L A B SOFT

LaboTex

Version 3.0

The Texture Analysis Software for Windows



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

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Determination of Volume Fraction of Texture Components Model Functions Method

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Determination of Volume Fraction of Texture Components Model Functions Method Example 1

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



Step 1 - Texture Components

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



We can use both methods : automatic and manual.

Automatic method (SORT)

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



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

ODF Values for Orientations from Database (Sort by OD	OF Values)	X
Project : wzorce-new Sample : Axial-ODF r Orientation Type	Symmetry: 0-Cubic Job: 3 ¬ Orientations in Basic Region	
No Orientation Type Name ODF (average)	(HKL)(UVW) 6/1 (HKL)(UVW) (HKL)(UVW)	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	(1 1 1 > fiber fiber 54.7 45.0 4.701)	
View Report OK	Cancel	

In the list from right side you can see ODF values for each symmetrically equivalent orientations of component. There is only one orientation for *<111>fiber* component (*<111>fiber* component has not symmetrically equivalent orientations).

When you click on the *<311>fiber* component you can see 3 symmetrically equivalent orientations, their ODF values and Euler angles:

ODF Values for Orientations from Database (Sort by OD	DF Values)	×
Project : wzorce-new Sample : Axial-ODF - Orientation Tupe	Symmetry : O-Cubic Job : 3 	
No Orientation Type Name ODF (average)	(HKL)[UVW] P ₁ Φ P ₂ OD	;
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	<pre>< 1 3 1 > fiber fiber 72.5 18.4 1.15 < 3 1 1 > fiber fiber 72.5 71.6 1.15 < 1 1 3 > fiber fiber 18.2 45.0 1.14 </pre>	223
View Report OK	Cancel	

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



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



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

Manual method

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



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

Near (HKL)[UVW] Orientations							Near (HKL)[UVW] Orientations							
	ODF		(HKL)[UVW]		Р ФР2			ODF		(HKL)[UVW]		Р <mark>Ф</mark>		
	0.749 1.149 1.080 0.614	< 1 < 1 < 1 < 1	1 2> fiber 1 3> fiber 1 4> fiber 2 4> fiber	fiber fiber fiber fiber	35.3 25.2 19.5 29.2	45.0 45.0 45.0 26.6		1.149 1.080 0.749 0.614	< 1 < 1 < 1 < 1	1 3>fiber 1 4>fiber 1 2>fiber 2 4>fiber 2 4>fiber	fib fib fib	er 25.2 er 19.5 er 35.3 er 29.2	45.0 45.0 45.0 26.6	
			Max. Value of	Miller Indice	= 15	÷				Max. Value	of Miller In	dice = 15	;	

You can also change maximal value of miller indices.

Step 2 - First approximation

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

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



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



or you can use a suitable item from menu 'Analysis'.

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

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

These parameters are grayed and user can't change them.

When you start dialog window LaboTex calculates average ODF values for components and sort components using average ODF values. Hence component No. 1 is the component which has the greatest average ODF value. LaboTex fill also initial parameters for model functions:

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

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

Crysta	Crystal Symmetry Sample Symmetry Grid Cells for Output ODF Step 0.50 O (Cubic) Axial \$.0*5.0 Diagram Range +/- 45.0											
100.0%	Centre of Orientation	100.0%		Centre	of Orientatio	on	100.0%					
No	FYHM 1/1 = fiber Texture Component	On Distri	u.50 oution	FYHMQ FYHMP	Р = 10.0 ГүнмФ	45. FWHM (% 2	.0 0. Volume	.50 FYHM ¥2 = 10.0 45.0 Show Sym. Eq.				
1	< 1 1 1 > fiber	💌 🗹 Gaus	s 🔻	fiber	10.0	10.0	13 I	% < 1 1 1 ≻ fiber 💌				
2	< 1 0 0 > fiber	🔽 🗹 Gaus	s 🔻	fiber	10.0	10.0	13 🛓	[%] Calculation Mode				
3	{ fiber , 0.00, 20.00} test	🔽 🔽 Gaus	s 🔻	fiber	10.0	10.0	13 🚔	%				
4	{fiber , 1.00, 24.00}	🔽 🗹 Gaus	s 🔻	fiber	10.0	10.0	12 🚔	%				
5	< 3 4 4 > fiber	🔄 🗹 Gaus	s 🔻	fiber	10.0	10.0	8 🕀	% Max. Iteration Number : 🚺 1 000 🚔				
6	< 3 3 2> fiber	Gaus	s 🔻	fiber	10.0	10.0	7 🚊	% Max. Fit Error % (*1000) : 🚺 100 📑				
7	< 3 411> fiber	Gaus	s 🔻	fiber	10.0	10.0	3 🕀	a Iteration :				
<u>8</u>	 A 115 Abor 			liber	10.0	10.0		% Fit Error% (*1000) :				
10	< 2 0.7 > fiber			fiber	10.0	10.0		* Fit Calculation Progress				
I M Linea	ax. Drientation Set Set from Dat	tabase (sort by	- - -	Jave Curren	t Set	ickground	25	%				
	Change Initial Parar	meters		Start Vo	olume Fracti	on Calculati	on	Exit Exit and Show				

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

Quantit	uantitative Analysis - Model Functions Method - Project: wzorce-new Sample:Axial-ODF Job:3												
Cryst	tal Syr <mark>O</mark>	nmetry (Cubic)	Sam	ole Symm Axial	ietry		Gr	id Cells for (Dutput ODF	0	7	Step 0.50 Diagram Range +/- 45.0	
100.0%	*	Centre ol	f Orientation	1(00.0%		Centre	of Orientatio	on 	100.0%		Centre of Orientation	<mark>0</mark>
		FYHM 🚧 =	fiber		0.5	50	<mark>F∀HM</mark> ₫) = 10.0	45	.o c	,).50	FWHM 192 = 10.0 45.0	
No		Texture Comp	oonent	On	Distribu	tion	FWHM 🍘	<mark>г∨нм</mark> Ф	FWHM 🖗	Volume Fraction		Show Sym. Eq.	
1	< 1	1 1 > fiber		• •	Gauss	•	fiber	10.0	10.0	13 🗧	%	<111>fiber	-
2	< 1	0 0 > fiber		• •	Gauss	•	fiber	10.0	10.0	13 🗧	%	Calculation Mode	-
3	{ fibe	er , 0.00, 20.00)} test	<u> </u>	Gauss	•	fiber	10.0	10.0	13 👙	%	• Automatic O Once	
4	{ fibe	er, 1.00, 24.00)}	- 2	Gauss	•	fiber	10.0	10.0	12 🕀	%		
5	< 3	4 4 > fiber		- 2	Gauss	•	fiber	10.0	10.0	8 🗧	%	Max. Iteration Number : 🚺 1 000 📑	3 E
6	< 3	3 2 > fiber		- 2	Gauss	•	fiber	10.0	10.0	7 🕀	%	Max. Fit Error % (*1000) : 📃 100 📑	3
7	< 3	4 11 > fiber		┛┖	Gauss	•	fiber	10.0	10.0	3 🗧	%	Iteration :	-
8	< 3	1 1 > fiber		_ <	Gauss	•	fiber	10.0	10.0	2 🕀	%	Ex Euro? (#1000) .	-
9	< 4	1 15 > fiber		- 2	Gauss	•	fiber	10.0	10.0	2 🗧	%	Fit Elfor% (*1000) : j	
10	< 2	07>fiber		- 2	Gauss	•	fiber	10.0	10.0	2 🕀	%	Fit Calculation Progress	
I Ine	vlax. earity	Orientation Set	Set from Dat	abase (si	ort by 💌] _	Save Currer	t Set Ba	ackground	25	%		
		Fis	Initial Paramet	ers			Start Vo	olume Fracti	on Calculati	ion		Exit Exit and Show	

You can change:

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

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

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



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



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

Save Set for Qua	ntitative Analysis	5			? ×
Zapisz w:	🔁 WORK		•	🗢 🗈 💣 🎟 •	
Historia Historia Pulpit Moje dokume	SET10.SET SET11.SET SET13.SET SET14.SET SET15.SET SET16.SET SET17.SET SET18.SET SET19.SET SET19.SET SET2.SET) SET3.SET) SET5.SET) SET6.SET) SET7.SET) SET8.SET) SET9.SET) SET9.SET) SET9.SET			
Mój komputer	•				•
Moje miejsca	Nazwa pliku: Zapisz jako typ:	axial.SET Set Files for Q.Analysis (*.S	ET)	•	Zapisz Anuluj

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

Orientation Set axial	•
-----------------------	---

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



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

Fix Initial Parameters

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

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

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

Calculation Mode-	
Automatic	O Once
L	10

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

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

Max. Iteration Number :	998	÷
Max. Fit Error % (*1000) : 🔽	100	÷
Iteration :	253	
Fit Error% (*1000) :	1363	0.
Fit Calculation Pr	ogress	

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



Next you can change initial parameters and start calculation once more.

When LaboTex has finished calculation it displays diagrams for each Euler angle, where LaboTex shows comparison between model and experimental ODF. There are two mode for comparison diagrams:

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

You can change mode by click mouse on the button 'Norm.' or 'Diff.'.

In 'Norm.' mode LaboTex displays diagrams using colors:

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



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



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



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

Juantitative Analysis - Model Functions Method - Project: wzorce-new Sample:Axial-ODF Job:3											
Crystal S O	ymmetry (Cubic)	- Sample Sy Axia	mmetry —— al		E Gri	id Cells for C	Jutput ODF)	v	Step Diagram Range +/-	0.50
100.0% Model Exper. Backgr. Norm.	tion	100.0%		Centre	of Orientatio	n	100.0%		Centre of Orientation	 	
No	Texture Component		-4: On Distribul	5.U tion <mark>I</mark>	FYHM 🌮	<mark>гүнмФ</mark>	45. F¥HM 🖗	.0 -4 Volume	45.0	Show Sym. Eq.	45.0
1	1 1 1 > fiber	~	🔽 Gauss	F	fiber	18.6	25.4	31 ÷	%	< 1 1 1 > fiber	•
2 < 3 <	1 0 0 > fiber 1 1 3 > fiber ber , 1.00, 24.00}	v v	✓ Gauss ✓ Gauss ✓ Gauss		fiber fiber	13.5 11.3 10.0	13.5 33.7 10.0	14 ÷	%	Calculation Mode	Once
5 <	3 4 4> fiber 3 3 2> fiber		Gauss		fiber fiber	10.0	10.0	8 2	% % N	Max. Iteration Number : 🗍 Max. Fit Error % (*1000) : 🗍	1 000 ÷
7 < 8 < 9 <	3 411>fiber 3 1 1>fiber 1 1 3>fiber	▼ ▼ ▼	Gauss Gauss Gauss		fiber fiber fiber	10.0 10.0 10.0	10.0 10.0 10.0	3 4 2 4 2 4	% % %	Iteration : Fit Error% (*1000) :	349 11668.
10 K Max. Linearity	0 C 10 C 10 10.0 10.0 2										
	Change Initia	l Parameters	:		Start Vo	lume Fracti	on Calculati	on		Exit	and Show

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

Quantit	ative Analys al Symmetry — <mark>O</mark> (Cubic)	is - Model Functio	ons Mel mple Syl Axia	thod mmet	d - Proje try	ect:	wzorce-n Gri	ew Sampl d Cells for C	e:Axial-OD Jutput ODF 5.0*5.0)F Job:3	~	Step	0.50
100.0% Misfit Good Backor		entre of Orientation	ļ	100).0%		Centre	of Orientatio	on	100.0%		Centre of Orientation	
Diff.	-45.0	e Component	45 (i.0 On (-45. Distributi	.0 0n	EVHMØ	гунмФ	45. EVHM (%	.0 -4 Volume	45.0	Show Sum Ea	45.0
	< 1 1 1 > fit	er	Ī	ান	Gauss	F	fiber	18.6	25.4	Fraction	%	< 1 1 1 > fiber	
2	< 1 0 0 > fit < 1 1 3 > fit { fiber = 1 00	per per 24.00}] 이 지 이 지	Gauss Gauss Gauss		fiber fiber	13.5 11.3	13.5 33.7	14 ÷	% % %	Calculation Mode	Once
5	< 3 4 4> fit	per per			Gauss Gauss		fiber fiber	10.0	10.0		%	Max. Iteration Number : Max. Fit Error % (*1000) :	1 000 ÷
7 8 9	< 3 411>n < 3 1 1>n < 3 1 1>n < 4 1 3>n < 4 1 15>n	ber			Gauss Gauss Gauss		fiber fiber fiber	10.0 10.0 10.0	10.0	3 I 2 I 2 I 2 I 1 2 I 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	Iteration : Fit Error% (*1000) : Eit Calculation Pr	349 11668.
Ine Ine	Image: Max. Drientation Set Taxial Save Current Set Background 41 %												
	Change Initial Parameters Start Volume Fraction Calculation Exit Exit and Show								and Show				

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



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



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



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



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

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

– Crystal Sy <mark>O</mark>	ymmetry (Cubic)	nple Symmetry Axial		àrid Cells for Outp	ut ODF	Step Diagram Range +/-	0.50
100.0% Model xper. Backgr.	Centre of Orientation	100.0%	Centr	e of Orientation	100.0%	Centre of Orientation	
No	Texture Component	-2 On Distribi	15.0 Ition FYHM 4		45.0	-45.0 Show Sym. Eq.	45.0
1 < 1	I 1 1 > fiber	Gauss	Fiber	18.6 2	5.4 S1	% 1 1 3> fiber	•
2 < 1	I 0 0 ≻ fiber	🔽 🗹 🖬 Gauss	fiber	13.5 1	3.5 14 🚊	% Calculation Mode	
3 < 1	1 1 3> fiber	Gauss	Fiber	11.3 3	3.7 14 🔅	🕺 📀 Automatic 🖉	O Once
4 Em	3 4 4 5 hber	Gauss	▼ fiber	10.0 1	0.0	% Max Iteration Number :	<u> 1000</u> 픤
6 < 3	3 3 2 > fiber	🔄 🗖 Gauss	Fiber	10.0 1	0.0 7 🗧	% Max. Fit Error % (*1000) :	100 ÷
7 🖂	3 4 11 > fiber	🔽 🗖 Gauss	Fiber	10.0 1	0.0 3 🚊] %	349
8 < 3	3 1 1 > fiber	🔽 🗖 Gauss	fiber	10.0 1	0.0 2 🗧	% Iteration :]	11668
9 < 1	I 1 3> fiber	Gauss	▼ fiber	10.0 1		[%] FitEli0i%(1000): [-
Image: Constant of the state of the stat							
Change Initial Parameters Start Volume Fraction Calculation Exit Exit and Show							

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

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

Volume	FWHM	FWHM	FWHM	
Fraction	Phil	Phi	Phi2	Orientation
Component N	No 1 -	Distrib	ution :Gauss	
30.1	fiber	18.9	24.7	<1 1 1 > fiber
Component N	No 2 -	Distrib	ution :Gauss	
12.7	fiber	13.0	13.1	< 1 0 0 > fiber
Component N	No 3 -	Distrib	ution :Gauss	
8.2	fiber	11.2	19.0	< 1 1 3 > fiber
48.99	Backqi	cound Vo	lume Fraction	
	2			

Step 3 to N - Second to N approximation

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



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



Example 2 Aluminium Sample

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



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

† ;+ V

We can use both methods : automatic and manual.

Automatic method (SORT)

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



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

PF values for orientatio Symmetry : O-Cubic	n from Databa	se (Sort by PF	Value)	PE values fo	r poles of orienta	tion (HKL)(LI\Av/1	×
Immunol Grientation 1 (3 6 2) 2 (7 4 14) 3 (7 4 14) 4 (6 300, 28) 5 (1 4 2) 6 (1 1 2) 7 (1 1 2) 8 (1 1 2)	on Type Name 2 -2 3 > 4 -7 4 > 4 -7 4 > 00, 58.00} 2 -1 1 > 1 -1 > copper 1 -1 > 1 -1 > A 4	PF (a 60.43 55.41 55.41 48.32 47.83 46.80 46.80 46.80 46.80	average) 5 5 16 4 7 7 7	HKL=111 24.9 85.3 54.7 65.6 HKL=100 64.6 73.4	RPF Sample: A 354.8 187.9 118.5 258.7 RPF Sample: A 55.0 316.9 10.2 2	PF - Value Vuminium-o-1 12.421 4.391 3.190 3.546 Aluminium-o-1 4.968 4.433 5.524	-
9 { 1 3 2 × 6 10 { 2 1 3 × 5 11 { 2 3 1 × 5 - Orientations in Basic Reg (HKL)(UVW) (6 -2 3)(-2 -3 2)	3 -4 3 > 5 -1 3 -6 4 > 5 -3 3 -4 6 > 5 -2 ion 12	45.11 45.11 45.11 Φ ^β ₂ 6 108.4	2 2 2 PF (sum) 60.433	31.0 HKL=110 24.6 59.7 66.2 72.4 84.2 36.1	197.2 RPF Sample: A 87.5 4.0 157.1 221.5 97.4 284.4	5.234 Aluminium-o-l 6.454 5.626 2.562 2.068 2.257 3.284	
$ \begin{bmatrix} 3 & -2 & 6 \\ 3 & -2 & 6 \\ 1 & 2 & 3 & 2 \\ 1 & 3 & -2 & 6 \\ 1 & 2 & 3 & 2 \\ 1 & 3 & -2 & 6 \\ 1 & 2 & 3 & 2 \\ 1 & 2 & 3 & 2 \\ 1 & 3 & 2 & 6 \\ 1 & 2 & 3 & 2 \\ 1 & 3 & -2 & 6 \\ 1 & 2 & 3 & 2 \\ 1 & 3 & -2 & 1 \\ 1 & 2 & -2 & 3 \\ 1 & 2 & -2 & 3 \\ 1 & 2 & -2 & 2 \\ 1 & 3 & -2 & 2 \\ 1 & 3 & -2 & 2 \\ 1 & 3 & -2 & 2 \\ 1 & 3 & -2 & 2 \\ 1 & 3 & -2 & 2 \\ 1 & 3 & -2 & 2 \\ 1 & 3 & -2 & 2 \\ 1 & 3 & -2 & 2 \\ 1 & 3 & -2 & 2 \\ 1 & 3 & -2 & 2 \\ 1 & 3 & -2 & 2 \\ 1 & 3 & -2 & 2 \\ 1 & 3 & -2 & 2 \\ 1 & 3 & -2 & 2 \\ 1 & 3 & -2 & -2 $	70.3 145 70.3 31 49.4 73 32.5 64 70.3 145 49.4 73 32.5 64 32.5 64 32.5 64 32.5 64 32.5 64 32.5 64 32.5 64 32.5 64 32.5 64 32.5 64 9.4 106 70.2 21	3.0 123.7 .0 236.3 .4 116.6 .6 288.4 3.0 303.7 5.6 333.4 .6 198.4 5.6 153.4 .0 146.2	60.433 60.433 60.433 60.433 60.433 60.433 60.433 60.433 60.433 60.433				
		OK	Can	cel			

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



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



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

Manual method

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

r	ear (HKL)	[UVW] Orientations		×
	PF	(HKL)[UVW]	<i>¶</i> Ф <i>¶</i>	Misorientation
	15.928 15.443 12.826 12.438 9.147 8.133 8.063 5.992 5.962 5.962	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	32.7 49.1 93.8 35.3 45.0 90.0 43.3 45.0 90.0 25.2 45.0 90.0 19.5 45.0 90.0 15.0 57.7 108.4 42.0 56.3 90.0 51.9 47.2 94.1 52.1 47.0 93.8 57.7 43.1 85.9	4.16 ▲ 2.31 6.40 11.93 17.67 20.96 11.09 17.84 17.81 17.81 ▼
			Max. Value of Miller Indice =	15 📫

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

First approximation

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

•	{ 1	3 2 }< 6 -4 3 >
•	{ 1	1 2 }< 1 1 -1 >
•	{ 1	4 6 }< 2 1 -1 >
•	{ 1	1 0 }< 1 -1 2>
•	{ 1	2 3 }< 4 1 -2 >
•	{ 1	$1 \ 0 < 0 \ 0 - 1 > 0$

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



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

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

These parameters are grayed and user can't change them.

When you start dialog window LaboTex calculates average ODF values for components and sort components using average ODF values. Hence component No. 1 is the component which has the greatest average ODF value. LaboTex fill also initial parameters for model functions:

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

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

Quantit	uantitative Analysis - Model Functions Method - Project: wzorce-new Sample:Axial-ODF Job:3							
Cryst.	al Symmetry Sam	ple Symmetry Axial	G	rid Cells for Output ODF 5.0*5	.0	Step 0.50 Diagram Range +/- 45.0		
100.0%	Centre of Orientation	100.0%	Centre	of Orientation	100.0%	Centre of Orientation		
	FWHM 1/4 = fiber	0.5	60 <mark>ғұнм</mark> (P = 10.0 45	, 5.0 0.50	FWHM 1/2 = 10.0 45.0		
No	Texture Component	On Distribut	ion <mark>FYHM</mark>	<mark>ЕЖНМФ</mark> ЕЖНМ 🖗	Volume Fraction	Show Sym. Eq.		
1	< 1 1 1 > fiber	💌 🔽 Gauss	✓ fiber	10.0 10.0	13 🔆 %	< 1 1 1 > fiber		
2	< 1 0 0 > fiber	🔽 🔽 Gauss	Fiber	10.0 10.0	13 🐺 %	Calculation Mode		
3	{ fiber , 0.00, 20.00} test	🔽 🔽 Gauss	Fiber	10.0 10.0	13 🔆 %	Automatic Once		
4	{ fiber , 1.00, 24.00}	🔄 🗹 🛛 Gauss	fiber	10.0 10.0	12 🛨 🎖			
5	< 3 4 4 > fiber	🔄 🗹 Gauss	fiber	10.0 10.0	8 🛨 %	Max. Iteration Number : 🚺 1 000 🌐		
6	< 3 3 2 > fiber	🔄 🗹 🖬 Gauss	fiber	10.0 10.0	7 😤 %	Max. Fit Error % (*1000) : 🗾 100 📑		
7	< 3 411 > fiber	🔄 🔽 Gauss	Fiber	10.0 10.0	3 🗧 %	Iteration :		
8	< 3 1 1> fiber	Gauss	fiber	10.0 10.0		Eit Error% (*1000) :		
9	< 4 115>fiber	🔄 🔽 Gauss	_ fiber	J10.0 J10.0				
10	10 < 2							
Line	Image: Max. Orientation Set Set from Database (sort by Save Current Set Background 25 %							
	Change Initial Parameters Start Volume Fraction Calculation Exit Exit. and Show							

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

Quantitative Analysis - Model Functions Method - Project: wzorce-new Sample:Axial-ODF Job:3						
Crystal Symmetry Sample S (Cubic)	Symmetry xial	Grid Cells for O	5.0×5.0	Step 0.50 Diagram Range +/- 45.0		
Centre of Orientation	100.0%	Centre of Orientatio	n 100.0%			
FWHM 14 = fiber	0.50	FWHMΦ = 10.0	45.0 0.5	50 <mark>F¥HM 🖗</mark> = 10.0 45.0		
1 < 1	Gauss Gaus Gaus	fiber 10.0 fiber 10.0	Fraction 10.0 13 5 10.0 13 5 10.0 13 5 10.0 13 5 10.0 12 5 10.0 7 5 10.0 7 5 10.0 2 5 10.0 2 5	% 1 1 > fiber % Calculation Mode % • Automatic • Once % • Automatic • Once % • Max. Iteration Number : 1000 ÷ % Max. Fit Error % (*1000) : 100 ÷ % Iteration : • % Iteration : • % Fit Error % (*1000) : •		
10 < 2						
Fix Initial Parameters Start Volume Fraction Calculation Exit Exit and Show						

You can change:

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

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

Now, you should set texture components 1 to 5 which you have found in previous step. Next components 6-10 you should turn off from further calculations.

uantitative Analysis - Model Functions Method - Project: Aluminium Sample:Aluminium-o-I Job:2										
Crystal 9	Symmetry Sample (Cubic)	Symmetry Orthorhombic		Gri	d Cells for C	lutput ODF 5.0*5.0)	7	Step Diagram Range +/-	0.50
100.0%	Centre of Orientation	100.0%		Centre o	of Orientatio	in	100.0%		Centre of Orientation	<mark>מ</mark> ך
0.	.50 <mark>FYHM 1<mark>4</mark> = 10.0</mark>	45.0 0. ¹	50	<mark>г∀нм</mark> Ф	= 10.0	45.	.0 0	.50	FWHM 🖗 = 10.0	45.0
No	Texture Component	On Distribu	tion	FYHM 🖗	г₩нмФ	FWHM 🌮	Volume Fraction		Show Sym. Eq.	
1 {	1 3 2 }< 6 -4 3 > S-1	🗹 🗹 🖬 🖬	•	10.0	10.0	10.0	28 🗧	% {	1 3 2 }< 6 -4 3 > S-1	•
2 {	1 1 2 \ 1 1 1 - 1 > Al 4	🗹 🔽 🖬 Gauss	•	10.0	10.0	10.0	25 🕂	× _C	alculation Mode	
3 {	1 4 6 }< 2 1 ·1 > Al2	🔽 🔽 🖬 🔽		10.0	10.0	10.0	17 🗧	%	Automatic	Manual
4 {	1 1 0)< 1 -1 2> Al3	🗹 🗹 🖬 🖸		10.0	10.0	10.0	9 🗄	%		
5 {	1 2 3 × 4 1 ·2 × Al 1	🖸 🗹 🖬 Gauss		10.0	10.0	10.0	6 🗄	% Ma	ax. Iteration Number : 🦵	1 000 🗦
6 {	1 1 0 × 0 0 ·1 × AI5	🗹 🗹 🖬 Gauss		10.0	10.0	10.0	5 🛨	% Ma	x.Fit Error % (*1000) : 厂	100 🗧
7 {	1 1 2 k 1 1 ·1 >	🗖 🗖 Gauss		10.0	10.0	10.0	9 🕂	%	Iteration :	
8 {	1 1 2 × 1 1 1 × AI4	🗖 🗖 Gauss		10.0	10.0	10.0	15 🚔	% га	F% (*1000) .	
9 {	4 1 6 }< -1 -2 1 >	🗖 🗖 Gauss		10.0	10.0	10.0	12 🗧	% гк	Enor% (*1000) : j	
10 {	10 { 4 1 6 }< -1 -2 1 > Gauss 🔽 10.0 10.0 10.0 14 🚍 % Fit Calculation Progress									
✓ Max Linearit	Imax. Orientation Set Set from Database (sort by Image: Save Current Set) Background 10 %									
	Fix Initial Parameters Start Volume Fraction Calculation Exit Exit and Show									

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



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

Save Set for Qua	ntitative Analysi	is				? ×
Zapisz w:	🔁 WORK			•	← 🗈 💣 🎟•	
Historia Historia Pulpit Moje dokume	SET10.SET SET11.SET SET13.SET SET14.SET SET15.SET SET16.SET SET17.SET SET19.SET SET19.SET SET2.SET SET2.SET		SET3.SET SET5.SET SET5.SET SET6.SET SET7.SET SET8.SET SET9.SET TI.SET			
Mój komputer	•					•
	Nazwa pliku:	axial.SET			•	Zapisz
Moje miejsca	Zapisz jako typ:	Set Files f	or Q.Analysis (*.SET))	~	Anuluj

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

Orientation Set	Set from Database (sort by	•
	,	

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

Fix Initial Parameters

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

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

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

Calculation Mode	
O Automatic	C Once

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

Start Volume	Fraction	Calculation
Start Volume	FIGUUUT	Calculation

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

Max. Iteration Number :	998 🗧				
Max. Fit Error % (*1000) :	100 🗧				
Iteration :	253				
Fit Error% (*1000) :	13630.				
Fit Calculation Progress					

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



Next you can change initial parameters and start calculation once more.

When LaboTex has finished calculation it displays diagrams for each Euler angle, where LaboTex shows comparison between model and experimental ODF. There are two mode for comparison diagrams:

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

You can change mode by click mouse on the button 'Norm.' or 'Diff.'.

In 'Norm.' mode LaboTex displays diagrams using colors:

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



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

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



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

Misfit Good Backgr. Diff.



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

Quantitative Analysis - Model Functions Method - Project: Aluminium Sample:Aluminium-o-I Job:1						
Crysl	tal Symmetry <mark>O</mark> (Cubic)	Sample Symmetry Orthorhombic	Gi	id Cells for Output OE	5.0 💌	Step 0.50 Diagram Range +/- 45.0
100.05 Misfit Good Backg	Centre of Orier	ntation 100.0%	Centre	of Orientation	100.0%	Centre of Orientation
	-45.0	45.0 -45	i.O		45.0 -45.0	45.0
No	Texture Componen	t On Distribut	ion <mark>FWHM 124</mark>	<mark>Е¥НМФ</mark> Е¥НМ{	Volume Fraction	Show Sym. Eq.
1	{ 1 3 2 }< 6 -4 3 > S-1	💌 🗹 Gauss	12.9	11.3 12.3	35 🛒 %	[29.25, 56.67, 9.46](Sym.Eq.) 💌
2	{ 1 1 2 }< 1 1 -1 > AI4	🔽 🔽 🖬 🖉	26.9	12.0 14.9	32 🚊 %	Calculation Mode
3	{ 1 4 6 }< 2 1 -1 > Al2	🔽 🔽 Gauss	7 16.1	11.9 12.2	18 🚔 %	Automatic C Manual
4	{ 1 1 0 }< 1 -1 2 > Al3	👻 🗹 🖬 🖉	9.3	8.4 8.2	2 🛫 %	S Addinate S Mandai
5	{ 1 2 3 }< 4 1 - 2 > Al 1	👻 🔽 Gauss	- 8.9	14.1 9.8	2 🗄 %	Max. Iteration Number : 🚺 1 000 📫
6	{1 1 0}< 0 0.1> AI5	🔽 🔽 Gauss	9.6	6.7 6.4	1 🗄 %	Max. Fit Error % (*1000) : 100 🕂
7	{ 2 3 1 }< -3 4 -6 > S-4	💌 🗖 Gauss	▼ 10.0	10.0 10.0	8 🕂 %	775
8	{ 2 1 3}<-3 -6 4>S-3	🔽 🗖 Gauss	▼ 10.0	10.0 10.0	16 👙 %	Iteration : 779
9	{1 1 2}< 1 1-1> cop	per 🔽 🗖 Gauss	▼ 10.0	10.0 10.0	18 🛨 %	Fit Error% (*1000) : 75421.
10	{1 1 2} 1 1 -1>	👻 🗖 Gauss	▼ 10.0	10.0 10.0	22 🕂 %	Fit Calculation Progress
Imax Internation Set Set from Database (sort by Save Current Set Background 10 %						
Change Initial Parameters Start Volume Fraction Calculation Ex						Exit Exit and Show

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



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



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



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

Finally, we receive results calculation:

LaboTex - Texture - Quantitative Analysis Report						
User: Ozg	a					
Project: A	luminiun	ı				
Sample: A	luminiun	1-0-I				
Job: 2						
Date:2006	5/03/18					
Time:18:2	8:32					
Volume	FWHM	FWHM	FWHM			
Fraction	Phi1	Phi	Phi2	Orientation		
Componer	nt No 1 -	Distribut	ion :Gaus	s		
37.4	12.6	12.0	12.5	$\{1 \ 3 \ 2\} < 6 \ -4 \ 3 > S - 1$		
Componer	nt No 2 -	Distribut	ion :Gaus	S		
34.5	29.7	11.9	15.7	$\{ 1 \ 1 \ 2 \} < 1 \ 1 \ -1 > Al 4$		
Componer	nt No 3 -	Distribut	ion :Gaus	S		
18.2	19.0	12.2	13.6	$\{ 1 \ 4 \ 6 \} < 2 \ 1 \ -1 > Al2$		
Componer	1t No 4 -	Distribut	ion :Gaus	S		
2.3	9.6	10.4	10.5	$\{ 1 \ 1 \ 0 \} < 1 \ -1 \ 2 > Al3$		
Componer	ıt No 5 -	Distribut	ion :Gaus	S		
0.1	5.9	<i>9.3</i>	9.1	$\{1 \ 2 \ 3\} < 4 \ 1 - 2 > Al 1$		
Componer	1t No 6 -	Distribut	ion :Gaus	S		
0.4	6.2	11.7	6.3	$\{ 1 \ 1 \ 0 \} < 0 \ 0 - 1 > Al 5$		

6.98 Background Volume Fraction

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



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







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