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LaboTex

Version 2.1

The Texture Analysis Software for Windows

Introduction

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1. Introduction

1.1. The Main Advantages of the Program

The LaboTex software is the Windows 95/98/Me/NT/2000/XP tool for complex and detailed analysis of crystallographic textures. This user-friendly program performs the different calculations and graphic analysis of Orientation Distribution Function (ODF), Pole Figures (PFs) and Inverse Pole Figures (IPFs):

- 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 or sets of individual orientations
- ODF, PF and IPF data measured, calculated and presented in a wide range of grid cells: 1x1, 1.2x1.2, 1.25x1.25, 1.5x1.5, 2x2, 2.5x2.5, 3x3, 3.75x3.75, 5x5, 6x6, 7.5x7.5, 10x10. From version 21.006 also: 1.8x1.8, 2.25x2.5, 3.6x3.6, 4.5x4.5 (exceptions: trigonal, hexagonal crystal lattice symmetry)
- texture analysis of all types of sample symmetry
- fiber texture analysis
- texture analysis for materials of all types of 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
- on-line qualitative and quantitative texture analysis
- rotations and symmetrizations of experimental pole figures
- plotting graphics on a wide range of mono and colour printers
- passing graphical objects to other Windows applications by a clipboard
- management of data and results collecting them for users, symmetries, projects, samples and jobs

1.2. Application Range of the Program

The program application range includes crystallographic textures of materials such as metals and alloys, ceramics and composites, semiconductors and superconductors, polymers and rocks:

- of all types of sample symmetry :
 - 1) orthorhombic,
 - 2) monoclinic,
 - 3) triclinic,
 - 4) axial,
- of all types of crystal lattice symmetry :
 - 1) triclinic (symmetries after Schoenflies: C_1),
 - 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. Crystal and sample coordinate systems. LaboTex Axis and Angles Convention.

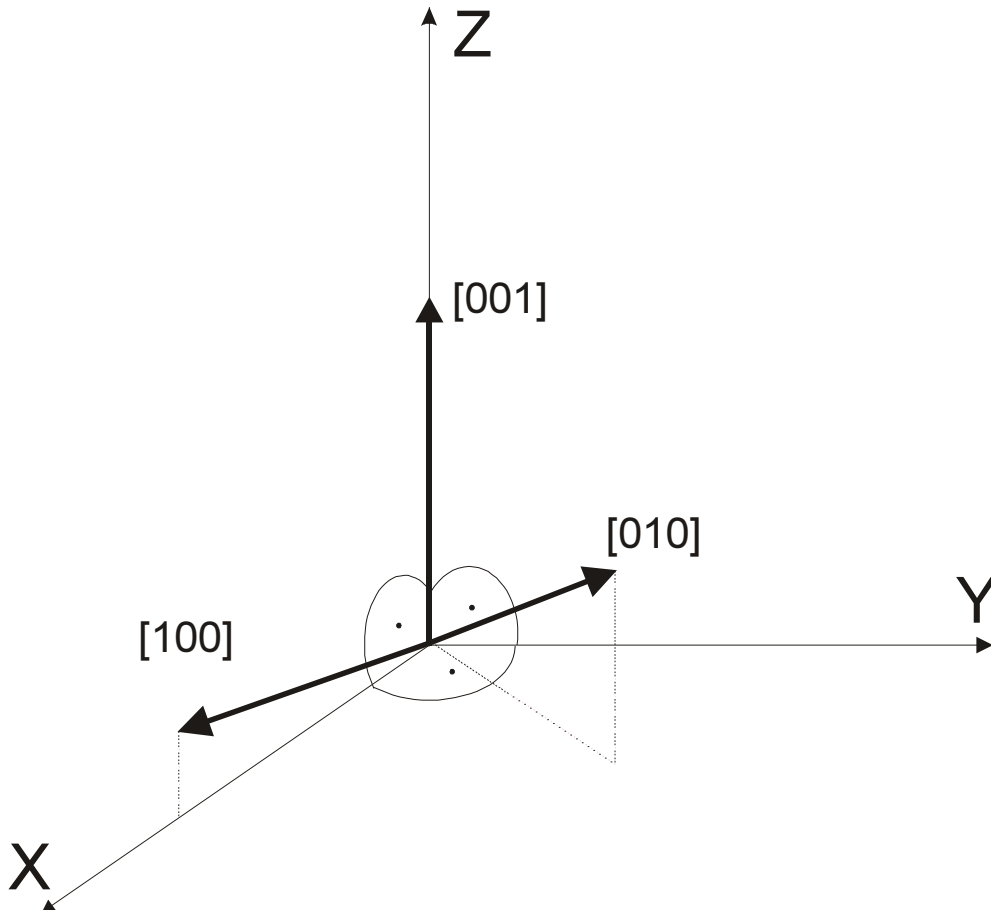


Figure 1

LaboTex uses 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. 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.

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

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

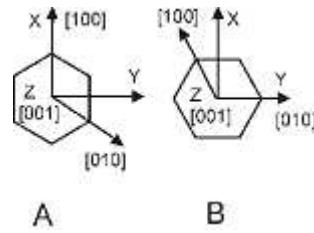


Figure 2

1.4. Representation of Orientations by Euler Angles.

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

- the crystal coordinate system is rotated by ϕ_1 angle around Z axis of the sample coordinate system,
- and next by Φ angle around X axis (in new position) of the crystal coordinate system,
- and finally by ϕ_2 angle around Z axis of the crystal coordinate system,

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 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 reduced basic range. The Euler angle space can be reduced because of the crystal and sample symmetries. Boundaries of the basic range of ODF in the Euler space and symmetry structure code used by LaboTex are collected in table below:

Symmetry		Cubic**		Hexagonal		Tetragonal		Trigonal		Ortho- rhombic	Mono- clinic	Triclinic
		O	T	D ₆	C ₆	D ₄	C ₄	D ₃	C ₃	D ₂	C ₂	C ₁
LaboTex structure code		7	6	11	10	5	4	9	8	3	2	1
ϕ_1	triclinic* (C ₁)	360°	360°	360°	360°	360°	360°	360°	360°	360°	360°	360°
	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°	180°
ϕ_2	90°	180°	60°	60°	90°	90°	120°	120°	180°	180°	180°	360°

* - sample symmetry

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

*** - for any ϕ_1 angle

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

1.7. Pole Figures

The experimental pole figures are obtained in X-ray and neutron measurement. LaboTex pole figures processing comprises the correction of pole figures on account of their defocusing and background, as well as preliminary normalization and the possibility of different kinds of symmetrization. ODF calculation from pole figures is the one of the main aim of the LaboTex program. Experimental pole figures are unnormalised i.e. measured intensities depend on type of X-ray or neutron source, type of a counter, collimating system, absorption properties of measured material and so on. So, experimental pole figures can not be comparable to each other. Only in ODF calculation process pole figures can be correctly normalized. Pole figures used in LaboTex program are of three types from point of view of normalization:

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

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

1.8. The ODF Calculation

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

- ODF calculation from Pole Figures by the ADC method [1-10]. The algorithm of the ADC method used in the program has been verified on a big number of model and experimental data. The results were published in many papers and proceedings (see - ADC Method References). The LaboTex program reproduces the orientation distribution function with 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 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

Texture index and definitions of fit error RP (controlling the iteration procedure of ODF calculation) are:

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

where :

f^2 – texture index,

$f(g)$ – value of ODF,

g – orientation,

G - orientation space.

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

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. Volume fraction of components

The volume fraction of each components, g , you can calculate by integrating over the appropriate subvolume in 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 $dg = \sin\Phi d\Phi d\phi_1 d\phi_2$

- ϕ_1, Φ, ϕ_2 are Euler angles that parametrize the orientation space.

Fundamentals for calculation of volume fraction of texture components are:

- LaboTex makes integration around 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 exit outside the basic region of ODF space (Euler angles space) LaboTex continues integration in equivalent area of the basic region.

1.10.1 The overlapping problem.

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

- i) Overlapping of integration ranges between symmetrically equivalent positions of component
- ii) Overlapping of integration ranges between different components

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

- "Simple Integration" - overlapping region is multiply integrated. Integration around any single component in full range of basic region gives (100% minus background)*number of symmetrically equivalent position.
- "Singlely Counts in Overlapping Area" - overlapping region is only singlely integrated for component. Integration around any single component in full range of basic region give 100% minus background.
- "Divide by Number of Symmetrically Equivalent Position" - LaboTex integrates for all symmetrically equivalent positions of the components with proper weight equal $1/\text{number of symmetrically equivalent positions}$. Integration around any single components in full range of basic region give 100% minus background.

To solve problem of overlapping of integration ranges between different components LaboTex offers (case ii):

- Total percent of overlapping (overlapping volume fraction) is displayed in special window ("Orientations Overlap"). Overlapping volume fraction can be limited by diminishing integration ranges of texture components.
 1. In case of "Simple Integration" overlapping volume fraction means sum of overlapping between different components and between symmetrically equivalent positions of all overlapped components.
 2. In case of "Singlely Counts in Overlapping Area" overlapping volume fraction means sum overlapping between different components.
 3. In case of "Divide by Number of Symmetrically Equivalent Position" overlapping volume fraction means excessive orientation overlap. Excessive orientation overlap area is defined in the points where sum of weights is greater than 1. The weight is equal to $1/\text{number of symmetrically equivalent positions}$. 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 excessive orientation overlap is the integral of excessive ODF values in mentioned area.
- 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 case of "Simple Integration" and "Singlely Counts in Overlapping Area" ODF values in overlapping areas are divided proportionally to number of symmetrically equivalent overlap orientations.
 2. in case of "Divide by Number of Symmetrically Equivalent Position" excessive ODF values in overlapping areas are divided among components proportionally to the weights and to number of symmetrically equivalent overlapping orientations.

1.11. 2D and 3D Graphics

The program includes on-screen graphic presentation of calculated ODFs, PFs and INVs in the form of contour levels (isolines) shown in 2D and 3D spaces. 3D objects plotted on the screen

are optionally increased, decreased, shifted, rotated and animated. Up to 100 PFs or INVs can be presented in one window. In Compare Mode the same kind (PFs vs PFs, or INVs vs INVs, or ODFs vs ODFs), or a different kind (PFs vs ODFs, PFs vs INVs, INVs vs ODFs) of objects can be shown in two separated windows.

1.12. Qualitative and Quantitative Texture Analysis

Identification of the orientation using cursors, giving their parameters in Euler angles and Miller indices can be done on the PF and ODF. Simultaneously identification of the orientation on the different types of objects (PF and ODF) is possible in 'Compare mode'. The Compare mode is very important for education (interdependence of orientations on PF and ODF). The values of PFs and ODFs are shown in the points chosen by the cursor. Orientations are optionally collected by the user in the orientation data base. User can add, edit and delete orientations from the database. Orientations can be entered in form of Miller indices (HKL UVW) or Euler angles (ϕ_1, Φ, ϕ_2). You may write angles or indices of orientation directly into the text windows on the toolbar. You can see the value of intensity for the selected orientation. Value of ODF or/and PF are displayed on the status bar (sums PF value(s) or/and ODF value). Qualitative analysis is very easy: you choose appropriate objects and next press 'SORT' button. You will see the window with assorted orientations from database by PF or ODF. You can also analyse near (HKL)[UVW] orientations by mouse click in selected point on the pole figure or ODF projection. "Near orientations" can be sorted by PF or ODF values, Miller indices or distance. Program includes on-line quantitative analysis of volume fraction of texture components (orientations).

1.13. 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

The LaboTex program may be executed in either Windows 95/98/NT/Me/2000/XP.

Minimal requirements:

Processor PENTIUM 200MHz, 64 MB RAM, 100 MB HD space, graphic card resolution 800x600, CD-ROM drive.

Recommended system configuration:

Processor PENTIUM IV/1GHz or higher, 1 GB HD space, 192 MB RAM, graphic card resolution 1024x768+OPNGL, CD-ROM drive. In case data are measured in the grid less than 5x5 degrees, double increase of the disk space is recommended.

2.2. Installation

To install LaboTex, follow these directions:

1. Switch off the computer.
2. Install the protect key in a parallel (printer) port.
3. Switch on the computer.
4. Note: If you use Windows NT/2000/XP Operating System, you have to be logged in as an "Administrator" when installing LaboTex
5. Insert the LaboTex CD-ROM. Then select Run... from the Start menu,
6. enter D:Setup.exe, and click OK. (or x:Setup where x – is a letter describing CD-ROM drive in your PC)
7. Read the Welcome screen, then click Next. The Software License Agreement is displayed.
8. Read the Software License Agreement and click Next.
9. Specify a directory to install LaboTex (use short name e.g. LaboTex2 in main directory),
10. then click Next.
11. Verify that the settings are correct, then click Next (or use the Back button if you need to
12. go back and make changes).
13. LaboTex is installed in the destination directory, and you are prompted whether or not
14. to view the README file. Click Yes.
15. Install protect key driver: from LaboSoft folder run "HASP Protect Key Installation"
16. application!
17. Start LaboTex from LaboSoft folder.

2.3. Configuration

The first time you run LaboTex, you should edit some of the configuration options in order to optimize workshop.

Select "LaboTex Options..." from the Edit Menu.

The fields you need to review are:

- Temporary Directory
- Experimental Data Directory (EPF and other)
- Correction Data Directory (COR)

You can set other initial (default) options.

3. LaboTex Objects and Object Containers

3.1 Introduction

Pole figures and orientations distribution functions (ODF) are LaboTex objects. Figure 3 shows diagram of creating objects, calculation and analysis in LaboTex program.

Labotex operates on 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, Orientation Distribution Function container :

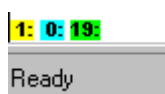
No	Container	Objects	Color
1	Pole Figures Container	CPF, NPF, RPF, APF	yellow color
2	Inverse Pole Figures Container	INV	blue color
3	Orientation Distribution Function container	ODF	green color

Exclusively the objects from one container can be shown at the same time in the single window. Objects from two containers can be shown simultaneously only in compare (double windows) mode (see: Compare Window Mode). To add or delete object from container click proper button on the object toolbar:

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

Numbers of objects in containers are indicated in the left bottom corner of the window (yellow color number for pole figures container, blue color number for inverse pole figures and green color number for orientation distribution function container). One projection only can be in container of the ODF objects simultaneously. For ODF container, the number indicates the number of 2-D ODF sections. Number of objects in specific container is presented in the left bottom corner of the window (yellow color numbers for pole figures container, blue color numbers for inverse pole figures and green color numbers for orientation distribution function).

In the following example Pole Figures Container contains 1 pole figure, Inverse Pole Figures



Container is empty (0 INV object), Orientation Distribution Function container contains ODF projection which has 19 2-D ODF sections

Objects Creations, Calculations and Analysis in LaboTex Program

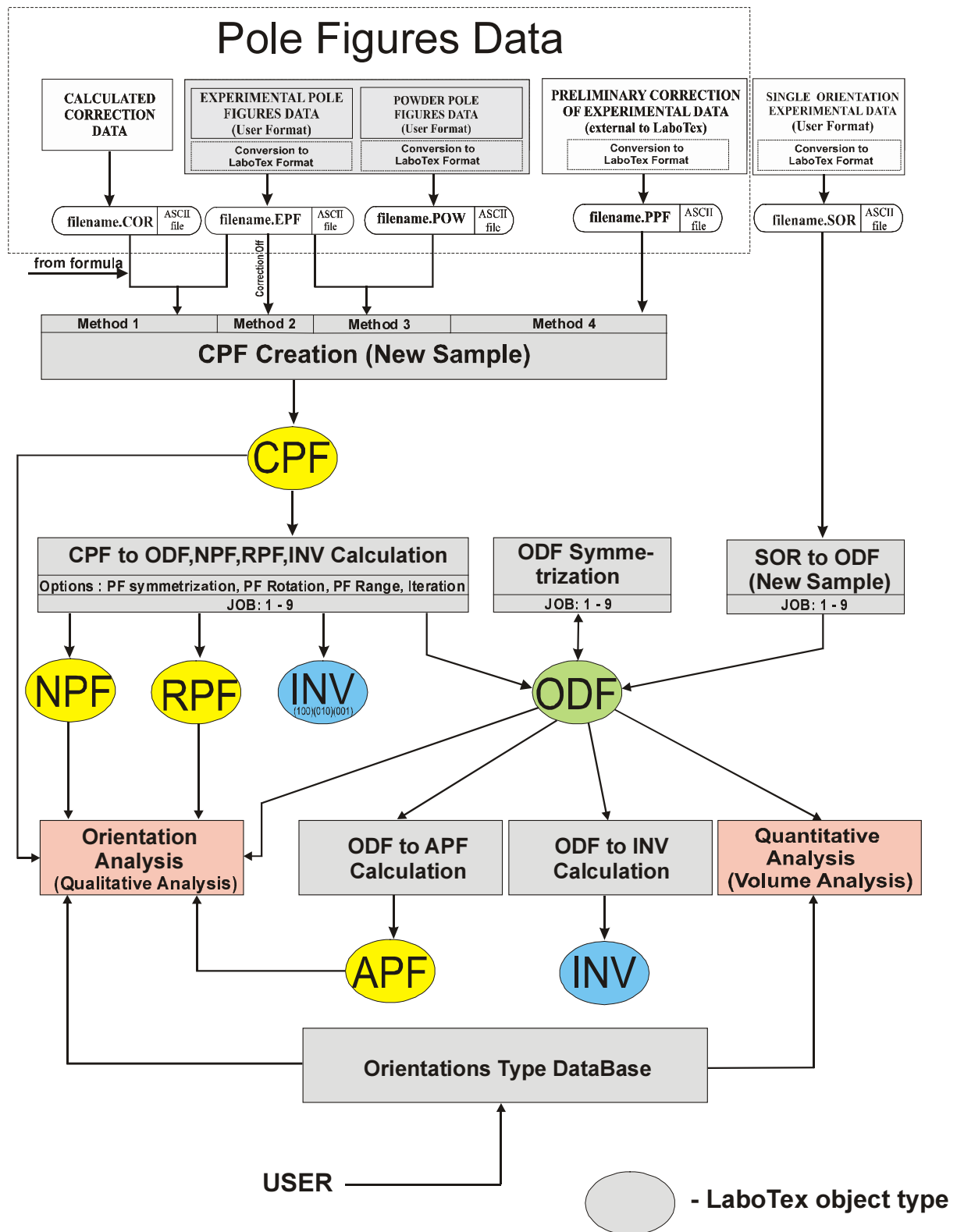



Figure 3

For the ODF objects only one projection ϕ_1 or ϕ_2 or Φ can be stored in container simultaneously. To add or delete objects from containers, click proper button on the object toolbar (for the pole figures container and 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 current session in Edit Menu – Arrangement.

To delete all objects in containers use "Clear All" Command in Edit Menu or  from toolbar.

3.2 LaboTex Objects Types

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

- i - unnormalised : EPF
- ii - approximately normalised : CPF
- iii - precisely normalised: NPF, RPF, and APF


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

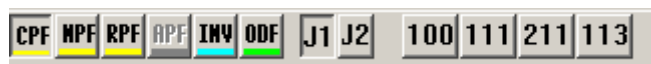
All comparisons between pole figures should be done inside pole figures of type iii.

Quantitative analysis can be made by the means of normalised pole figures.

3.2.1 CPF - Corrected Pole Figures

Experimental pole figures obtained from X-ray or neutron diffraction are unnormalised i.e. measurement intensities depend on type of X-ray or neutron source, type of a counter, colimating system, absorption properties of measured material and other. So, experimental pole figures can not be comparable to each other. Only in ODF calculation process pole figures can be correctly normalized.

Corrected Pole Figures (CPF) are corrected (according to background and de-focussing) and only **preliminary** normalized experimental pole figures **prepared for ODF calculation**. CPF object should not be used to analysis. CPF objects contain single pole figures of hkl type. To create CPF objects from experimental files, open "New Sample" Window or click the icon of the toolbar : . You can calculate ODF after creating CPF objects and create other objects. To display CPF objects click the CPF button of the object toolbar, next click one or more buttons with hkl indices:

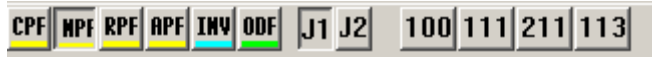


Note: CPF object are the same for all jobs.

3.2.2 NPF - Normalized Pole Figures

Normalized Pole Figures are completely normalized (in ODF calculation process) experimental pole figures. They are correctly normalized and they can be comparable to each other. They are

created after ODF calculation. To display NPF object click the NPF button on the object toolbar, next click one or more buttons with *hkl* indices:



Note: If more than one job are created, choose proper job from job buttons (J1,J2 ..) on the object toolbar.

3.2.3.RPF - Recalculated Pole Figures


Recalculated Pole Figures are calculated from ODF, equivalent to those PFs used as data to ODF reproduction. They are **complete** pole figures.

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



Note: If more than one job is created, choose proper job from job buttons (J1,J2 ..) on the object toolbar.

3.2.4.APF - Additional Pole Figures


Additional Pole Figures, i.e. calculated from the ODF pole figures of HKL types which were **not used for ODF determination**. APF objects contain collection of a single additional pole figure. To calculate additional pole figures (APF) open "ODF to APF" dialog from "Calculation menu" or click the button  from the toolbar.

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



Note: If more than one job is created, choose proper job from buttons (J1,J2 ..) on the object toolbar.


3.2.5.INV - INVerse pole figures

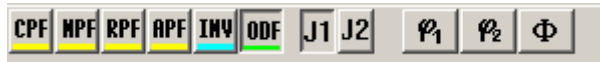
INVerse pole figures are calculated from the ODF. Inverse pole figures object, INV object, contains collection of a single inverse pole figure of XYZ types. INV objects: (100),(010) and (001) are ever created after ODF calculation. To calculate other inverse pole figures (INV) open "ODF to INV" dialog from "Calculation menu" or click the button  from the toolbar. To display an INV object click the INV button on the object toolbar, next click one or more buttons with XYZ indices:



Note: If more than one job is created, choose proper job from job buttons (J1,J2 ..) on the object toolbar.

3.2.6.ODF - Orientation Distribution Function

Orientation Distribution Function 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 "CPF to ODF,NPF,RPF,INV" dialog from "Calculation menu", "SOR to ODF" or click the button  from the toolbar. The ODF objects are 2-D ODF projections: ϕ_1 , ϕ_2 and Φ . To display ODF object click ODF button on the object toolbar, next click the button with ODF projection:



Note: If more than one job is created, choose proper job from job buttons (J1,J2 ..) on the object toolbar.

3.3. Example CPF, NPF, RPF objects

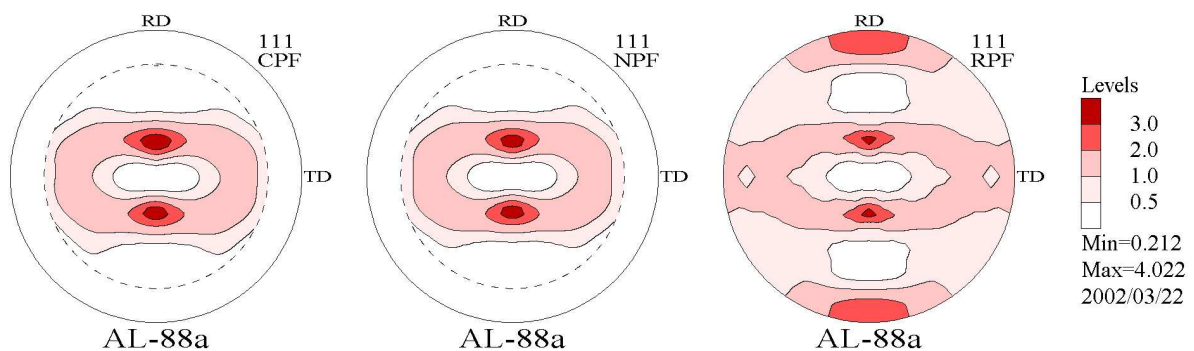
In this example:

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).



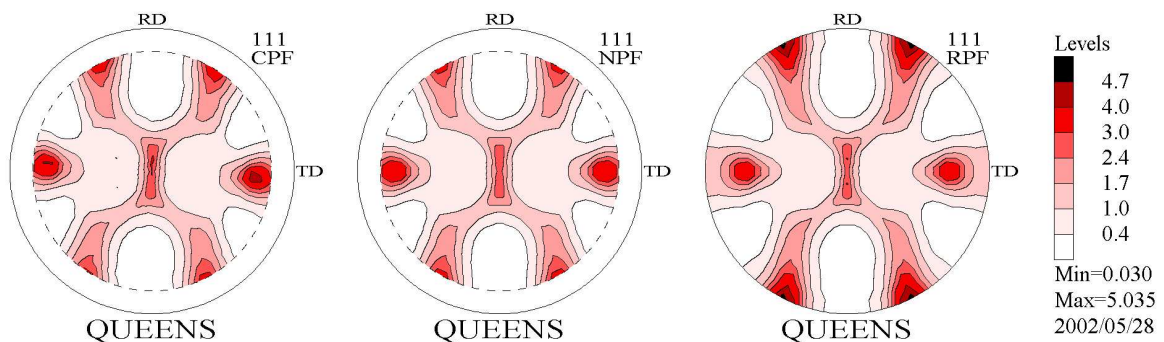
In this example:

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).



3.4. LaboTex Jobs

Second and next calculation of ODF from the same sample creates new job. If more than one job is created, choose proper job from job buttons (J1,J2 ..) on the object toolbar. New job is also created when you make ODF symmetrization.

Job buttons:



Note: Maximal number of jobs = 9

4. LaboTex Formats

4.1. EPF file format

It needs correction file: COR or POW

Experimental Pole Figures, i.e. raw experimental data and their background.

Description of *filename.EPF* data format:

Line	No of data in line	Description	Type
1 – 2		Arbitrary title	Character
3		Remarks for data in line 4	
4	1	Structure Code (symmetries after Schoenflies): 1 - C ₁ (triclinic) 2 - C ₂ (monoclinic) 3 - D ₂ (orthorhombic) 4 - C ₄ (tetragonal) 5 - D ₄ (tetragonal) 6 - T (cubic) 7 - O (cubic) 8 - C ₃ (trigonal) 9 - D ₃ (trigonal) 10 - C ₆ (hexagonal) 11 - D ₆ (hexagonal)	Integer
4	2	Lattice constant, a (absolute or relative)	Real
4	3	Lattice constant, b (absolute or relative)	Real
4	4	Lattice constant, c (absolute or relative)	Real
4	5	Lattice angle, α in degrees	Real
4	6	Lattice angle, β in degrees	Real
4	7	Lattice angle, γ in degrees	Real
5	1	Number of Pole Figures (including background PFs) (N)	Integer
6		Remarks for data in line 7	Character
7 to 7+N	1	2 θ Bragg angle in degrees	Real
7 to 7+N	2	α_s - beginning of polar angle in degrees	Real
7 to 7+N	3	α_e - ending of polar angle in degrees	Real
7 to 7+N	4	$\Delta\alpha$ - step of polar angle in degrees. Permissible value: 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
7 to 7+N	5	β_s - beginning of azimuthal angle in degrees (0 or 2.5)	Real Positive values for pole figures drawn clockwise or negative values for counter-clockwise
7 to 7+N	6	β_e - ending of azimuthal 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 azimuthal angle in degrees . Permissible values: 1.0, 1.2, 1.25, 1.5, 2.0, 2.5, 3.0, 3.75, 5.0, 6.0, 7.5, 10.0. for textured pole figures, and the same values or multiplicity of above-mentioned values for background PFs	Real Positive values for pole figures drawn clockwise or negative values for counter-clockwise
7 to 7+N	8	Index - must be 0	Real
7 to 7+N	9	Index <i>h</i> of <i>hkl</i> pole figure	Integer
7 to 7+N	10	Index <i>k</i> of <i>hkl</i> pole figure	Integer
7 to 7+N	11	Index <i>l</i> of <i>hkl</i> pole figure	Integer
7 to 7+N	12	Type of Data (1-Pole Figure, 0-Background)	Integer
7+N+1		Blank line	
7+N+2	1 to 8	Data 1 to 8 (1 st Pole Figure)	Real
7+N+3	1 to 8	Data 9 to 16 (1 st Pole Figure)	Real
7+N+4 to end of data for 1 st PF	1 to 8	Data for 1 st Pole Figure	Real
...		Blank line (separates block of data)	
...	1 to 8	Data for 2 nd 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

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 also: EPF Example, COR file format , POW file format , PPF file format , SOR file format.

4.2. EPF Example

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

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

See also: EPF file format , COR file format , POW file format , PPF file format , SOR file format .

4.3. PPF file format

filename.PPF - Preliminary Corrected Pole Figures^K i.e. experimental data after the background and de-focussing effects corrections using procedures external to LaboTex program.

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

See also: EPF file format, COR file format, POW file format , SOR file format .

4.4. SOR file format

filename.SOR – Single ORientation File i.e. experimental, single orientation set in LaboTex format

Description of *filename.SOR* data format:

Line	No of data in line	Description	Type
1 - 2		Arbitrary title	Character
3		Remarks for data in line 4	
4	1	Structure Code (symmetries after Schoenflies): 1 - C ₁ (triclinic) 2 - C ₂ (monoclinic) 3 - D ₂ (orthorhombic) 4 - C ₄ (tetragonal) 5 - D ₄ (tetragonal) 6 - T (cubic) 7 - O (cubic) 8 - C ₃ (trigonal) 9 - D ₃ (trigonal) 10 - C ₆ (hexagonal) 11 - D ₆ (hexagonal)	Integer
4	2	Lattice constant, a (absolute or relative)	Real
4	3	Lattice constant, b (absolute or relative)	Real
4	4	Lattice constant, c (absolute or relative)	Real
4	5	Lattice angle, α in degrees	Real
4	6	Lattice angle, β in degrees	Real
4	7	Lattice angle, γ in degrees	Real
4	8	Step for output ODF (grid cells). Permissible values (deg): 1.0, 1.2, 1.25, 1.5, 2.0, 2.5, 3.0, 3.75, 5.0, 6.0, 7.5, 10.0*	Real
4	9	Weight for data (1 – present, 0 – absent)	Integer
4	10	Angle Unit: 0 – deg, 1 – rad	Integer
4	11	Angle Convention: 0 – Bunge 1 – Roe	Integer
5 to the end	1	ϕ_1	Real
5 to the end	2	Φ	Real
5 to the end	3	ϕ_2	Real
5 to the end	[4]	Weight (optionally) (if parameter <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 also: EPF file format, COR file format, POW file format , PPF file format.

4.5. POW format

filename.POW - **POW**der 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 help to find out the absorption curve for defocusing correction.

The structure of file **filename.POW** is identical to the **filename.EPF**.

See also: EPF file format, COR file format, SOR file format , PPF file format.

4.6. COR format

filename.COR - **COR**rection coefficients for the de-focussing effect.

File contains set of correction coefficients for the de-focussing effect.

Description of **filename.COR** data format:

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

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

See also: EPF file format, PPF file format, SOR file format, POW file format.

4.7. Other formats

List of the compatible LaboTex data formats:

- **'TSV'** Single Orientations Files,
 - Single orientations data files: *.tsv (input from "Choose Experimental Data" list)
- **'PLF'** Queens Univ. PF Format files (4*5deg) - (corrected pole figures),
 - Pole figures data files : *.plf (input from "Choose Experimental Data" list)
- **'PLF'** 5*5deg - (corrected pole figures),
 - Pole figures data files : *.plf (input from "Choose Experimental Data" list)
- **'CON'** McGill University PF Format files - (corrected pole figures),
 - Pole figures data files : *.con (input from "Choose Experimental Data" list)
- **'HKL'** HKL - Kawasaki KTEC Format files - (corrected pole figures),
 - Pole figures data files : *-hkl. (input from "Choose Experimental Data" list)
- **'hkl'** AGH main format,

- Pole figures data files : *.hkl (input from "Choose Experimental Data" list)
- Background pole figures data files: *-b.hkl (input from "Choose Experimental Data" list)
- Random(powder) pole figures data files: *-p.hkl (input from "Choose Experimental Data" list)
- Background random(powder) pole figures data files: *-t.hkl (input from "Choose Experimental Data" list)
- 'xfb' AGH second format (corrected pole figures),
 - Pole figures data files : *.xfb (input from "Choose Experimental Data" list)
- 'CTF' HKL Single Orientations Files,
 - Single orientations data files: *.CTF (input from "Choose Experimental Data" list)
- 'SNG' TSL Single Orientations Files,
 - Single orientations data files: *.sng (input from "Choose Experimental Data" list)
- 'TXT' HKL Single Orientations Files,
 - Single orientations data files: *.txt (input from "Choose Experimental Data" list)
- 'UXD' (file version 1) - BRUKER D-8 Discover (corrected pole figures - ASCII files). 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 (input from "Choose Experimental Data" list)
- 'UXD' (file version 2) - BRUKER GADDS (corrected pole figures - ASCII files). 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 (input from "Choose Experimental Data" list)
- 'HKL' Chalk River Neutron Diffraction Data (corrected pole figures)
 - Pole figures data files: *.* (input from "Choose Experimental Data" list)
- 'ANA' - EMSE Format files (corrected pole figures)
 - Pole figures data files: *.ana (input from "Choose Experimental Data" list)
- 'epf' - popLA PF Format files (corrected pole figures). Warning: Files in popLA format have the same extension as LaboTex files: "EPF". Select "epf" (small letter!!!) data format in LaboTex Options for files in popLA format.
 - Pole figures data files: *.epf (input from "Choose Experimental Data" list)
- 'RAW' - popLA Format files
 - Pole figures data files: *.raw (input from "Choose Experimental Data" list)
 - Defocussing correction data files: *.dfb (input from "Choose Defocussing Correction" list)

- 'ASC' - Rigaku ASC format (1PF/file)
 - Pole figures data files: *.asc (input from "Choose Experimental Data" list)
 - Random(powder) pole figures data files: : *.asc (input from "Choose Defocussing Correction" list)
- 'XPF' - BEARTEX data format (corrected pole figures)
 - Pole figures data files: *.xpf (input from "Choose Experimental Data" list)
- 'PFG' - RIST data format from RIGAKU (ASCII)
 - Pole figures data files: *.pfg (input from "Choose Experimental Data" list)
 - Random pole figures data files: *.pfg (input from "Choose Defocussing Correction" list)
- 'TXT' - RIST data format from PHILIPS (ASCII- corrected pole figures)
 - Pole figures data files: *.txt (input from "Choose Experimental Data" list)
- 'RW1' - PHILIPS X'Pert binary data format (Binary)
 - Pole figures data files: *.rw1 (input from "Choose Experimental Data" list)
 - Background pole figures data files: *.bgr (input from "Choose Experimental Data" list)
 - Defocussing correction data files: *.cor (input from "Choose Defocussing Correction" list)
- 'NJA' - Seifert ASCII data format
 - Pole figures data files: *.NJA (input from "Choose Experimental Data" list)
 - Random pole figures data files: *.NJA (input from "Choose Defocussing Correction" list)

4.8. How make given format accessible for LaboTex

To make format accessible for creation of CPF files you should:

- a) select EDIT menu in LaboTex
- b) select LaboTex Options
- c) select Data Formats
- d) select name of format from selection windows 4 -7

You may use several files simultaneously:

in "New Sample" dialog box select (click mouse) several files simultaneously holding CTRL (control) key.

If extensions of files with data differ from higher indicated please to change it.

For example: (case RW1 format) background pole figures data files have a COR extension as default which is the same as defocussing correction data files. Change extension of background pole figures data files to BGR before input to LaboTex.

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5. LaboTex - Frequently Asked Questions (FAQ)

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

A: Yes, you can use incomplete pole figures without any problem.

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 in your case.

A: In demo version we have not used the background values but, on the whole, if you check the structure of EPF file (see HELP menu) you will notice that LaboTex program 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: The LaboTex program calculates ODF for all crystal symmetries. You can use whichever you wish.

Q: Max 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. measured intensities depend on type of X-ray source, type of a counter, colimating system, absorption properties of measured material and so on. So, pole figures from X-ray machine can not be comparable to each other. Only in ODF calculation process pole figures can be normalised.

Pole figures used in LaboTex program are of two types:

I - approximately normalised : .CPF

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

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

Q: Does the accuracy, or I can say 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, accuracy of different texture components does not depend on the type of texture component in calculation by ADC method (LaboTex program).

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

A: The algorithm used in LaboTex program is different from the WIMV method. In Labotex program is used

an original ADC algorithm. Similarities in WIMV and ADC methods:

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

series methods

2) both use iteration procedures

Differences between ADC and WIMV methods:

1) different principles of the iteration procedure

2) different principles of "ghosts" correction

See:

1) 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.

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

3) "... 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

4) Principles of the ADC method are described in the reference papers: see → The ADC Method References

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 $\{554\}\langle 225 \rangle$ and I can calculate these angles if I know what to look for, but its very tedious to index some higher order reflections by guessing what they might be and then calculating the angles- checking, reguessing, calulating... I would like a program which takes inputs of Euler angles and lists the closest $\{hkl\}\langle uvw \rangle$ 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 may doing it simulatonously!

Q: What indices I should use for hexagonal symmetry?

A: In case of hexagonal symmetry you should transform $\{hkil\}$ ---> $\{hkl\}$ by excluding indice $\{i\}$! e.g.: $\{01-11\}$ to $\{011\}$;

- for pole figure, if first or second indice 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.

e.g. $\{-2110\}$ to $\{11-20\}$ and final $\{110\}$;

- for crystal directions $\langle uvw \rangle \implies \langle UVW \rangle$ please calculate:

$$U=u-t$$

$$V=v-t$$

$$W=w$$

e.g. $\langle 11-20 \rangle$ to $\langle 330 \rangle$ and final $\langle 110 \rangle$;

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

$$\{0,1,-1,1\} \langle 2,-1,-1,0 \rangle \implies \{0,1,1\} \langle 1,0,0 \rangle$$

Q: The format of the raw data as we get 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 absent in LaboTex (see: Edit --> LaboTex Options ---> Data Formats),

I have two suggestions:

I) Please, take a look at the description of data file structure in the HELP menu of LaboTex Demo. See the "LaboTex Format of Experimental Data" option and the examples of Filename.EPF , Filename.COR and Filename.POW

Then you can transform your data to EPF and COR type format.

or:

II) 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)

Q: Can I create CPF file myself? We would like to calculate the 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 complicated structure. So I give you another suggestions:

I - You can make your special data as a 'PPF' file (please, check in help). This file does not include background data and you do not need to use .COR file.,

or

II - You can use your special pole figures as 'EPF' file including at the end of file the proper number of "0" values for the beckground for each pole figure. Remember to add the lines

describing data (at the beginning of the file) for each pole figure background. In that case you need to make a 'COR' file including correction coefficients as "1".

Q: What should I do to read Rigaku data?

A: For Rigaku data files, please remember:

- 1) use only one pole figure in one file,
 - 2) extension of file has to be ASC (for example: 53110.ASC, 53200.ASC, 53211.ASC)
 - 3) to make ASC files accessible for creation of CPF files you should:
 - I) select EDIT menu in LaboTex
 - II) select LaboTex Options
 - III) select Data Formats
 - IV) select "ASC - Rigaku ASC format (1PF/file)" in one of "selection windows" 4 - 7then
 - 4) select "new sample" (from File menu or third icon from toolbar),
select "ASC" data format, if you do not use defocusing correction,
please select "off" for "Correction"
 - 5) select ASC pole figures files by the mouse clicking
 - 6) select the proper crystal symmetry for your sample
-

Q: Could you please let me know whether Labo Tex for Windows could be used for files generated with Bruker equipment?

A: Yes (File version 1 and 2). Use only one pole figure in one file (files extension: UXD). "_sample" has to contain Miller indices of PF (in triangle brackets) for example: "Ir<111>".

Q: When using ASC format only one PF file can be input and other APF can be calculated by the soft. Is that meant that it is not necessary to measure other PFs experimentally? Can I input other PF such as 200 and 112, besides the 110 in BCC structure? But 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 "New Sample" dialog box select (click mouse) ASC files simultaneously holding CTRL (control) key!!!. Calculation ODF from one PF not ever is enough!. If it is possible you should use more PF.

Q: Do you have any simple way to transfer the ASC into EPF format, with 8 columns?

A: When you create CPF file from ASC files LaboTex convert ASC files to the EPF/POW or PPF files. This files you can find in LaboTex temporary directory (e.g C:\Labotex2\user\username.LAB\tmp...)

Q: As for the background data, I find no way to input to the file when a ASC has been input. Can the background data only be used in the EPF format?

A: Usually measured pole figures must be corrected according to the background and defocusing absorption. So, you should measure these values for your samples. These both corrections of raw pole figures data, sometimes are done by software of experimental x-ray device (especially in the case of using PSD-Position Sensitive Detector). You should check what case is in your x-ray device ? Inside the ASC file format you can find two places in which the background values can be included. Please find the lines with words: *LOW , *HIGH. In these places there are zero values in your files. You should decide if this is correct or you must read the manual of your x-ray device to find out 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 in inputting the data?

A: To defocus correction you should measure the pole figures of the powder sample (from the same material as the "textured samples" - in your case steel). The powder sample is treated as "non texture" sample, which help to find out the absorption curve for defocusing correction. The files of the powder sample should have extension POW (LaboTex format) or ASC (Rigaku format), and should be included in COR directory (for proper user) of LaboTex. In your case of the steel samples you should choose the O-cubic symmetry. All symmetries are indicated according to the Schoenflies symbols (International Tables for Crystallography - ed.T.Hahn - 1983, D.Reidel publishing company. Dordrecht/Boston).

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

A: Yes.

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

A: Yes.

Q: What does "Azimuthal angle steps different for pole figures. Pole figures {1 1 0}. ... CPF file will not be created." mean?

A: In actual version of LaboTex (2.0,2.1) the step of polar angle (alpha) has to be equal the step of azimuthal angle (beta) (permissible values: 1.0, 1.2, 1.25, 1.5, 2.0, 2.5, 3.0, 3.75, 5.0, 6.0, 7.5, 10.0). In your case these angle steps are different: 2.0 and 5.0. You should measure with the grid of the same alpha and beta steps. Only in the case of background data, alpha step can be different than beta step. But the alpha step for the texture data and the alpha step for the background must be equal !

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

A: This option is in version 2.1 (menu File-->ODF export). Upgrade version 2.0 to 2.1 is free of charge by e-mail.

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:

I) select EDIT menu in LaboTex

II) select LaboTex Options

III) select Data Formats

IV) select "EPF - popLA EPF files format" in one of "selection windows"

V) select "new sample" (from File menu or third icon from toolbar),

VI) select "epf" (small letter!!!) data format (in this format data are after correction)

VII) now select your data file by the mouse clicking

VIII) select the proper crystal symmetry for your sample

Q: How does LaboTex define sample and coordinate system?

A: LaboTex convention (from the version 2.1.006):

1) X,Y,Z axis 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 paralel 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 should be :{38,43,30} (Zr Alloy - hexagonal system).

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

(there is the possibility of the choice of the axial convention in hexagonal system in LaboTex from version 2.1.008 !!!)

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

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

Q: When I run the HASP Protect Key Instalation from the windows system,

a message apears :

"user has no access to the database registry 0x20 10000 0x0 0x0"

and the installation is stopped.

A: Before installation of the HASP Protect Key on NT/2000/XP system you should:

- 1) Switch off your PC with Win NT/2000/XP system.
- 2) Install HASP Protect Key to the parallel printer port in PC.
- 3) Switch on your PC with Win NT/2000/XP system.
- 4) Very important !!! Login to the NT/2000/XP system as Administrator.
- 5) As Administrator install HASP device driver. Remember to reboot the computer after complete HASP installation.
- 6) Now, you can login every time to the NT/2000/XP system as a ordinary user and run Labotex program.

6. References

1. K.Pawlik - *phys.stat.sol.(b)* 134 (1986), p477, "Determination of the Orientation Distribution Function from Pole Figures in Arbitrarily Defined Cells"
2. K.Pawlik, J.Pospiech - Proc. of Int. Workshop, Clausthal-Zellerfeld, Germany, (1986), p127
3. K.Pawlik, J.Pospiech, K.Lucke - Proc. of ICOTOM-8, Santa Fe, USA, (1987), p105, "The Development of a New Direct Method of ODF Reproduction From Pole Figures and its Testing with the Help of Model Functions"
4. K.Pawlik, W.Truszkowski, J.Pospiech, T.Pawlik - Proc. of ICOTOM-8, Santa Fe, USA (1987), p531
5. K.Pawlik, J.Pospiech, K.Lucke - Proc. of ICOTOM-9, Avignon, France, (1990), p25, "The ODF approximation from pole figures with the aid of the ADC-method".
6. K.Pawlik - Proc. of EPDIC-2, Enschede, The Netherlands, (1992), p151
7. K.Pawlik - Proc. of ICOTOM-10, Clausthal-Zellerfeld, Germany, (1993), p401
8. K.Pawlik, P.Ozga: LaboTex: The Texture Analysis Software, 'Göttinger Arbeiten zur Geologie und Paläontologie', SB4, 1999.
9. 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
10. H.R.Wenk, K.Pawlik, J.Pospiech and J.S.Kallend - 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 (1994), p233-260.
11. U.F.Kocks, C.N.Tome, H.R.Wenk, "Texture and Anisotropy", Cambridge University Press

The Calculation of the Volume Fraction of Texture Components - reference :

8. J.W.Flowers, "Volume Fractions of Texture Components of Cubic Materials", *Textures and Microstructures*, 1983, Vol.5, pp. 205-218, "A method for obtaining volume fractions in regions about ideal texture components of cubic materials by integration of the orientation distribution function is described".

7. LaboTex: Technical specifications

Item		Comments
Full Windows application from version 2.0.	YES	Windows 95 - OSR2/98/Me/NT 4/2000/XP.
Management of data and results.	YES	Simple access to data and results. Collecting them for 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	
The fiber texture analysis.	YES	
High resolution ODF option.	YES	
Calculation of fit error (RP).	YES	
Calculation of texture index.	YES	
ODF calculation report.	YES	Every 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 input data in 25 data formats.
The possibility accomodation of the Software to the Customer data format.	YES	Free of charge
Correction for defocussing using powder pole figures.	YES	
Correction for defocussing from correction coefficients.	YES	
Correction for defocussing from Schulz equation.	YES	
Input data in any grid.	No	Only: 1x1, 1.2x1.2, 1.25x1.25, 1.5x1.5, 2x2, 2.5x2.5, 3x3, 3.75x3.75, 5x5, 6x6, 7.5x7.5, 10x10 degrees and extra: 1.8x1.8, 2.25x2.5, 3.6x3.6, 4.5x4.5 but with exceptions: trigonal and hexagonal crystal lattice symmetry.
Maximal/minimal value of Miller indices H,K,L for input PF	9/-9	

Item		Comments
ODF calculation from incomplete pole figure(s).	YES	
Information about too small number of data to ODF calculation.	YES	During ODF calculation.
Possibility of the ODF calculation for different parameters for the same sample.	YES	Up to 9 job for sample.
Choice of the symmetrization of pole figures before ODF calculation.	YES	Viewing of symmetrized PF.
Choice of the sample symmetry for ODF (ODF symmetrization).	YES	Available after ODF calculation.
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
Possibility of the rotation of pole figure(s) before ODF calculation.	YES	For all pole figures or separately in range -90 to 90 degrees.
Possibility of the cut off the pole figure(s) in the center before ODF calculation.	YES	For all pole figures or separately. User choose angle ranges.
Possibility of the cut off the pole figure(s) in the edge before ODF calculation.	YES	For all pole figures or separately. User choose angle ranges.
Possibility of change parameters finishing calculation in ODF calculation.	YES	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, model calculation and other.
Roe/Bunge notation of angles in SOR.	YES/YES	Notation chosen by user.
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 sample symmetry after ODF calculation (ODF symmetrization).
Calculation of volume fraction of texture components.	YES	10 components simultaneously.
Choice of integration ranges.	YES	For each Euler angle separately with the viewing.

Item		Comments
The possibility of the evaluation of parameters of component peak.	YES	
The possibility of the choice of the components (volume fraction).	YES	From files or from database.
Possibility of the choice of the method of calculation of volume fraction.	YES	3 methods.
Display of orientation overlapping.	YES	
Correction of overlapping.	YES	Divide ODF among overlapping orientation.
Report from calculation of volume fraction of texture components.	YES	Ready to print or copy.
Orientations database.	YES	100 position for each crystal system.
Introduce orientations to database in Miller indices ($\{HKL\}\langle UVW\rangle$).	YES	
Maximal/minimal value of Miller indices H,K,L,U,V,W for orientation $\{HKL\}\langle UVW\rangle$	15/-15	
Introduce orientations to database in Euler angles.	YES	
Introduce fiber orientations to database.	YES	
Display of orientation from database on the ODF and PF(s).	YES	The choice from combobox, Automatic mode, Next, Previous
Display of symmetrically equivalent position on the ODF and PF(s).	YES	The choice from combobox or from listbox.
Presentation of symmetrically equivalent position.	YES	In basic region for ODF and full Euler space for PF, in Miller indices and Euler angles.
On-line identification of the orientations.	YES	in Euler angles and Miller indices, ODF and pole figures (exclude IPF). In cursor position.
Help in finding of near orientations.	YES	Near orientation sort by: PF/ODF, Miller indices, distance.
Compare orientation analysis. Important for educational purpose!	YES	LaboTex shows simultaneously orientation on: ODF and ODF (the same and different projection), ODF section and ODF, pole figure(s) and ODF, pole figure and ODF section.
Shows ODF/PF values using mouse.	YES	For PF LaboTex shows sum PF values under poles of orientation and separately for in option SORT.
Qualitative orientations analysis for PF/ODF.	YES/YES	Sorted orientations from database.
Report from qualitative analysis.	YES	Only for ODF. Ready to print and copy.

Item		Comments
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.
Export of ODF as ASCII files.	YES	
Export of Pole Figures as ASCII files.	YES	
Export of Inverse Pole Figures as ASCII files.	YES	
Choice of convention for hexagonal system.	YES	
2D and 3D pole figures presentation.	YES	
Choice of pole figures presentation convention	NO	Only clockwise rotation from the NS direction.
Maximal number of pole figures/inverse pole figures on the window.	100	
Pole figures descriptions.	YES	HKL,sample name,directions (3 characters, edited by user), type of figure. (CPF,RPF,NPF,APF)
Pole figures descriptions turn off.	YES	Separately for each description kind.
Fill option in 2D/3D presentation.	YES/NO	3 isoline mode in fill option: normal/black/white.
User defined sets of colors.	YES	15 sets.
Isoline mode.	YES	3 mode. Automatic, manual, from user defined sets.
The possibility of change parameter of pole figures presentation.	YES	Number of isoline (maximal 14), color, color set, value, fill.
2D ODF presentation for Phi1, Phi and Phi2 projections.	YES	
2D ODF presentation for section of projection.	YES	
Bunge definition of 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/NO	Fill and orientation analysis is non-active for this option.

Item		Comments
The possibility of the save of the set of isolines.	YES	color,value and activity.
Export 2D and 3D images as bitmap.	YES	BMP or TIF format.
Export 2D and 3D images by the clipboard.	YES	Bitmap or EMF.
Possibility of the choice of the resolution of the exported image.	YES	
Online help.	YES	
Manuals/Technical Reports.	YES	<ol style="list-style-type: none"> 1. <i>Short Introduction to LaboTex</i> 2. <i>Menu and Toolbars Commands</i> 3. <i>Determination of Volume Fraction of Texture Components Using LaboTex</i>
Examples	YES	<p>Following examples are available:</p> <ol style="list-style-type: none"> 1. Examples for all crystal symmetry. 2. Examples for all sample symmetry. 3. Example for high resolution pole figures and ODF (1x1 deg) . 4. Examples for fiber texture (demo version). 5. Additional examples (download from labotex web pages).
Demo version.	YES	Special demo version can be prepared from customer data.
Support.	YES	Free e-mail support (at least one year).
Protection.	YES	HASP Key: to Parallel Port or USB
Minimal system configuration:		Processor PENTIUM 200MHz or higher, 100 MB HD space, graphic card resolution 800x600, CD-ROM drive.
Recommended system configuration:		Processor Athlon or PENTIUM IV/1.6 GHz or higher, 1 GB HD space, graphic card resolution 1024x768 (+OPENGL), CD-ROM drive. In the case the data are measured in the grid less than 5x5 degrees, the double increase of the disk space is recommended.