conducted on the basis of two ODFs. LaboTex creates a new ODF which is one of:

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

1.17. 2D and 3D Graphics

The program includes an on-screen graphic presentation of calculated ODFs, PFs and INVs in a form of contour levels (isolines) shown in 2D and 3D spaces. 3D objects plotted on the screen can be increased, decreased, shifted, rotated and animated. Up to 100 PFs or INVs can be presented in one window. In Compare Mode the objects of the same kind (PFs vs PFs, or INVs vs INVs, or ODFs vs ODFs) or of different kinds (PFs vs ODFs, PFs vs INVs, INVs vs ODFs) can be shown in two separated windows. Users can use pole figures cuts.

In order to do that, define the starting and end points on the pole figure and Labotex will show you the intensity along the selected section. The following cuts are available:

- 'Arc' (in the range from 0 to 360 degrees);
- **'Radial'** (in the range from 0 to 90 degrees);
- **'Radial (full)'** (in the range 90 0 90 degrees).

Users can define a grid for the alpha angle and/or a grid for the beta angle of the PF.

1.18. Detailed Manuals (www.labosoft.com.pl and www.labotex.com)

You can find more details about LaboTex in our manuals:

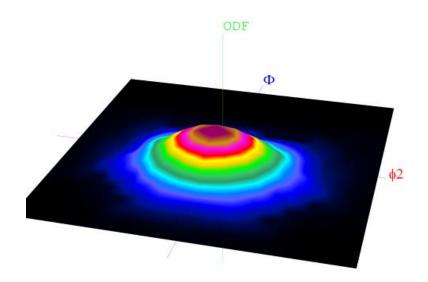
- 1) Introduction to LaboTex 3.0
- 2) Menu Guide to LaboTex

3) Determination of Volume Fraction of Texture Components Using LaboTex - Integration Method

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

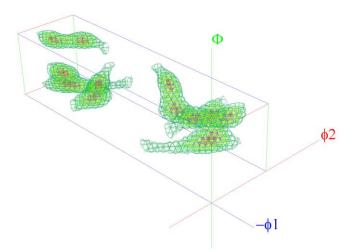
- 5) Nomenclature of Inverse Pole Figures Use in LaboTex
- 6) Pole Figures: Registration and Plot Conventions
- 7) LaboTex: Modeling of ODF, Pole Figures and Inverse Pole Figure
- 8) Texture Analysis on the Base of the EBSD Data
- 9) "Device-independent" pole figures for quantitative texture analysis (Techniques: PIM and IM)
- 10) Fundamentals of 3-D Texture Analysis. Symmetry aspects of 3-D texture analysis
- 11) Hexagonal Axes: Conventions & Conversions
- 12) LaboTex The Texture Analysis Software Getting Started
- 13) LaboTex: Modelling of ODF, Pole Figures and Inverse Pole Figure
- 14) LaboTex: Skeleton Lines and Misorientation Diagrams

All manuals are available on our websites www.labosoft.com.pl and www.labotex.com



1.19. ADC method: Opinions and Applications

- "... The strong and weak points of each method are examined showing that the iterative discrete methods (ADC and WIMV) are better suited for the reproduction of the texture function in the present case. In comparing these two discrete methods, it is evidenced that the ADC method reproduces more accurately both the experimental and synthetic texture functions over the entire range of texture sharpness considered ..." F.Caleyo, T.Baudin, M.H.Mathon and R.Penelle Comparison of several methods for the reproduction of the orientation distribution function from pole figures in medium to strong textured materials Eur. Phys. J. AP 15 (2001), p85-96.
- "... A discrete method (called as the Arbitrarily Defined Cells method) was applied to calculate the ODF. The 3-D distribution of orientations of the cellulose crystalline areas was reconstructed in the space of the Euler angles. Additionally, the complete pole figures as well as the inverse ones were recalculated. The presented analysis of the cellulose texture provides more extensive information on the space organisation of microfibrils than the standard methods...", Olek W., Pawlik K., Bonarski J. (2000): Space orientation of the crystalline areas of cellulose. Proceedings of the International Conference on Wood and Wood Fiber Composites, 13-15 April 2000, Stuttgart, Germany: 37-46.
- "... Direct Methods (WIMV, ADC) With 1 Degree Resolution Are Preferred...", K.J.Kozaczek,D.S.Kurtz, Quantitative texture analysis of blanket films and interconnects, Workshop on Texture in Electronic Applications NIST, Gaithersburg, MD, October 10-11, 2000.



2. Getting started

2.1. System Requirements

LaboTex runs on MS Windows OS 7,8 or 10 platforms.

1.2 Minimal hardware requirements

Computer PC, Processor PENTIUM IV (or compatible) 2 GHz, 512 MB RAM, 1 GB HD space, graphic card - resolution 1024x768, USB port.

To use the full version of LaboTex, you need to install the protection key (you will need a USB port to do this).

1.3 Recommended hardware requirements

Processor Intel Core 2 Duo or Athlon 64 X2 or higher, 10 GB HD space, 4 GB RAM, graphic card resolution 1920x1080, USB port, color laser jet or inkjet printer.

If your data are measured in the grid less than 5x5 degrees, double free disk space (20 GB) is recommended.

2.2. Installation

To install LaboTex:

- 1. Switch off the computer.
- 2. Insert the USB Sentinel/HASP dongle (includes Protect Key & Electronic Media) to USB port.
- 3. Switch the computer on.

You have to have Administrator credentials to complete the installation procedure!

4. Select drive assigned to USB dongle drive (using Windows Explorer on My Computer icon).

Execute *Setup.exe* file and click *OK*.

5. You will see the '*Welcome*' screen, click *Next*. The Software License Agreement will be displayed.

- 6. Read the Software License Agreement and click *Next* to accept it.
- 7. Specify a directory to install LaboTex (we strongly recommend that you install LaboTex in the

default directory to avoid further possible conflicts) and click Next.

- 8. Enter the data for the main user, institution and serial number. The serial number can be found on the dongle and in the License Agreement.
- 1. Double check if all settings are correct and click *Next*. If you need to change any of the settings, click the *Back* button.
- 10. Now LaboTex is installed and you are prompted whether or not you want to view the *README* file. To proceed further click *Yes*.
- 11. In order to install protect key driver (Sentinel/HASP) from the LaboSoft folder run "HASP Protect Key Installation" (double click the "HASP Protect Key Installation" file).

If you experience any problems during the installation process, please contact us via email <u>office@labosoft.com.pl</u>

2.3. Configuration

The first time you run LaboTex, you will need to configure a few options to your further optimize work: 1) From the main menu select '*Edit'*> '*LaboTex Options*...'

2) In the Tab *Miscellaneous* check if the following directories point to the right space on your hard drive:

A) Temporary Directory

B) Experimental Data Directory (EPF and other)

C) Correction Data Directory (COR

You may change the default setup of the directories by clicking the 'New' button.

3. LaboTex Objects and Object Containers

3.1 Introduction

Pole figures and orientations distribution functions (ODF) are LaboTex objects. Figure 3 shows a diagram for creating objects, calculation and analyses in LaboTex. Labotex operates six types of objects:

No	Denotation	Object Types
1	CPF	Corrected Pole Figures
2	NPF	Normalized Pole Figures
3	RPF	Recalculated Pole Figures
4	APF	Additional Pole Figures
5	INV	INVerse Pole figures
6	ODF	Orientation Distribution Function

These six types of objects can be stored in three types of containers: Pole Figures Container, Inverse Pole Figures Container and Orientation Distribution Function container :

No	Container	Objects	Color
1	Pole Figures Container	CPF, NPF, RPF, APF	yellow color
2	Inverse Pole Figures Container	INV	blue color
3	Orientation Distribution Function	ODF	green color
	container		

Objects from one container can be only shown in a single window at a time. Objects from two containers can be shown simultaneously only in the comparison mode (double windows - see: *Compare Window Mode*). To add or delete an object from a container click the relevant button on the object toolbar:

Button	Objects
HKL	CPF,NPF,RPF,APF
XYZ	INV
Projection	ODF

The number of objects in containers is shown in the left bottom corner of the window (yellow for the pole figures container, blue for the inverse pole figures and green for the orientation distribution function container). There can only be one projection in the container of the ODF objects at a given time. For the ODF container the number of objects indicates the number of 2-D ODF sections.

The figure below shows an example when the Pole Figures Container contains 1 pole figure, the Inverse Pole Figures Container is empty (0 INV object) and the Orientation Distribution Function container contains a ODF projection which has 19 2-D ODF sections



Objects Creations, Calculations and Analysis in LaboTex Program

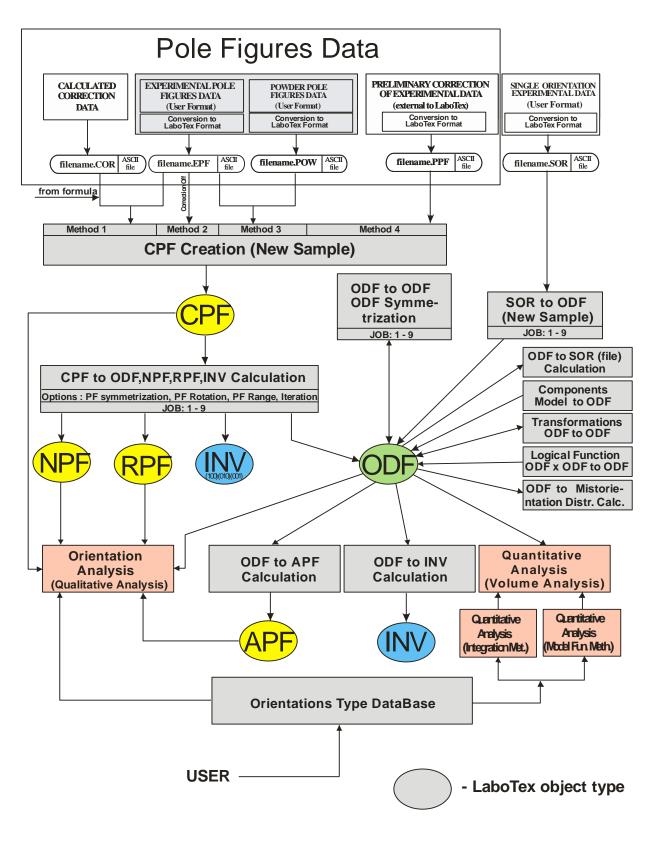


Figure 3

For the ODF objects only one projection $\phi_{\Box\Box}$ or $\phi_2\Box$ or $\Box\Phi$ can be stored in a container at a given time. To add or delete objects from the containers, click the relevant button on the object toolbar (for the pole figures container and the inverse pole figures container).

Container	Objects	Limitation
HKL	CPF,NPF,RPF,APF	maximum up to 100 objects
XYZ	INV	maximum up to 100 objects
Projection	ODF Projection	maximum up to 360 2D ODF sections

All objects in the container have to be in the same crystal symmetry. Objects arrangement on the screen can be changed as a new default (in *LaboTex Options -> Edit Menu*) or temporarily for the current session in *Edit Menu -> Arrangement*.

To delete all objects in containers use *Edit Menu -> Clear All* or select the toolbar button

3.2 LaboTex Objects Types

Pole figures used in LaboTex are of three types from the point of view of normalization:

- $i\ \ \text{-}\ \ \text{unnormalised}: EPF$
- ii approximately normalised : CPF
- iii precisely normalised: NPF, RPF, and APF

Pole figures from the experiment EPF and CPF have usually different intensities from pole figures of type iii (NPF, RPF and APF).

All comparisons between pole figures should be done inside pole figures of type iii. Quantitative analysis can be conducted using normalised pole figures.

3.2.1 CPF - Corrected Pole Figures

Experimental pole figures obtained from X-ray or neutron diffraction are unormalised i.e. measurement intensities depend on the type of the X-ray or neutron source, the type of the counter, the collimating system, the absorption properties of measured material and so on. Therefore experimental pole figures are not comparable between each other. Pole figures can be correctly normalized only during the ODF calculation process.

Corrected Pole Figures (CPF) can be corrected (according to background and de-focussing) and only **preliminary** normalized to experimental pole figures **prepared for the ODF calculation**. CPF object should not be used for analysis. CPF objects contain single pole figures of the hkl type.

To create CPF objects from your experimental files, select *File*->*New Sample* or click \square on the toolbar. You can calculate ODFs after creating CPF objects and create other objects.

To display CPF objects click the CPF button on the object toolbar, then click one or more buttons with the hkl indices:

CPF NPF RPF APF INV ODF J1 J2 100 111 211 113

Note: CPF objects are the same for all jobs.

3.2.2 NPF - Normalized Pole Figures

Normalized Pole Figures are completely normalized (during the ODF calculation process) experimental pole figures. They are correctly normalized and they can be compared between

each other. They are created after the ODF calculation. To display an NPF object click the NPF button on the object toolbar and then click one or more buttons with the *hkl* indices:

CPF NPF RPF APF INV ODF J1 J2 100 111 211 113

Note: If more than one job have been created, choose the relevant job using the job buttons (J1,J2 ..) on the object toolbar.

3.2.3. RPF - Recalculated Pole Figures

Recalculated **P**ole **F**igures are calculated from ODFs, equivalent to those PFs used as data to ODF reproduction. They are **complete** pole figures.

To display RPF objects click the RPF button object toolbar, then click one or more buttons with the hkl indices:

CPF NPF RPF APF INV ODF J1 J2 100 111 211 113

Note: If more than one job have been created, choose the relevant job using the job buttons (J1,J2 ..) on the object toolbar.

3.2.4. APF - Additional Pole Figures

Additional Pole Figures are calculated from the ODF pole figures of HKL types which were **not used for ODF determination**. APF objects contain a collection of single additional pole figures. To calculate additional pole figures (APF) select *Calculation menu -> ODF to APF* or click the button I from the toolbar.

For displaying APF object click the APF button on the object toolbar, then click one or more buttons with the hkl indices:

```
CPF NPF RPF APF INV ODF J1 J2 111
```

Note: If more than one job have been created, choose the relevant job using the job buttons (J1,J2 ..) on the object toolbar.

3.2.5. INV - INVerse pole figures

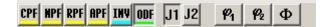
INVerse pole figures are calculated from ODFs. An inverse pole figures object (INV object) contains a collection of single inverse pole figures of XYZ types. INV objects: (100),(010) and (001) are always created after the ODF calculation. To calculate other inverse pole figures (INV) select *Calculation menu ->ODF to INV* or click the button \square on the toolbar. To display an INV object click the INV button on the object toolbar, then click one or more buttons with the XYZ indices:

CPF NPF RPF APF INV ODF J1 J2 100 010 001

Note: If more than one job have been created, choose the relevant job using the job buttons (J1,J2 ..) on the object toolbar.

3.2.6.ODF - Orientation Distribution Function

Orientation **D**istribution **F**unction is calculated from experimental pole figures (CPF objects) by the ADC method or from sets of single orientations. To calculate ODF and create ODF objects open the *Calculation menu ->CPF to ODF*, *NPF*, *RPF*, *INV*, *Calculation menu ->SOR to ODF* or click the button \blacksquare from the toolbar. The ODF objects are 2-D ODF projections: $\phi 1$, $\phi 2 \square \square$ and Φ . To display an ODF object click ODF button on the object toolbar, then click the button with the ODF projection:



Note: If more than one job have been created, choose the relevant job using the job buttons (J1,J2 ..) on the object toolbar.

3.3. Example CPF, NPF, RPF objects

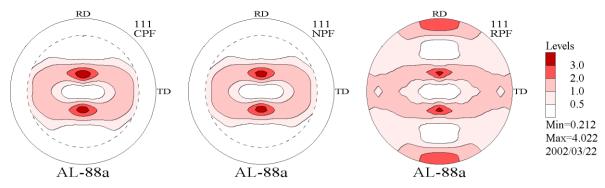
In the example below:

CPF – experimental {111} pole figure (incomplete pole figure).

ODF - calculated for symmetrization : triclinic to orthorhombic.

NPF – normalized $\{111\}$ pole figure.

RPF - recalculated from ODF {111} pole figure (complete pole figure).

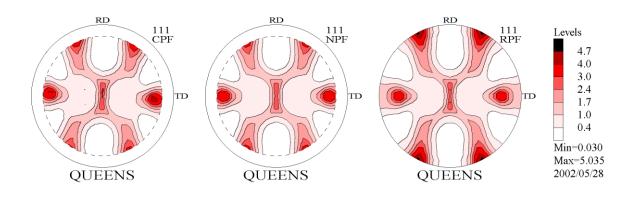


In the example below:

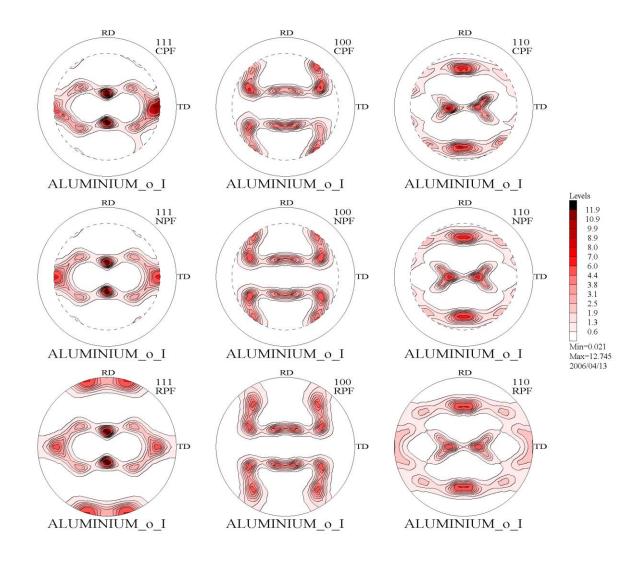
CPF – experimental {111} pole figure (incomplete pole figure).

ODF - calculated for symmetrization : triclinic to orthorhombic and rotation of PF(s)= -2.5 deg.

- NPF normalized **{111}** pole figure.
- RPF recalculated from ODF $\{111\}$ pole figure (complete pole figure).



Experimental pole figures - aluminium - pole figures: CPFs, NPFs, RPFs



3.4. LaboTex Jobs

When one calculation (job) is already running, selecting next calculations of ODFs from the same sample creates new jobs. If more than one job has been created, select the relevant job using the job buttons (J1,J2 ..) on the object toolbar. A new job is also created when the ODF symmetrisation is launched

Job buttons:



Note: The maximal number of jobs is 9

4. LaboTex Formats

4.1. EPF file format

*.EPF (Experimental Pole Figures) files refer to the raw experimental data and their background. In order to use the EPF files you will need a correction file: *.<u>COR</u> or *.<u>POW</u> The table below provides a detailed description of the *. *EPF* data format:

No of data Description Line Туре in line 1 – 2 Arbitrary title Character 3 Remarks for data in line 4 4 1 Structure Code (symmetries after Schoenflies): Integer 1 - C₁ (triclinic) 2 - C₂ (monoclinic) 3 - D₂ (orthorhombic) $4 \ \text{-} \ C_4 \ \text{(tetragonal)}$ 5 - D₄ (tetragonal) 6 - T (cubic) 7 - O (cubic) 8 - C₃ (trigonal) 9 - D₃ (trigonal) 10 - C₆ (hexagonal) 11 - D₆ (hexagonal) 2 Lattice constant, a (absolute or relative) Real 4 4 3 Lattice constant, b (absolute or relative) Real 4 4 Lattice constant, c (absolute or relative) Real 4 5 Real Lattice angle, α in degrees 4 6 Real Lattice angle, β in degrees 4 7 Real Lattice angle, γ in degrees Number of Pole Figures (including background PFs) (N 5 Integer 1 6 Remarks for data in line 7 Character 7 to 7+N 1 20 Bragg angle in degrees Real 7 to 7+N 2 α_s - beginning of polar angle in degrees Real 7 to 7+N 3 Real α_e - ending of polar angle in degrees 7 to 7+N 4 $\Delta \alpha$ – step of polar angle in degrees. Permissible value: 1.0, 1.2, 1.25, Real 1.5, 2.0, 2.5, 3.0, 3.75, 5.0, 6.0, 7.5, 10.0. 7 to 7+N 5 Real β_{s} - - beginning of azimutal angle in degrees (0 or 2.5) Positive values for pole figures drawn clockwise or negative values for counter-clockwise 7 to 7+N 6 β_e - ending of azimutal angle in degrees Real Positive values for pole figures drawn clockwise or negative values for counter-clockwise 7 to 7+N 7 $\Delta\beta$ – step of azimutal angle in degrees . Permissible values: 1.0, 1.2, Real Positive values for 1.25, 1.5, 2.0, 2.5, 3.0, 3.75, 5.0, 6.0, 7.5, 10.0. for textured pole pole figures drawn figures, and the same values or multiplicity of above-mentioned values clockwise or for background PFs negative values for counter-clockwise Index - must be 0 7 to 7+N 8 Real 7 to 7+N Index h of hkl pole figure 9 Integer 7 to 7+N 10 Index k of hkl pole figure Integer 7 to 7+N 11 Index I of hkl pole figure Integer 7 to 7+N 12 Type of Data (1-Pole Figure, 0-Background) Integer 7+N+1 Blank line Data 1 to 8 (1st Pole Figure) Real 7+N+2 1 to 8 Data 9 to 16 (1st Pole Figure) 7+N+3 1 to 8 Real Data for 1st Pole Figure 7+N+4 to end 1 to 8 Real of data for 1st PF Blank line (separates block of data) 1 to 8 Data for 2nd pole figure Real Blank line (separates block of data) 1 to 8 Data for the next PF (up to end followed by blank line) Real

Please note: Real and integer input data must be separated by one or more space signs.

*LaboTex version 2.1.006 and higher allows new grid cell 1.8x1.8,2.25x2.5,3.6x3.6,4.5x4.5 (exceptions: trigonal,hexagonal and crystal lattice symmetry)

See the specifications below for: EPF Example, COR file format, POW file format, PPF file format, SOR file format.

4.2. EPF Example

Example of an experimental data file *.*EPF* - test.epf:

line 1: Test of LaboTex program - ADC method for ODF calculation. 2: Sample: FeSi, pole figures: 200 110 112 line line 3: Structure Code b с alfa beta gamma а 1 90 90 90 line 4: 7 1 1 line 5:6 number of Pole Figures line 6: 2theta alf-s alf-e d-alf bet-s bet-e d-bet indx HKL P/B 45.250 0.0 85.0 5.0 0.0 355.0 5.0 0 200 1 line 7: line 8: 52.050 85.0 0.0 5.0 0.0 355.0 5.0 0 110 1 line 9: 77.450 0.0 85.0 5.0 0.0 355.0 5.0 0 112 1 line 10: 48.500 0.0 85.0 5.0 0.0 270.0 90.0 0 200 0 line 11: 70.000 0.0 85.0 5.0 0.0 270.0 90.0 110 0 0 line 12: 80.000 0.0 85.0 5.0 0.0 270.0 90.0 0 112 0 line 13: line 14: 172763. 172763. 172763. 172763. 172763. 172763. 172763. 172763. 172763. 172763. 172763. 172763. 172763. 172763. 172763. 172763. line 15: line 16: 172763. 172763. 172763. 172763. 172763. 172763. 172763. 172763. ... (line 17-172) line 173: 12871. 15208. 15536. 13571. 10464. 7874. 6977. 7874. line 174: 10464. 13571. 15536. 15208. 12871. 9947. 7753 6885 23949. line 175: 7512. 9977. 15302. 32907. 36331. 32369. 25152. line 176: 12319. 12319. 12319. 12319. 12319. 12319. line 177: 12319. 12319. line 178: 12319. 12319. 12319. 12319. 12319. 12319. 12319. 12319. 12319. 12319. 12319. 12319. 12319. 12319. 12319. 12319. line 179: ... (line 180-335) 13260. 19655. 23043. 23659. 22398. 23659 line 336: 11977. 15924 line 337: 23043. 19655. 15924. 13260. 11977. 12233. 14581. 19084. 40462. 38757. 30857. line 338: 24630. 30445. 36111. 21645. 15090. line 339: 142442. 142442. 142442. 142442. 142442. 142442. 142442. line 340: 142442. line 341: 142442. 142442. 142442. 142442. 142442. 142442. 142442. 142442. line 342: 142442. 142442. 142442. 142442. 142442. 142442. 142442. 142442. ... (line 343-498) 15387. 15200. 19467. 22203. line 499: 19467. 17249. 16302. 15782. 15068. 15200. line 500: 15782. 16302. 17249. 15387. 22229. 18484. line 501: 13296. 9168. 7555. 7739. 8997. 11247. 13362. 14321. line 502: line 503: 830. 792. 679. 717. 830. 792. 679. 717. 710. line 504: 822. 784. 672. 814. 777. 666. 703. 806. 769. 653. 689. line 505: 659. 696. 798. 762. ... (line 506-508) line 509: 519. 495. 424. 448. 441. 421. 361. 381. 346. 296. 313. 287. 274. 235. line 510: 362. 248. line 511: 220. 210. 180. 190. 164. 157. 134. 142. line 512: 2258. 2156. line 513: 1848. 1951. 2258. 2156. 1848. 1951. 2156. line 514: 2258. 1848. 1951. 2236. 2134. 1830. 1931. line 515: 2236. 2134. 1830. 1931. 2236. 2134. 1830. 1931. ... (line 516-518) line 519: 1981. 1891. 1621. 1711. 1851. 1767. 1515. 1599. 1562. 1413. line 520: 1637. 1339. 1329. 1268. 1087. 1147. line 521: 922. 880. 754. 796. 330. 315. 270. 285. line 522: 9209. 8791. 7535. 7954. 9209. 8791. 7535. 7954. line 523: line 524: 9118. 8704. 7460. 7875. 9118. 8704. 7460. 7875. line 525: 9029. 8618. 7387. 7798. 8941. 8535. 7315. 7722. ... (line 526-528) line 529: 7265. 6227. 6573 6977. 6660. 5708 6025 7611 line 530: 5903. 5635. 4830. 5098. 4723. 4508. 3864. 4079. line 540: 3143. 3000. 2572. 2715. 1246. 1190. 1020. 1076.

See the specifications below for: EPF file format, COR file format, POW file format, PPF file format, SOR file format.

4.3. PPF file format

*.*PPF* (Preliminary Corrected Pole Figures^K) files refer to the experimental data after conducting the background and de-focussing effects corrections using external procedures (not conducted in LaboTex).

The structure of a *.*PPF* file is identical to *.*EPF* and *.**POW** except for the data for the background of pole figures.

See the specifications below for: EPF file format, COR file format, POW file format, SOR file format.

4.4. SOR file format

*.SOR (Single Orientation) files refer to experimental, single orientation set in the LaboTex format

The table below provides a detailed description of *.*SOR* data format:

Line	No of data	Description	Туре
	in line		
1 - 2		Arbitrary title	Character
3		Remarks for data in line 4	
4	1	Structure Code (symmetries after Schoenflies): 1 - C ₁ (triclinic)	Integer
		2 - C ₂ (monoclinic)	
		3 - D ₂ (orthorhombic)	
		4 - C ₄ (tetragonal)	
		5 - D ₄ (tetragonal)	
		6 - T (cubic)	
		7 - O (cubic)	
		$8 - C_3$ (trigonal)	
		9 - D_3 (trigonal)	
		$10 - C_6$ (hexagonal)	
4		11 - D_6 (hexagonal)	Deal
4	2	Lattice constant, a (absolute or relative)	Real
4	3	Lattice constant, b (absolute or relative)	Real
4	4	Lattice constant, c (absolute or relative)	Real
4	5	Lattice angle, α in degrees	Real
4	6	Lattice angle, β in degrees	Real
4	7	Lattice angle, γ in degrees	Real
4	8	Step for output ODF (grid cells). Permissible values (deg): 1.0, 1.2, 1.25, 1.5, 2.0, 2.5, 3.0, 3.75, 5.0, 6.0, 7.5, 10.0*	Real
4	9	Weight for data (1 – present, 0 – absent)	Integer
4	10	Angle Unit: 0 – deg, 1 – rad	Integer
4	11	Angle Convention: 0 – Bunge 1 – Roe	Integer
5 to the end	1	φ ₁	Real
5 to the end	2	Φ	Real
5 to the end	3	ϕ_2	Real
5 to the end	[4]	Weight (optionally) (if parameter <i>weight</i> in line 4 is 1)	Real

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

*LaboTex allows new grid cell from version 21.006: 1.8x1.8,2.25x2.5,3.6x3.6,4.5x4.5 (exceptions: trigonal,hexagonal crystal lattice symmetry

See the specifications below for: EPF file format, COR file format, POW file format , PPF file format.

4.5. POW format

*.*POW* (*POW*der pole figures) files refer to the powder sample pole figures measured, if possible, for a specific sample.

You should measure the pole figures of the powder sample for defocusing correction from the same material as the "textured samples". The powder sample is treated as "non-texture" sample which helps to identify the absorption curve for defocusing correction. The structure of *. *POW* file is identical to *.*EPF*.

See the specifications below for: EPF file format, COR file format, SOR file format, PPF file format.

4.6. COR format

*.*COR* (*COR* rection) files refer to coefficients for the de-focussing effect.

*.COR files contain a set of correction coefficients for the de-focussing effect.

The table below provides a detailed description of *.*COR* data format:

Line	No of data in line	Description	Туре
1 – 2		Arbitrary title	Character
3	1 to n	α in degrees (polar angle)	Real
4	1	<i>{hkl}</i> of first pole figure (three digits number)	Real
4	2 to n+1	correction coefficients for de-focussing effect	Real
5	1	<i>{hkl}</i> of second pole figure (three digits number)	Real
5	2 to n+1	correction coefficients for de-focussing effect	Real
3+N*2	1	<i>{hkl}</i> (three digits number) N - number of pole figure	Real
4+N*2	2 to n+1	correction coefficients for de-focussing effect	Real

Please note: Real and integer input data must be separated by one or more space signs.

See the specifications below for : EPF file format, PPF file format, SOR file format, POW file format.

4.7. Other data formats

List of the compatible LaboTex data formats.

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(For the updates and the current list of LaboTex compatible file formats see: www.labosoft.com.pl)

- 'TSV' Single Orientations Files,
- Single orientations data files: *.tsv can be selected from *File->New Sample-> Choose Experimental Data*
- 'PLF' Queens Univ. PF Format files (4*5deg) (corrected pole figures),
- Pole figures data files : *.plf can be selected from *File->New Sample-> Choose Experimental Data*
- 'PLF' 5*5deg (corrected pole figures),
 - Pole figures data files : *.plf can be selected from *File->New Sample-> Choose Experimental Data*
- 'CON' McGill University PF Format files (corrected pole figures),
- Pole figures data files : *.con can be selected from *File->New Sample-> Choose Experimental Data*
- 'HKL' HKL Kawasaki KTEC Format files (corrected pole figures),
- Pole figures data files : *-hkl. can be selected from *File->New Sample-> Choose Experimental Data*
- 'hkl' AGH main format,
- Pole figures data files : *.hkl can be selected from *File->New Sample-> Choose Experimental Data*
- Background pole figures data files: *-b.hkl can be selected from *File->New Sample-> Choose Experimental Data*

- Random(powder) pole figures data files: *-p.hkl can be selected from *File->New Sample-* > *Choose Experimental Data*
- Background random(powder) pole figures data files: *-t.hkl can be selected from *File*->*New Sample*-> *Choose Experimental Data*
- 'xfb' AGH second format (corrected pole figures),
- Pole figures data files : *.xfb can be selected from *File->New Sample-> Choose Experimental Data*
- 'CTF' HKL Single Orientations Files,
- Single orientations data files: *.CTF can be selected from *File->New Sample-> Choose Experimental Data*
- 'SNG' TSL Single Orientations Files,
- Single orientations data files: *.sng can be selected from *File->New Sample-> Choose Experimental Data*
- 'TXT' HKL Single Orientations Files,
- Single orientations data files: *.txt can be selected from *File->New Sample-> Choose Experimental Data*
- 'UXD' (file version 1) SIEMENS/BRUKER (corrected pole figures, ASCII-files!,GADDS/D-8 Discover XRD). Use only one pole figure in one file. Parameter "_sample" has to contain Miller indices of PF (in triangle brackets) for example: "Ir<111>".
 - Pole figures data files: *.uxd can be selected from *File->New Sample-> Choose Experimental Data*
- **Please note:** Convert the binary files from the GADDS/D-8 Discover XRD to the the ASCII UXD files using software from Siemens/Bruker (XCH or other).
- 'UXD' (file version 2) BRUKER (corrected pole figures, ASCII-file!,GADDS/D-8 Discover XRD).
- Pole figures data files: *.uxd can be selected from *File->New Sample-> Choose Experimental Data*
- **Please note:** Convert the binary files from the GADDS/D-8 Discover XRD to the ASCII UXD files using the software from Bruker (XCH or other).Use only one pole figure in one file. The parameter "_sample" has to contain Miller indices of PF (in triangle brackets), for example: "Ir<111>".

LaboTex can read background files for the UXD format: 1) mark the data for background with 'B' letter in indices of pole figure (for example, the filename should be '<111B>cu brut').

```
_FILEVERSION=2
_SAMPLE="<111B> cu brut"
_SITE='UNIV ...'
_USER='LAMBDA'
...
```

2) LaboTex requires one pole figure in one UXD file.

Each pole figure and background file has to be in a separate file with the extension *.UXD.

For example: sample_100.UXD, sample_100BL.UXD, sample_100BR.UXD, ...

(the filenames which terminate with 'BL' or 'BR' include the background from the 'left' and 'right' side of PF. LaboTex average BL and BR values.)

3)You may use only BL or BR file.

4) Background files in the UXD format can have <u>only one background value for one alpha value</u>! For example, if you have one pole figure, Cu-brut_111.UXD, you should make 3 files in XRD software:

a) Cu-brut_111.UXD (pole figure data+ parameter sample: _SAMPLE="<111> cu brut")

b) Cu-brut_111BL.UXD (left background data + parameter sample: _SAMPLE="<111B> cu brut")

c) Cu-brut_111BR.UXD (right background data+ parameter sample: _SAMPLE="<111B> cu brut")

 \circ Many pole figures in a file (2 cases). Please convert XCH (or any other format) to UXD with options: 2Theta-Intensity and with one column of intensity values. You can input data for azimuthal (KHI) angle in ranges: 0.0-360.0,0.0-180.0,0.0-90.0 or 0.0-X degrees (where 0.0 < X < =50.0)

• enter manually the hkl indices in triangle brackets to the UXD file in places where the pole figure data starts (available from version 3.0.004)::

------... (header) _ANODE='Cu' <111> ; (Data for Range number 1) <---- start (data for first pole figure) _DRIVE='PHI' _STEPTIME=5.000000 ... ; (Data for Range number 17) <---- start (data for second pole figure) _DRIVE='PHI' _STEPTIME=5.000000 ...

For the background data add 'B' letter to the hkl indices (for example: <111B>). The background data in UXD format can have <u>only one background value for one alpha/PHI value</u>!

You can also enter defocussing correction data (from version 3.0.004).

Random (powder) pole figures data files: *.UXD can be selected "Choose Defocussing Correction" list.
(available from version 3.0.006):

enter manually the hkl indices in triangle brackets to the UXD file from the second line in the file. For the background data please add 'B' letter to the hkl indices (for example: <111B>).

;remarks line (first line) <111> <111B> <111B> <200> <200B> <200B> <311> <311B> <311B> _FILEVERSION=2 _SAMPLE='Copper' ...

Background data in UXD format can have <u>only one background value for one alpha/PHI value</u>! If your file contains background data with a label "_RATE_BKG=", LaboTex will automatically correct your pole figure. In such case do not enter the hkl indices for the background into your file. You can enter the defocussing correction data in the same way. Random (powder) pole figures data files: *. can be selected from *File->New Sample-> Choose Defocussing Correction*.

- 'UXD' As 'UXD' formats above (SIEMENS/BRUKER file version 1 and 2) only with reversed radial direction! Corrected pole figures (ASCII-files).
- 'HKL' Chalk River Neutron Diffr. Data (corrected pole figures)
- Pole figures data files: *.* can be selected from *File->New Sample-> Choose Experimental Data*
- 'ANA' EMSE Format files (corrected pole figures)
- Pole figures data files: *.ana can be selected from *File->New Sample-> Choose Experimental Data*
- 'epf' popLA PF Format files (corrected pole figures).

Please note: Files in popLA format have the same extension as LaboTex files: "EPF". Select "epf" (**small capitals!**) data format in LaboTex Options for files in popLA format.

- Pole figures data files: *.epf can be selected from *File->New Sample-> Choose Experimental Data*
- 'RAW' popLA Format files
- Pole figures data files: *.raw can be selected from *File->New Sample-> Choose Experimental Data*
- Defocussing correction data files: *.dfb can be selected from *File->New Sample-> Choose Defocussing Correction*
- 'ASC' Rigaku ASC format (1PF/file)
- Pole figures data files: *.asc can be selected from *File->New Sample-> Choose Experimental Data*
- Random(powder) pole figures data files: *.asc can be selected from *File->New Sample-> Choose Defocussing Correction*
- 'XPF' BEARTEX data format (corrected pole figures)
- Pole figures data files: *.xpf can be selected from *File->New Sample-> Choose Experimental Data*
- 'PFG' RIST data format from RIGAKU (ASCII)
- Pole figures data files: *.pfg can be selected from *File->New Sample-> Choose Experimental Data*
- Random pole figures data files: *.pfg can be selected from *File->New Sample-> Choose* Defocussing Correction
- 'TXT' RIST data format from PHILIPS (ASCII- corrected pole figures)
- Pole figures data files: *.txt can be selected from *File->New Sample-> Choose Experimental Data*

- 'RW1' PHILIPS X'Pert binary data format (Binary)
- Pole figures data files: *.rw1 can be selected from *File->New Sample-> Choose Experimental Data*
- Background pole figures data files: *.bgr can be selected from *File->New Sample-> Choose Experimental Data*
 - Defocussing correction data files: *.cor can be selected from *File->New Sample-> Choose Defocussing Correction*

Please note: Background pole figures data files may have the same extension as defocussing correction data files ('COR'). Please change 'COR' extension for the background files to 'BGR'!

- 'NJA' Seifert ASCII data format (compatible also with data from PSD)
- Pole figures data files: *.NJA can be selected from *File->New Sample-> Choose Experimental Data*
- Random pole figures data files: *.NJA can be selected from *File->New Sample-> Choose Defocussing Correction*
- 'NJC' Seifert binary data format (compatible also with data from PSD)
- Pole figures data files: *.NJC can be selected from *File->New Sample-> Choose Experimental Data*
- Random pole figures data files: *.NJC can be selected from *File->New Sample-> Choose Defocussing Correction*
- 'DAT' Seifert ISO-DEBYFLEX 3003 ASCII data format. Use only one pole figure in one file. Pole figure indices are 3 last characters before the period in the filename (example: PC_200.DAT for 200 pole figure). Optionally you may add the parameter "2THETA" before label "XDATA" in the file (for example 2THETA=33.45). Values of 2THETA are essential for defocussing correction from Schultz equation. You may also use non equal angle step: 5deg for inclination angle (chi or alpha) and 10 deg for the azimuthal angle (phi or betha) data are approximated to 5x5 grid. Background data (one data for each value of inclination angle) are first after the label "XDATA".
 - Pole figures data files: *.DAT can be selected from *File->New Sample-> Choose Experimental Data*
 - Random pole figures data files: *.DAT can be selected from *File->New Sample-> Choose Defocussing Correction*
- 'COA' COA data format (corrected pole figures).
- 'POL' The University of Birmingham/HiltonBrooks Texture Data.
- Pole figures data files: *.POL can be selected from *File->New Sample-> Choose Experimental Data*
- Random pole figures data files: *.POL can be selected from *File->New Sample-> Choose Defocussing Correction*
- 'DAT' TU Berlin data format (1PF/file)
- Pole figures data files: *.DAT can be selected from *File->New Sample-> Choose Experimental Data*

- 'POL' The University of Birmingham with background (add '_b' to filename for background data).
- Pole figures data files: *.POL can be selected from *File->New Sample-> Choose Experimental Data*
- Background data for pole figures (filename_b.pol): *.POL can be selected from *File*->*New Sample*-> *Choose Experimental Data*
- Random pole figures data files: *.POL can be selected from *File->New Sample-> Choose* Defocussing Correction
- Background data for random pole figures (filename_b.pol): *.POL can be selected from *File->New Sample-> Choose Defocussing Correction*
- '000' U.Paris-Sud (Neutron Diffr.Data) (1PF/file) (add '_b' to filename for background data)
 - Pole figures data files: *.DAT can be selected from *File->New Sample-> Choose Experimental Data*
 - Background data for pole figures (filename_b.000): *.DAT can be selected from *File*->*New Sample*-> *Choose Experimental Data*
- 'RWA' Philips ATC3 (add '_b' to filename for background data)
 - Pole figures data files: *.RWA can be selected from *File->New Sample-> Choose Experimental Data*
 - Background data for pole figures (filename_b.RWA): *.RWA can be selected from *File*->*New Sample*-> *Choose Experimental Data*
 - Random pole figures data files: *.RWA can be selected from *File->New Sample-> Choose Defocussing Correction*
 - Background data for random pole figures (filename_b.RWA): *.RWA can be selected from *File->New Sample-> Choose Defocussing Correction*
- 'M ' University of Northeastern (Shenyang) (add '_b' to filename for background data)
 - Pole figures data files: *.M can be selected from *File->New Sample-> Choose Experimental Data*
 - Background data for pole figures (filename_b.M): *.M can be selected from *File->New Sample-> Choose Experimental Data*
 - Random pole figures data files: *.M can be selected from *File->New Sample-> Choose Defocussing Correction*
 - Background data for random pole figures (filename_b.M): *.M can be selected from *File*->*New Sample*-> *Choose Defocussing Correction*
- 'EXP' (also 'CAL' and 'COR') (add '_b' to filename for background data) Experimental data RWTH Achen
 ('CAL' recalculated pole figures and 'COR' corrected pole figures can be also used.)
 - Pole figures data files: *.EXP (or *CAL or *COR) can be selected from *File->New* Sample-> Choose Experimental Data;

- Background data for pole figures (filename_b.EXP,) can be selected from *File->New Sample-> Choose Experimental Data* ;
- Random pole figures data files: *.EXP can be selected from *File->New Sample-> Choose Defocussing Correction*
- Background data for random pole figures (filename_b.EXP) can be selected from *File*->*New Sample*-> *Choose Defocussing Correction*
- 'HPF' (add '_b' to filename for background data) Experimental data pole figures
 - Pole figures data files: *.HPF can be selected from *File->New Sample-> Choose Experimental Data;*
 - Background data for pole figures (filename_b.HPF) can be selected from *File->New Sample-> Choose Experimental Data*;
 - Random pole figures data files: *.HPF can be selected from *File->New Sample-> Choose Defocussing Correction*
 - Background data for random pole figures (filename_b.HPF) can be selected from *File*->*New Sample*-> *Choose Defocussing Correction*

4.8. How make given format accessible for LaboTex

To enter experimental or modeling data to LaboTex select *File> New Sample*. You can change the data formats using the radio buttons in the top of the *New Sample* window (see below). If your data format is not listed (for example like on the screenshot below it is not "EPF", PPF", "SOR", "TSV", "PLF", "CON", "HKL"), you can select your data format from *Edit>LaboTex Options>Data Formats* tab (see below for the detailed instructions).

LaboTex allows a maximum of 7 active data formats in the *New Sample* window. The formats EPF, PPF and SOR are the default fixed active formats. You can choose up to 4 more active data formats (non-LaboTex). LaboTex allows you to choose from **36 different** data formats.

New Sample	×
Choose Experimental Data (LaboTex Experimental Pole Figure Files) • EPF • PPF • S0R • TSV • PLF • C0N • HKL Selected 0	Crystal Symmetry O (Cubic)
Dis_Trictinic.epf D6. Hexagonal.epf C2_Monochnic.ept U_Ubic.ept C3_Trigonal.epf 0_Ubic_acb.epf C4_Tetragonal.epf 0_Cubic_acb.epf C6_Hexagonal.epf 0_Cubic_d2.epf D3_Trigonal.epf 0_Cubic_cb.epf D3_Trigonal.epf 0_Cubic.ept D4_Tetragonal.epf 0_Lubic.ept P4_Tetragonal.epf 0_Lubic.ept	Project Name Demo
Info	Project Name : Demo
Choose Defocussing Correction Correction (On/Off) Correction Data from File (COR,PDW,DFB,ASC) Correction Data from Formula Cor(5x5).cor	Sample Name
Path C:\LaboTexd\USER\Demo version.LAB\COR\ Info	Sample Name :
Cancel Create of Binary File in LaboTex Fo	rmat (Corrected Pole Figure(s) (CPF))

To select the active data formats for the window *New Sample* for creation of CPF files: a) from the main menu select *Edit>LaboTex Options*



b) in the window LaboTex-Options select the tab Data Formats

c) the first three formats (EPF, PPF, SOR) are preselected and fixed out but you can change formats 4 to 7 using the drop down list (see the screenshot below).

Captions and Draw						
Miscellaneous	Section Contractor					
Print Setup		34				
Choose Additional Da 1, 🥅 Cclockwise					100 C 100 C 100	
LaboTex Experiment		10		2010 - MARCON		EPF
2. 🔲 Cclockwise	• Non	• O	90 de	g. O	180	deg.
LaboTex Preliminary	Corrected	I PF File	es		*	PPF
3. 🔲 Cclockwise	Non	e O	90 de	g. Č	180	deg.
LaboTex Single Orie	ntations F	iles			-	SOR
4. I_ Cclockwise	. Non	e O	90 de	g. C	180	deg.
TSV Single Orientati	ons Files				•	TSV
5. 🔲 Cclockwise	Non	e O	90 de	g. C	180	deg.
CTF - HKL Single Or	ientations	Files			-	CTF
6. 🗖 Cclockwise	• Non	e O	90 de	g. C	180	deg.
ANG - TSL Single O	rientations	Files			•	ANG
7. 🗖 Cclockwise	• Non	e O	90 de	g. C	180	deg.
TXT - HKL Single Oi	ientations	Files			-	TXT
If background data i	s greater t	han pol	le figure	e data th	en :	а.
•	Set'0' va	lue	О Ма	ke all da	ata po	ositive

For example, to make format PFG (Rigaku ASCII or binary data format) accessible for creation of CPF:

a) from the main menu select *Edit>LaboTex Options*...

b) in the window LaboTex-Options select the tab Data Formats

c) from one of the drop down lists (from 4 to 7) select 'PFG' - RIST data format 3014 (see the following screenshot).

LaboTex - Options	? ×
Captions and Draw 3D View Arrangement Miscellaneous 0DF Calculation Act	Isoline No
	Conventions
Choose Additional Data Formats and their Default Se	
1. □ Cclockwise ○ None ○ 90 deg. ○ LaboTex Experimental Pole Figure Files	180 deg.
· · · · · · ·) 180 dea.
LaboTex Preliminary Corrected PF Files	
· · · · · · · · · · · · · · · · · · ·) 180 deg.
LaboTex Single Orientations Files	SOR
4. 🔲 Cclockwise 💿 None 🔿 90 deg. 📿) 180 deg.
EXP - RWTH Achen	▼ EXP
RAW - popLA Format files ASC - Rigaku ASC format (1PF/file)	▲) deg.
CTF - HKL Single Orientations Files ANA - ANA Format files	UXD
XPF - BEARTEX data format	deg.
PFG - RIST data format from RIGAKU txt - RIST data format from PHILIPS	
RW1 - PHILIPS XPert binary data format NJA - Seifert ASCII data format	
If background data is greater than pole figure data t	
⊙ Set '0' value ⊂ Make all c	
OK	Anuluj

You can change the default parameters for data format using relevant the checkboxes or radio buttons.

Now when you open the *New Sample* window (*File>New Sample*), you will see the "*PFG*" file format listed.

New Sample	X
Choose Experimental Data (TXT - Rigaku 3014)	Crystal Symmetry
CEPF C PPF C SUN O EXE C ANG C EXP C UUU	O (Cubic)
002_corrected.txt n4752001xt 100_corrected.txt New File.txt	Project Name
101_corrected.txt New File2.txt	0000000
102_corrected.txt A-200.inatxt	0000000x
alfa-Few5.xpe.txt file-1.txt	000acc 000ak
file-2.txt	000akar
Path G:\w3000\USER\SMITH.LAB\EPF\	000avv 000ax
	000nja 🗾
Info	Project Name : 0000000
Choose Defocussing Correction	- Sample Name
Correction (On/Off)	111
Correction Data from File Correction Data from Formula	111_fiber 🗖
(COR,POW,DFB,ASC,PFG,NJA,DAT,POL,NJC,COA,RWA,UXD,EXP) 111fcc.cor AA40601 b.POL A-Random211.nja Austenii	111aa
200fcc.cor Al.pow A-Random220.nja Austenil	111bb 111dd 🔓
220fcc.cor A-Radom111.nja A-RAVI-NML.POW CHRIS4 A1-P1.COR A-Random200.nja Austenite.pow CHRIS4	1111ff °
	111fff 111bb
Path G:\w3000\USER\SMITH.LAB\COR\	111-POeL
	1111-POL
Info	Sample Name :
Cancel Create of Binary File in LaboTex For	mat (Corrected Pole Figure(s) (CPF))

To <u>simultaneously</u> use <u>several files</u> with <u>the data from the same sample</u> :

select the relevant files in the files selection box by holding the Ctrl key on your keyboard and left-clicking the filenames with your mouse. The selected files will be highlighted in blue (see the screenshot below).

If you have files with corrected pole figures, select these files from the file list in the *New Sample* window ("Choose Experimental Data").

If you have files with non-corrected pole figures and files with data for defocussing and background correction, set the extension for all these files to PFG (*.**pfg**). The files with the background correction data should also have "_B" in their filename before file extension ".PFG" (for example: *ferrite_B.PFG*). Once you adjusted all file extensions, you can select the data from the lists in the 'New Sample' window:

- Pole figures data files: *.pfg (from the "Choose Experimental Data" list)
- Background of pole figures data files: *_B.pfg (from the ''Choose Experimental Data'' list)
- Defocussing correction data files (files with pole figures from a 'random' (powder) sample): *.pfg (from the "Choose Defocussing Correction" list)
- Background of pole figures with defocussing correction data files: *_B.pfg (from the "Choose Defocussing Correction" list)

New Sample	×
Choose Experimental Data (PFG - RIST data format from RIGAKU) C EPF C PPF C SOR • PFG C ASC C EXP C NJA Selected : 10	Crystal Symmetry D ₆ (Hexagonal)
Ti_002.PFG Ti_110.PFG Ti_002_b.PFG Ti_110_b.PFg Ti_100.PFG Z00000.PFG Ti_100_b.PFG Ti_101_b.PFG Ti_101_b.PFG Ti_102_PFG Ti_102_b.PFg	Project Name Demo Fabien IIS
Path G:\w3000\USER\SMITH.LAB\EPF\KIM\binary\ Ti_002.PFG	
Info .PFG08-MAR-02 10:35:35C-1(110)	Project Name : Fabien
Choose Defocussing Correction Correction (On/Off) Correction Data from File Correction Data from File COR,POW,DFB,ASC,PFG,NJA,DAT,POL,NJC,COA,RWA,UXD,EXP) RANDOM_002,PFG RANDOM_002,PFG RANDOM_100,PFG TI,RANDOM_002,B,PFG RANDOM_101,PFG TI,RANDOM_002,B,PFG RANDOM_101,PFG TI,RANDOM_101,B,PFG RANDOM_102,PFG TI,RANDOM_102,B,PFG RANDOM_110,PFG TI,RANDOM_102,B,PFG Path G:\w3000\USER\SMITH.LAB\EPF\KIM\binary\No TI_RANDOM_	Sample Name W042at RLaboTe Zr-Fabien Zr-Fabien01 Zr-Fabien02 Zr-Fabien03 Zr-Fabien04 Zr-Fabien04 Zr-Fabien-bc Zr-Fabien-bc Zr-Fabienn zw042at_RLaboTe
Info PFG06-MAR-02	Sample Name : Ti_ROLU
Cancel Create of Binary File in LaboTex Format (Corrected Pole Figure(s) (CPF))	

For more details see 'Pole Figures: Plot and Registration Conventions' PDF file on <u>www.labosoft.com.pl</u> or <u>www.latotex.com</u>

Please note:

LaboTex can input data for different azimuthal and radial steps (azimuthal step is adjusted to radial step by linear interpolation).

Azimuthal step has to be within the range 1-10 deg., one of radial steps from: 1., 2., 1.2, 1.25, 1.5, 2., 2.5, 3., 3.75, 5., 6., 7.5, 10. degrees and extra: 1.8, 2.25, 3.6, 4.5 except from trigonal and hexagonal crystal lattice symmetry.

The radial step for defocussing correction data has to be the same as for the pole figures(!).

To make format accessible for creation of CPF files:

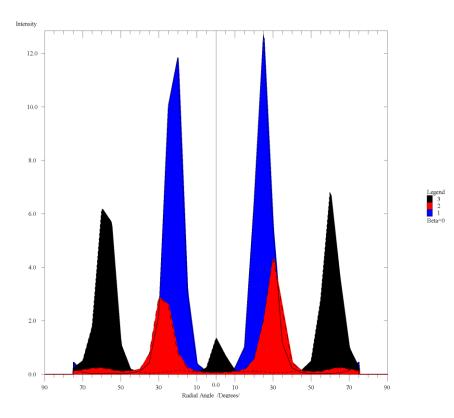
a) select *Edit->LaboTex Options;*b) select the *Data Formats* tab;
c) select the names of desired format from the drop down menus 4 -7.

To **simultaneously** use **several files** with **the data from the same sample** :

select the relevant files in the files selection box by holding the Ctrl key on your keyboard and left-clicking the filenames with your mouse. The selected files will be highlighted in blue (see the screenshot below).

If the extensions of your data files differ from those available, please to change them: for example, (in RW1 format) background pole figures data files have the *.COR extension by default. This extension is the same as for defocussing correction data files. Change the extension of the background pole figures data files to *.BGR before entering them to LaboTex.

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5. LaboTex - Frequently Asked Questions (FAQ)

Q: In the LaboTex demo version the raw data for the pole figure contains the data from 0 to 90 deg alpha angle tilt. In our pole figure the data obtained by the reflection method ranges from 0 to 75 deg as at the higher angles the beam is parallel to the sample surface leading to defocussing. Is the incomplete pole figure data obtained by us using the back reflection method enough to conduct analysis?

A: Yes, you can use incomplete pole figures for analysis. LaboTex accepts pole distances smaller than 90 deg. It can be 85, 80, 75 deg. and so on. You can cut off the pole figure in the center as well and start the pole distance not from 0 deg. but from 5, 10, 15.... deg. (for the transmision technique).

Q: At each alpha tilt angle we get the background values. There is no information in the software how to do the background correction by using these values. Also the raw data does not give the background values.

A: In the demo version we have not used the background values. However, if you check the structure of an EPF file (see *HELP* menu), you will see that LaboTex accepts the background data.

Q: We need to do the ODF for the HCP metals like Titanium, Zirconium and some cubic metals like steel. We may not need the other crystal geometry.

A: LaboTex calculates ODF for all crystal symmetries. You can use whichever you wish.

Q: The maximum intensity value of PF data which is obtained by X-ray machine is different from the one appearing on the computer screen of LABOTEX PF analysis. Any reason?

A: Experimental pole figures obtained from X-ray diffraction are unnormalized. The measured intensities depend on the type of the X-ray source, the type of a counter, the colimating system, the absorption properties of measured material and so on. Therefore the pole figures from an X-ray machine are not comparable between each other. Pole figures can be normalised in the ODF calculation process.

Pole figures used in LaboTex program are of two types:

I - approximately normalysed : .CPF

II - precisely normalysed: .NPF, .RPF, and .APF

Pole figures and the maximum intensities from X-ray and .EPF and .CPF usually have different intensities than pole figures of type II (.NPF, .RPF, and .APF). All comparisons between pole figures should be done inside the pole figures of type II! Quantitative analysis can be made using only normalyzed pole figures!

Q: Does the accuracy or the reliability of PF-to-ODF conversion depend on the type of the feature of the textures concerned? For example, is there any difference in the accuracy between Goss and cube oriented textures?

A: No, the accuracy of different texture components does not depend on the type of texture component in calculation by the ADC method in LaboTex.

Q: Is the algorithm for calculation of ODF's different from the 'WIMV' algorithm in the POPLA package?

A: The algorithm used in LaboTex is different from the WIMV method. LaboTex implements the original ADC algorithm.

There are some similarities between WIMV and ADC methods:

1) both methods belong to the same group of so called direct methods (or discrete methods) in opposition to Fourier series methods;

2) both methods use iteration procedures.

The main differences between ADC and WIMV methods:

1) different principles of the iteration procedure;

2) different principles of "ghosts" correction.

For more details see:

H.-R. Wenk, K. Pawlik, J. Pospiech and J.S. Kallend (1994) *Deconvolution of superposed pole figures by discrete ODF methods: Comparison of ADC and WIMV for quartz and calcite with trigonal crystal and triclinic specimen symmetry.* Textures and Microstructures 22, 233-260.

U. F. Kocks, C. N. Tomi, H. R. Wenk, "Texture and Anisotropy", Cambridge University Press

F.Caleyo, T.Baudin, M.H.Mathon and R.Penelle, *Comparison of several methods for the reproduction of the orientation distribution function from pole figures in medium to strong textured materials* - Eur. Phys. J. AP 15 (2001), p85-96

("... The strong and weak points of each method are examined showing that the iterative discrete methods (ADC and WIMV) are better suited for the reproduction of the texture function in the present case. In comparing these two discrete methods, it is evidenced that the ADC method reproduces more accurately both the experimental and synthetic texture functions over the entire range of texture sharpness considered ...")

There are more papers describing the principles of the ADC method. For the references see the *ADC Method* section on our website <u>www.labosoft.com.pl</u>

Q: I am looking for a better reference or way to index ODF patterns. Mostly, I use figures from Bunge's book which show low index orientations. Working with steel, I come across many higher order reflections like {554}<225> and I can calculate these angles if I know what to look for, but it's very tedious to index some higher order reflections by guessing what they might be and then calculating the angles- checking, guessing again, calculating... I would like a program which takes Euler angles from the input and lists the closest {hkl}<uv> indices. I guess I'll program something like this unless anyone can suggest a better method or point me towards something that has already been written.

A: Your problem of indexing ODF patterns can be solved using LaboTex. LaboTex is performing texture analysis using pole figures and ODF. LaboTex can do it simultaneously!

Q: What indices I should use for hexagonal symmetry?

A: In case of hexagonal symmetry you should transform {hkil} -> {hkl} by excluding {i} indices. For example: {01-11} to {011};

For pole figures, if the first or second index is negative, please rearrange it so that the first two indices are positive and exclude the third index (which is the negative sum of the first two). The last index remains the same.

For example: {-2110} to {11-20} and final {110};

For crystal directions < uvtw > ==> < UVW > please calculate:

U=u-t

V=v-t

W=w

For example: <11-20> to <330> and final <110>;

Please, check this for calculate orientation $\{0,1,-1,1\} < 2,-1,-1,0 >$:

 $\{0,1,-1,1\} < 2,-1,-1,0 > ==> \{0,1,1\} < 1,0,0 >$

Q: The format of the raw data as we get it is different than the one used by you. How do you propose to change the data structure so that it can be suitable for the software?

A: If format your data is not available in LaboTex (see: *Edit -> LaboTex Options -> Data Formats*), we have two suggestions:

1) Take a look at the description of data file structure in the *LaboTex Demo HELP* menu. Check the "*LaboTex Format of Experimental Data*" option and the examples of *.*EPF*, *.*COR* and *.*POW*. Then you can transform your data to EPF and COR type format.

2) You can send us examples of your data files and the LaboSoft team will prepare the LaboTex input to accept your data format, free of charge for our customers.

Q: Can I create a CPF file myself? We would like to calculate an ODF with pole figures which have been multiplied by corrected factors and which were not re-normalised after this multiplication.

A: .CPF files are binary files with a complicated structure. We can suggest two solutions:

1) You can save your special data as a 'PPF' file (for more details how to see *Help* section). This file does not include background data and you do not need to use .COR file.

2) You can save your special pole figures as 'EPF' file including the proper number of "0" values for the background for each pole figure at the end of the file. Remember to add the lines describing your data (at the beginning of the file) for each pole figure background. In such cases, you need to make a 'COR' file which includes correction coefficients equal to "1".

Q: What should I do to read Rigaku data?

A: For Rigaku data files, remember to use only one pole figure per file and to set the extension of your files to *.ASC (for example: 53110.ASC, 53200.ASC, 53211.ASC).

To make the *.ASC files accessible in LaboTex for creation of CPF files:

- a) select *Edit->LaboTex Options;*
- b) select the *Data Formats* tab;
- c) select "ASC Rigaku ASC format (1PF/file)" one of the from the drop down lists 4 -7;
- d) select *File -> New sample* then select "ASC" data format. If you do not use defocusing correction, select "off" for "Correction";
- e) select ASC pole figures files;
- f) select the proper crystal symmetry for your sample.

Q: Could you please tell me whether LaboTex for Windows could be used for files generated with Bruker equipment?

A: Yes. UXD file version 1 and 2 and the UXD data format with reversed radial angle direction are all compatible with LaboTex. For more details see <u>www.labotex.com/format.htm</u>

Q: When using ASC format only one PF file can be included and other APF can be calculated by the software. Does that mean that it is not necessary to measure other PFs experimentally? Can I include other PFs such as 200 and 112 apart from 110 in the BCC structure? On the other hand, in the EPF format several PFs can be input simultaneously. How about the difference in the EPF and ASC cases?

A: It is possible use more PFs (files). You may use 110, 200 and 112 PFs simultaneously. In *File->New Sample* window select (by a mouse click) several ASC files simultaneously by holding the *CTRL* (control) key. Calculating the ODF from one PF is not always enough. In such cases, you should use more PFs.

Q: Is there any simple way to transfer ASC format into EPF format with 8 columns?

Q: As for the background data, I cannot find a way to input that to the file when an ASC has been included. Can the background data only be used in the EPF format?

A: Usually the measured pole figures must be corrected according to the background and the defocusing absorption. You should measure these values for your samples. These both corrections of the raw pole figures data are sometimes done by the software used with the experimental X-ray device (especially if you use PSD-Position Sensitive Detector). You should check whether this can be done with your x-ray device (i.e. whether it is a type of a PSD detector). Inside the ASC file format you can find two places in which the background values can be included. Find the lines with words: **LOW*, **HIGH*. Your files will have zero values in these places. You should decide whether this is the correct value. If it is not, consult the manual for your X-ray device to find how to measure and include the background values to your ASC files in positions *LOW and *HIGH inside the files.

Q: I am studying the texture in steel. Which correction file and the symmetry type should I choose when including the data?

A: In order to defocus the correction, measure the pole figures of the powder sample (from the same material as the "textured samples", which in your case is steel). The powder sample is treated as a "non-texture" sample. This helps to find the absorption curve for the defocusing correction. The files related to the powder sample should have the extension *.POW (LaboTex format), *.ASC (Rigaku format) or other (for details see <u>www.labotex.com/format.htm</u>). The files should be in the COR LaboTex directory (for the current user). In your case (the steel samples), you should choose the O-cubic symmetry. All symmetries are indicated according to the Schoenfliess symbols (International Tables for Crystallography - ed.T.Hanhn - 1983, D.Reidel publishing company. Dordrecht/Boston).

Q: As for the powder sample should I measure it in the same condition with the ordinary ones?

A: Yes.

Q: Can I choose a Corr file also in the ASC format?

A: Yes.

Q: How can I have the same numerical values of the odf as in the file .pod which we had beefore? We need these values for our calculations to determine the stored energy.

A: This option is available from the version 2.1 onwards (menu *File-->ODF export*). If you use version 2.0, the upgrade to version 2.1 is free of charge. For more details, please contact us via e-mail: <u>office@labosoft.com.pl</u>

Q: When LaboTex reads my data file (sample.epf) I get a message ''Error: Improper data. Check data file''. Please check my input data file.

A: Your data file is in popLA format which has the same extension as LaboTex files (.EPF). To make popLA *.EPF files accessible for creation of CPF files you should:

- a) select *Edit->LaboTex Options;*
- b) select the *Data Formats* tab;
- c) select "*EPF popLA EPF files format*" from the drop down lists 4 -7;
- d) select *File -> New sample* then select "**epf**" (<u>small capitals</u>!) data format (in this format the data is after the correction);
- e) select your data file;
- f) select the proper crystal symmetry for your sample.

Q: How does LaboTex define the sample and coordinate system?

A: LaboTex convention (from the version 2.1.006 onwards) for defining the sample and coordinate system is:

1) X, Y, Z axis are perpendicular to each other,

2) X, Y axis are in the (001) crystallographic plane and Z axis is perpendicular to (001) crystallographic plane,

3) X axis is parallel to the [100] crystallographic plane,

4) Crystal coordinate system and sample coordinate system should be at the same order i.e. both right-handed or both left-handed,

5) Bunge definition of Euler angles.

Q: LaboTex shows bad Euler angles for orientation (01-12)<2-201>= (012)<2-21>={38.11,42.61,0.0}. From my diagram it should be :{38,43,30} (Zr Alloy - hexagonal system).

A: Your diagram is made in a different convention than the LaboTex one. In the hexagonal system (for the hexagonal division: a=b,c(non equal a),alpha=beta=90,gamma=120) two conventions are used for the sample and coordinate system. This is the reason for the difference between the values of Phi2 angle of about 30.

In <u>LaboTex version 2.1.008</u> and higher it is possible to <u>choose the axial convention in the hexagonal system</u>.

Q: I have cell parameters for the trigonal system: a=b=c, alpha=beta=gamma <120. In the example for the trigonal system LaboTex has the same cell parameters as for the hexagonal system. Is this an error?

A: No. Rhombohedral crystal can always be described in terms of hexagonal axes. In the trigonal division of the hexagonal system two conventions are used: (1) rhombohedral axes (like for your data) and (2) hexagonal axes. LaboTex uses hexagonal axes and cell parameters have to be the same as for the hexagonal division.

You can find more details about the convention of cell parameters used in our report: <u>"Pole Figures: Plot and Registration Conventions"</u> available in PDF from our website <u>www.labosoft.com.pl</u> and <u>www.labotex.com</u>

Q: The volume fraction calculated in the software does not agree with the ones I calculated. I calculated it by the C coefficient from the texture data. Can you tell me how you calculate it?

A: The results of the volume fraction calculation can be different due to the following reasons:

1) When you use C coefficients with l=22 or l=34, in the case of strong texture peaks you obtain the truncation error of the Fourier series. This causes the error in the volume fraction calculation

2) When you use C coefficients, in reality you calculate the volume of the ideal model components not your real experimental texture peaks. This is the second reason for the error.

3) In LaboTex we eliminated the truncation error of the peaks by not using the harmonic series (the ODF calculation is based on ADC method which calculates the real ODF peaks not the truncated ones).

4) In LaboTex calculates the volume fraction by integration of the real texture peaks on ODFs (LaboTex does not use Gauss models). Additionally users can independently decide about integration width of the peak in 3 Euler angles. In the case of C coefficients you are not able to change the different width of the Gauss model in the 3 Euler angles.

5) You can see the comparison of different ODF calculation methods (including ADC method which is the base of the LaboTex software) which are described in the reference papers: <u>The ADC Method References</u>

Q: I would like to use the same values of contour pole density in the analysis of ODF for several samples. Is it possible in your program?

A: You can plot contour lines by any scale in LaboTex program.

In order to do this:

- 1. Plot any PF, ODF, or INV object using "AUTOMATIC" contours.
- 2. Press the "i" icon on the program toolbar.
- 3. Change the "AUTOMATIC" option to "MANUAL" in "PF isolines mode/ Load PF isolines".
- 4. Edit all isolines values you want in the "isolines/values" windows.
- 5. Tick the box "Value" (or/and "Color", "State").
- 6. Press the "Save PF Isolines" and save the isolines to the file.
- 7. Now, you can load these isolines from the file at any time.

Q: How do you get the COR file? Where is it generated? Can we get it from LaboSoft? Can I use our dbf file instead of the cor file?

A: COR files are automatic generated when powder samples are processed (used as *.POW files in LaboTex - see *HELP*). You can create this file manual when you know the correction coefficients (see the manuals about LaboTex formats and pole figures conventions on our website <u>www.labosoft.com.pl</u>). *.DBF files can be used instead of *.COR files

Q: What is the meaning of rotation of the PF step, lower and upper ranges?

A: You can rotate pole figures around the normal axis before the ODF calculation. Sometimes it is useful to correct the sample coordinates. Lower and upper ranges mean the ability to cut off the pole distance range from both sides (in the centre and in the maximum distance).

Important! You can use <u>simultaneously the rotation</u> and cut off for all pole figures or <u>separately</u> for each one. Check the appropriate switch!

Q: It is so difficult to use the X-ray data for every two degree scan! The reason is that we do a lot of work on textured thin films and 1 or 2 degrees are what would be ideal for us!

A: There is no problem to do that. LaboTex is able to use data measured with 1 or 2 deg. step. The ODF calculation time will be longer of course. That is because the data set (the amount of data) is bigger in that case.

Q: There is a 90 deg. rotation between the PF plotted between my old texture software and LaboTex.

A: There are two issues here:

I) Different ways of pole figures plotting:

- (1) clockwise rotation from the NS direction
- (2) counterclockwise rotation from the NS direction
- (3) clockwise rotation from the WE direction
- (4) counterclockwise rotation from the WE direction

LaboTex uses the pole figures presentation as in point A.1.

If the ODF from LaboTex and the ODF from your old software are the same, then the difference is only in the pole figure presentation (a different pole figures plotting convention).

If ODF from LaboTex and ODF from your old texture software are different then pole figures measurements convention are different.

II) Different ways of registration of pole figures in the dependence from the motion of the texture goniometer are :

- (1) clockwise rotation from the RD direction
- (2) counterclockwise rotation from the RD direction
- (3) clockwise rotation from the TD direction
- (4) counterclockwise rotation from the TD direction

LaboTex uses the convention **B.1**.

You can find more details about the adjustment of LaboTex to different plot and registration conventions in our technical report: <u>"Pole Figures: Plot and Registration Conventions"</u> which is available on our website <u>www.labosoft.com.pl</u> and <u>www.labotex.com</u>

Q: I didn't find any information about how to use the delta Phi1, Phi, Phi2 range for the calculation of the quantitative texture analysis. If for example I choose a phi integration range of 20° for a phi angle of 45 °, does it mean that the calculation will integrate in phi between 25 and 65 ° or between 35 and 55 °?

A: In quantitative analysis DeltaPhi1, DeltaPhi and DeltaPhi2 denote the half width of the integration range around the chosen orientation. So, if orientation is PHI1, PHI2, then the volume fraction is integrating in the range:

[PHI1 - DeltaPhi1 , PHI1 + DeltaPhi1]

[PHI - DeltaPhi , PHI + DeltaPhi]

[PHI2 - DeltaPhi2 , PHI2 + DeltaPhi2]

Of course, you can choose different Delta for each Euler angle and for each selected orientation (using the view of the orientation profiles in each Euler angle cross section). The calculation will then integrate in Phi between 25 and 65 $^{\circ}$ for your example.

Q: How can I make defocusing correction?

A: The best way for making the defocusing correction is by measurement of a "random" sample. Firstly, you should take the measurement of a "random" sample just like a normal sample. A "random" sample has to be made from the same or similar material as the material of your sample. Secondly, enter the files with pole figures of the sample and the files with pole figures of the "random" sample can be selected from a different list in the same dialog window. Preparation of a good quality "random" sample is difficult. We offer a set of "random" samples (texture and strain free). For more details see our website <u>www.labosoft.com.pl</u> section <u>Prices&Orders</u>

Q: How can I check the quality of my texture measurement?

A: The best way in this case is using the measurements of texture standards. LaboSoft offers texture standards of different sample symmetry which also contain a "random" sample. All results of measurements pole figures are provided by the Accredited Testing Laboratorie. For more details see our website <u>www.labosoft.com.pl</u> section <u>Prices&Orders</u>

Q: Does LaboTex cooperate with VPSC texture modeling software packages?

A: Yes. You can input the data from a file with a set of single orientations. You can also generate a file which contains a set of single orientations on the base of ODFs.

Q: When I run the HASP Protect Key Installation on Windows, I get the following error message: "user has no access to the database registry 0x20 10000 0x0 0x0" and the installation is stopped.

A: In order to avoid this error when installing the HASP Protect Key on Windows NT/2000/XP, please follow the steps below:

1) Switch off your PC / laptop.

2) Plug in the HASP Protect Key into the USB slot (for earlier versions and older HASP Keys use the parallel printer slot).

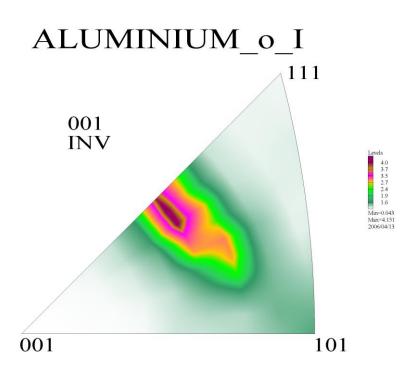
3) Switch your PC/ laptop on.

4) Login to the Windows NT/2000/XP with the Windows Administrator credentials

(otherwise you will not be able to carry out the installation!).

5) Install the HASP device driver. Remember to reboot the computer after the installation is complete.

6) To use LaboTex you do not need the Windows Administrator credentials. These are only needed during the installation.



6. References

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6.2 ADC Method - Main References:

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6.3 Other selected references on LaboTex and ADC:

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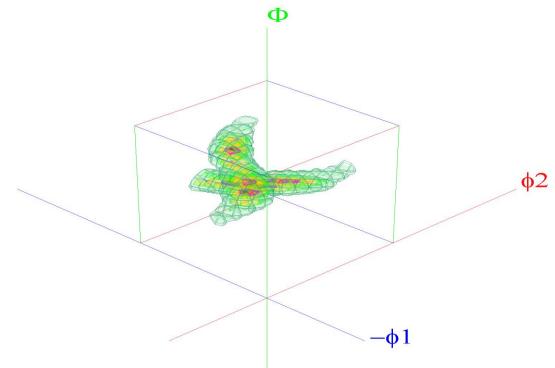
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7. LaboTex: Technical specifications

Version 3.0.54

Specification / Feature	3.0.22	Comments
Windows OS compatible application (from version 2.0.)	Yes	Windows 7/8/10
Management of data and results.	Yes	Simple access to data and results. Collecting them per: users, symmetries, projects, samples and jobs.
ODF calculation (direct - ADC Method).	Yes	The best ODF calculation method.
Texture analysis of all types of sample symmetry.	Yes	
Texture analysis for materials of all types of crystal lattice symmetry.	Yes	
Fiber texture analysis.	Yes	
High resolution ODF option.	Yes	
Calculation of a fit error (RP).	Yes	
Calculation of texture index.	Yes	
ODF calculation report.	Yes	Any available.
Ghost correction.	Yes	
Truncation errors of the series.	No	
ODF calculation using pole figures.	Yes	Data from X-Ray or Neutrons measurements.
Input data in non-LaboTex data format.	Yes	LaboTex acceptes data in 31 formats. For more details see www.labosoft.com.pl
Adjusting the customer data format for LaboTex	Yes	Free of charge
Correction of the pole figure for the background of pole figure.	Yes	
Indicating when background values are greater than pole figure data values.	Yes	LaboTex displays the percentage for the data
Choice of the correction method for the background.	Yes	 When the background data of the pole figure is greater than the pole figure data for some values LaboTex makes: a) negative values of pole figure after the correction for background is set to zero; b) adds to all the pole figure data an absolute value of the lowest values of the pole figure after the correction for background (LaboTex makes all data positive). Option "a" is the default one.
Correction for defocusing using powder pole figures.	Yes	Correction of the powder pole figure for the background is also available
Correction for defocusing from correction coefficients.	Yes	
Correction for defocusing from Schulz equation.	Yes	
Input data in any grid.	No	Only for radial angle: 1., 1.2, 2., 1.25, 1.5, 2., 2.5, 3., 3.75, 5., 6., 7.5, 10. degrees and extra: 1.8, 2.25, 3.6, 4.5 but with exception of the trigonal and hexagonal crystal lattice symmetry. If the azimuthal angle step is different from the radial step, the azimuthal step is adjusted to the radial step by linear interpolation. Azimuthal step has to be in the range of 1-10 deg.

Choice of the pole figures plot convention.	Yes	Users can choose to start to plot pole figures from "N","E","S" or "W". Users can also adjust the description of pole figure axis (e.g. denotation 'RD') to the new plot convention. ODF calculations are independent of the choice of plot convention.
Adjusting the pole figures registration convention to the LaboTex convention.	Yes	 Users can choose: counter-clockwise; none rotate; +90 deg pole figure rotate; +180 deg pole figure rotate. Users can set up the default for the registration convention for each available format of the pole figures. ODF calculations are dependent on the choice of the registration convention (ODF may be shifted).
Maximal/minimal value of Miller indices H,K,L for input PF	9/-9	
ODF calculation from the incomplete pole figure(s).	Yes	
Indication of too small number of data for the ODF calculation.	Yes	During the ODF calculation.
ODF calculation for different parameters for the same sample.	Yes	Up to 9 jobs per sample.
Choice of the symmetrization of pole figures before the ODF calculation.	Yes	Viewing of symmetrized PF.
Choice of the sample symmetry for ODF (ODF symmetrization).	Yes	Available after the ODF calculation.
A number of the symmetrization possibilities.	8	None,triclinic to monoclinic,triclinic to orthorhombic,triclinic to axial, monoclinic to orthorhombic, monoclinic to axial, orthorhombic to axial, custom to axial.
Rotation of pole figure(s) before the ODF calculation.	Yes	For all pole figures or separately for each PF in range -90 to 90 degrees.
Cutting off the pole figure(s) in the center before the ODF calculation.	Yes	For all pole figures or separately for each PF. Users can choose the angle ranges.
Cutting off the pole figure(s) in the edge before ODF calculation.	Yes	For all pole figures or separately for each PF. Users can choose angle ranges.
Changing the parameters finishing calculation in ODF calculation.	Yes	A number of iterations (1-70), RP and dRP finishing calculation (0.1-10%).
Creation of complete pole figures.	Yes	Complete pole figures (RPF) are created during ODF calculations.
Creation of complete inverse pole figures.	Yes	
ODF calculation from sets of individual orientations (SOR).	Yes	Data from EBSD, the model calculation and other.
Roe/Bunge notation of the angles in SOR.	Yes/Ye s	Notation chosen by users.
Weights of orientations in SOR.	Yes	
Choice of ODF grid (ODF from SOR).	Yes	1x1, 1.2x1.2, 1.25x1.25, 1.5x1.5, 2x2, 2.5x2.5, 3x3, 3.75x3.75, 5x5, 6x6, 7.5x7.5, 10x10.
Choice of sample symmetry (ODF from SOR).	No	Choice of the sample symmetry after the ODF calculation (ODF symmetrization).

Modelling of ODF, pole figures and	Yes	Users can choose:
inverse pole figures.	1 65	Crystal Symmetry;
inverse pole ligures.		 Sample Symmetry:
		Grid cells for output ODF;
		 Up to 10 components.
		• Op to to components.
		For each texture component users can choose:
		 volume fraction;
		FWHM for each Euler angle (phi1, phi2 and phi);
		 distribution (Gauss or Lorentz).
		Users can create any model pole figures or/and any model inverse
		pole figures from model ODF using appropriate dialog for creating
		APF (additional pole figures) or IPF (inverse pole figures). Model
		ODF is created as a new job or as a new sample.
Choice of methods for the	Yes	Users can use 2 methods: Integration and/or Model Function.
determination of volume fraction of		control and a methodo, integration and of Wodel I and for
texture components.		
Calculation of the volume fraction of	Yes	Up to 10 components simultaneously.
texture components by Integration	- 00	op to to components simulations sy.
Methods.		
Choice of integration ranges.	Yes	For each Euler angle separately, with the viewing.
		Tor each Euler angle separatery, with the viewing.
Evaluation of parameters of the	Yes	
component peak (Integration		
Methods).		
Choice of the components (Integration	Yes	From files or from a database.
Methods).		
Choice of the method of the calculation	Yes	3 methods.
of volume fraction in Integration		
Methods.		
Display of orientation overlapping	Yes	
(Integration Methods).		
Correction of overlapping (Integration	Yes	Dividing ODF among overlapping orientation.
Methods).		
Reporting from the calculation of the	Yes	Ready to print or copy to clipboard.
volume fraction of texture components		
by Integration Methods.		
Calculation of volume fraction of	Yes	Up to 10 components simultaneously. For each texture component
texture components by Model Function		users can choose initial parameters for fitting calculation from:
Methods.		volume fraction, FWHM for each Euler angle (phi1, phi2 and phi),
		distribution (Gauss or Lorentz).
Choice of the components (Model	Yes	From files or from a database.
Function Methods).		
Choice of the mode of work during	Yes	Automatic and Manual ('Once' step). In the manual mode LaboTex
calculation of volume fraction in Model		calculates relative error between the experimental ODF and the
Function Methods.		model ODF made by the user. In the automatic mode LaboTex
		adjusts the model parameters (angles and volume fraction) to the
		optimal values.
Comparison of the 'experimental' ODF	Yes	LaboTex shows the calculated and 'experimental' ODF in two modes:
with the best fit model.	100	 common area - in blue color, different area - in red color;
		 'experimental' ODF - in blue color, model ODF - red line.
		Users can also save calculated ODF as a new job (Option: "Save and
		Show"). Then they can continue with the ODF comparison in
		LaboTex 'Compare Mode'.

Reporting the calculation of the volume fraction of texture components by Model Function Method.	Yes	The report is available after saving the fitted model. It is ready to print, copy to clipboard or view.
Components (orientations) database.	Yes	100 positions for each crystal system. The orientation introduced to the database is also the denotation of the component. In texture analysis LaboTex shows all sym. equivalent positions (orientations) for orientation from the database.
Introduce orientations (components) to database in Miller indices ({HKL}< UVW>).	Yes	Equivalent Euler angles for {HKL}< UVW> depend on the cell parameters when the crystal symmetry is lower than cubic. When users introduce an orientation (component) in the Miller indices, LaboTex automatically calculates Euler angles on the basis of the cell parameters. Hence for the samples with different cell parameters LaboTex shows the same orientation in the Miller indices on the different places in the Euler space.
Maximal/minimal value for the Miller indices H,K,L,U,V,W for orientation {HKL}< UVW>	15/-15	Users can set up the maximal value for the Miller indices in the conversion from Euler angles (in the range 5 to 15).
Introduce orientations (texture components) to the database in the Euler angles.	Yes	
Introduce fiber orientations (components) to the database.	Yes	
Displaying the orientation from a database on the ODF and PF(s).	Yes	Selecting via a combo-box, Automatic mode, Next and Previous.
Displaying the symmetrically equivalent position on the ODF and PF(s).	Yes	Selecting via a combo-box or from list-box.
Presentation of the symmetrically equivalent position.	Yes	In the basic region for ODF and the full Euler space for PFs, in the Miller indices and Euler angles.
On-line identification of the orientations (components).	Yes	In Euler angles and Miller indices, ODF and pole figures (except from IPFs). In the cursor position.
Help in finding near orientations.	Yes	Near orientations sorted by: PF/ODF, Miller indices and distance.
Comparing the orientation analysis. Very useful educational purposes!	Yes	LaboTex shows simultaneously the orientation on: ODF and ODF (the same and different projection), an ODF section and ODF, pole figure(s) and ODF, pole figure(s) and an ODF section.
Showing ODF/PF values using a mouse.	Yes	For PF LaboTex shows the sum of PF values under poles of the orientation and separately for the option SORT.
Qualitative orientations analysis for PF/ODF.	Yes/Ye s	Sorted orientations from database.
Report from qualitative analysis.	Yes	Only for ODF. Ready to print and copy into the clipboard.
Creation of additional, complete pole figures (APF) from ODF.	Yes	User input only HKL. Available after ODF calculation.
Creation of additional, complete inverse pole figures from ODF.	Yes	User input only XYZ. Available after ODF calculation.
Exporting ODF to ASCII format.	Yes	
Exporting Pole Figures as ASCII format.	Yes	
Exporting Inverse Pole Figures to ASCII format.	Yes	
Choice of the convention for the hexagonal system.	Yes	
2D and 3D pole figures presentation.	Yes	·

Choice of the pole figures plot convention.	Yes	Users can choose to start to plot pole figures from "N", "E", "S" or "W". Users can also adjust the description of the pole figure axis (for example denotation 'RD') to a new plot convention. ODF calculations are independent of the choice of the plot convention.
Adjust of pole figures registration convention to LaboTex convention	Yes	 User can choose: counter-clockwise; none rotate; +90 deg pole figure rotate; +180 deg pole figure rotate. User can set up default for registration convention for each available format of pole figures. ODF calculation are dependent on the choice of registration convention (ODF may be shift).
The maximal number of pole figures/inverse pole figures in one window.	100	
Pole figures descriptions.	Yes	HKL, the sample name, directions (3 characters, edited by user) and the type of a figure (CPF,RPF,NPF,APF).
Switching off pole figures descriptions.	Yes	Separately for each kind of description.
Fill-in option in 2D/3D presentation.	Yes/Ye s	4 modes of the fill-in option: normal/black/white and continuous.
User defined sets of colors.	Yes	15 sets.
Isoline mode.	Yes	3 modes: automatic, manual and from user defined sets.
Changing the parameter of the pole figures presentation.	Yes	Number of isolines (maximum of 14), color, color set, value and fill-in.
2D ODF presentation for Phi1, Phi and Phi2 projections.	Yes	
2D ODF presentation for a section of a projection.	Yes	
Bunge definition of the Euler angles.	Yes	ODF presentation and export.
3D ODF presentation.	Yes	
The possibility changes of parameters of 3D ODF presentation.	Yes	Rotate, distance, shift, color, axis(on,off,length),parallel/perspective projection, top/bottom contour, animation (cycle rotation).
The possibility of the choice of isolines.	Yes	14
Arrangements mode.	3	Automatic /optimal arrangements/, automatic /vertical close horizontal and custom.
Drawing basic region of PF/INV.	Yes	IPF in a standard stereographic triangle (only for: cubic, hexagonal, trigonal and tetragonal systems)
Saving the set of isolines.	Yes	Saved features: color, value and activity.
Exporting 2D and 3D images to the bitmap format (bmp).	Yes	BMP or TIF format available.
Exporting (copying) 2D and 3D images to the clipboard.	Yes	In the bitmap format (bmp).
Choosing the resolution of the exported image.	Yes	
Online help.	Yes	
ODF section (cuts) defined by users	Yes	Users can define two points in the Euler Space. LaboTex shows ODF intensity along the section defined by these points. Users can also choose initial points from an orientations database (to access the database select 'Start Point' or 'End Point'). Comparisons up to 12 ODFs are available. Users can save current parameters and/or samples.

Skeleton lines	Yes	 Users can create diagrams such as: alpha-fiber, beta-fiber, gamma fiber etc. Users can choose skeleton lines on the basis of the Euler angle (Phi1, Phi or Phi2) and : maximal intensity; integral intensity. Users can also change ranges in which LaboTex looks for the maximum odf value or makes integration (from +/-2 to +/-20 deg). Users can compare up to 12 skeleton lines. The current parameters and/or samples can be saved.
Misorientation histograms	Yes	Users define the starting point in the Euler Space from which LaboTex shows misorientation diagrams. The misorientations diagrams are calculated on the basis of ODFs in a range from 0 to 80 deg from the starting point (the starting orientation). LaboTex shows a relative intensity i.e. this intensity is relative to the intensity of the random sample (I=I(sample)/I(random sample)) for the same range of the misorientation angle. Users can make comparison of up to 12 misorientations histograms. Histogram steps can be changed within the range from 1 to 10 degrees. Current parameters and/or samples can be saved.
Optimization of diagrams : ODF section, Skeleton lines, Misorientation histograms, PF section (arc, radial, radial-full)	Yes	 Scale (within the percentage of the maximum intensity value: from 0.1% to 100%); colors (defined by the user); types of lines (14 types with different dots + solid pattern); line options (all solid, all black or black contours); width of lines (0 to 10 pixels); diagram fill.
ODFs - logical operations	Yes	 In order to activate this option switch LaboTex to Compare Mode, then choose two ODFs for comparison: one in the left window and the other one in the right window (<i>LaboTex Compare Mode</i>). On the basis these two ODFs (A - from the left window and B from the right window) LaboTex creates a new ODF which can be: an intersection of the ODF A and the ODF B, a difference between the ODF A and the ODF B (or B-A), a union of the ODF A and the ODF B, a sum of the ODF A and the ODF B, a ODF difference: A or B minus the intersection of A&B, an inverted ODF (only for the ODF A). The new ODF is created within the new job for the sample of ODF A. These diagrams can be copied to other applications or exported as images in 'BMP' or 'TIF' format (menu '<i>Edit</i>').

Transformations of ODF	Yes	 There are two kinds transformations: Frame rotations - users can rotate a sample frame along any Euler angles. This option gives the opportunity to see the ODF for other (different) sample position. For example, to see the ODF for the perpendicular surface with relation to the surface which was measured, transform the initial ODF by Phi=90deg. Users can create changes of the sample symmetry for a new ODF. Model builder rotations - (crystalites/planes rotations). Firstly, build a rotation model and save it. Secondly, in the rotation model you can choose up to 10 orientations for which you set: the ranges of the Euler angle around center of orientation (and for symmetrically equivalent positions); the vector "hkl" around which crystalites/planes will be rotated (only these which are included in chosen ranges); the percentage of the rotated crystalites/planes (from 0 to 100%). Now choose the rotation model and make the ODF transformation. LaboTex calculates the new ODF which is a result of the transformation of the initial ODF.
Generation of single orientations	Yes	LaboTex creates a set of single orientations on the basis of the current ODF. Users can choose a number of single orientations from 10000 to 9999999. This option is very useful for example for users who model deformation (VCS users). A random set of single orientation can be also generated using this option. *.SOR files created by LaboTex can be then used as a new sample for the ODF calculation.
Pole figures sections (cuts)	Yes	 Users define the starting and ending points on the pole figure and LaboTex shows the intensity along this section. The following cuts are available: 'Arc' (in the range of 0 to 360 degrees); 'Radial' (in the range of 0 to 90 degrees); 'Radial (full)' (in the range of 90 - 0 - 90 degrees). To see the position of the section line on the pole figure, select the 'View' button. Up to 12 pole figures can be compared. The information about compared PFs is displayed in the <i>information window</i> on the left hand. Users must choose all pole figures for which the sections are displayed before pressing the '2D' button. If more than 12 pole figures are chosen, LaboTex shows only the first 12 pole figures sections. There is a number of options to optimize the quality of diagrams : scale (the percentage of the maximum intensity value: from 0.1% to 100%); colors (defined by the user); types of lines (14 types – dots and solid); line options (all solid, all black or black contours); diagram ill. Users can save the current parameters. These diagrams can be copied over to other applications or saved as images in *.BMP or *.TIF formats (menu 'Edit').
On-line view of alpha (radial angle), beta (azimuthal angle) and pole figure value using the mouse cursor.	Yes	LaboTex displays this data in the format: (alpha,beta) PF='value of PF'.

User defined grid for pole figures.	Yes	Users can define a grid for the alpha angle and/or a grid for the beta angle of PF.
User Manuals and Technical Reports.	Yes	 Short Introduction to LaboTex Menu and Toolbars Commands Description Determination of the Volume Fraction of Texture Components Using LaboTex - Integration Methods Determination of the Volume Fraction of Texture Components Using LaboTex - Model Functions Method Pole Figures: Registration and Plot Conventions Nomenclature of the Inverse Pole Figures in LaboTex LaboTex: Modelling of ODF, Pole Figures and Inverse Pole Figures
Usage examples.	Yes	 The following examples are available: Examples for all crystal symmetry. Examples for all sample symmetry. Example for high resolution pole figures and ODFs (1x1 deg). Examples for the fibre texture (in the demo version). Additional examples (available on our website www.labosoft.com.pl)
Demo version.	Yes	The demo version is based on the version 2.1.012
Support.	Yes	Free full e-mail support and updates for 24 months
Protection.	Yes	HASP Key: Parallel Port or USB socket.
Minimal system configuration.		 Processor PENTIUM IV 2 GHz or higher; 1 GB HD space; graphic card resolution 1024x768; CD-ROM drive; OpenGL Graphic Card is required for 3D View in "Continuous" fill mode; USB port.
Recommended system configuration.		 Processor Intel Core I5 or I7; 20-50 GB HD space; 4 GB RAM; graphic card resolution 1920x1200 + OpenGL USB port; color laser jet or inkjet printer, if data are measured in the grid less than 5x5 degrees, double free disk space is recommended.

