Quick Start Guide

X'Pert Texture

PW3211

Winning by Sharing

PANalytical

X'PERT

TEXTURE

QUICK START GUIDE

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This is the Second Edition of this publication, it is intended for use with version 1.1 of the X'Pert Texture software.

ACKNOWLEDGMENTS

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X'PERT TEXTURE

QUICK START GUIDE

Contents

CHAPTER 1

INTRODUCTION

Contents

1.1 INTRODUCTION

This Quick Start Guide is intended to help you to use the X'Pert Texture software quickly and efficiently. The examples show you how to start and use the software to perform fairly simple tasks.

In order to follow these examples you must start with Chapter 2 and then follow the examples through the rest of the chapters.

This Quick Start Guide is not designed to show in detail or explain all the various possibilities of the software. For each of the examples shown in this document only one route to perform the task is shown, there may be other methods that you can use but you will have to experiment with the system and learn the other possibilities yourself.

Note: There may be differences between the example screens given in this Quick Start Guide and what you see on your screen. In all cases, where there is a difference, follow what you see on your screen.

1.2 CONTENTS OF THE QUICK START GUIDE

The worked examples in this Quick Start Guide are:

Chapter 2: Getting Started

This chapter describes a few basic concepts of X'Pert Texture and how to get started with it.

Chapter 3: Viewing Graphs

This chapter describes how to customize X'Pert Texture to view graphs for analysis. It describes how to display a graph, how to handle one and two dimensional graphs and how to attach labels to the graphs.

Chapter 4: Enhanced Display

In this chapter answers the following questions about 2.5D and 3D graphs:

What does "Enhanced Display" mean?
How do I get a 3D graph displayed on screen?
How can I make it bigger?
How can I rotate it?
How can I change the look of the graph?
How can I enhance the 3D effect?

Chapter 5: Manipulating Graphs in the Gallery

This chapter describes how to display multiple graphs and how to apply all changes simultaneously.

Chapter 6: Analyzing Texture Data

This chapter shows you how to set-up an ODF Project, calculate the Orientation Distribution Function and a Pole Figure and then observe the ODF in 2D and 3D graphics.

Chapter 7: Processing Graphics and Tables

This chapter shows you how to process the various data generated by X'Pert Texture for other texture or Windows applications.

Chapter 8: Automating Viewing of Texture Data

This chapter shows you how to use X'Pert APP to automate the viewing of texture data in X'Pert Texture.

1.3 TERMS AND CONVENTIONS USED

In this section, we describe the terms and conventions used in this Quick Start Guide and how they relate to the user interface.

1.3.1 Terms Used to Denote an Action

In this Guide there are several terms that indicate an action.

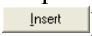
Check (✔)	Also referred to as a tick mark.
Click	Press the mouse button and quickly release it.
Double-click	Press the mouse button twice (quickly) on an icon, item, file or program.
Drag	Press and hold down the mouse button and move the pointer to define an area or move an object
Enter	Type in information. This can be either text or numerical data.
Press	A key on the keyboard, or a push-button in a window.
Right-click	Press the right mouse button and quickly release it.
Select	Move the mouse cursor to the option you want and click the left mouse button.
Tick (✔)	Also referred to as a check mark.
Toggle	Switch between parameters or states (for example: On-Off-On).
OK	In the examples in this Guide we terminate most actions by saying "press OK", you can if you prefer press ***Enter*** instead of OK.
	The instruction to click (or press)  is used in this Guide as an instruction to close the window that you are currently working in, **not** the program.

1.3.2 Instructions and Descriptive Text

An instruction is preceded by a bullet "●". Any descriptive text relating to an instruction is given directly after the instruction.

Generally, screen captures are preceded by an instruction and intend to reproduce what you will see on your screen. However, if there are any differences, follow what you see on your screen.

1.3.3 Push-Buttons and Fields

All push-buttons on a window are shown as the actual push-button (for example: 

), or in bold text (for example: **Apply** or **Cancel**).

All fields are shown between "quotation marks".

1.3.4 Menu Items and Keys

All menu items are printed in italics, for example: *File - Open* etc.

All keys are shown bold in an italic font. For example: ***Enter, Ctrl, Alt, Del*** etc.

CHAPTER 2

GETTING STARTED

Contents

2.1 INTRODUCTION

X'Pert Texture is a stand-alone analytical module for texture analysis by means of X-ray diffraction. X'Pert Texture's easy-to-use interface enables you to perform calculations of Pole figures, Inverse pole figures and Orientation Distribution Functions (ODF) based on the Williams-Imhof-Matthies-Vinel (WIMV) method. In addition, background and defocusing corrections can be easily applied. Graphical representations of data in 1, 2, 2.5 and 3D modes provide a clear overview of your analytical data. Data collection is performed by the X'Pert Data Collector.

In this Guide, we will introduce the basic concepts used in X'Pert Texture and then describe the functionality using a series of worked examples.

2.2 BEFORE YOU START

Before you can start to do the worked examples in this Quick Start Guide you must have some suitable data available. This data is contained in files (listed below) which are delivered with your X'Pert Texture. Following a standard installation of X'Pert Texture these files are located at: C:\Program Files\PANalytical\X'Pert Texture.

The ODF project file: "Example project.wtx" contains all these files.

Cu111.rw1	Cu200.rw1	Cu220.rw1	Cu311.rw1
Cu111bkg.cor	Cu200bkg.cor	Cu220bkg.cor	Cu311bkg.cor
Cu111def.cor	Cu200def.cor	Cu220def.cor	Cu311def.cor

Although X'Pert Texture is an easy-to-use program you will still need to understand a few basic concepts.

2.2.1 ODF Projects & Views

There are two basic types of file in X’Pert Texture, they are: “ODF Projects” and “Views”.

ODF Projects are the container of all your data for, and generated by, calculations on experimental pole figures, corrected pole figures, corrections, ODF, calculated pole figures or inverse pole figures.

Three View windows are available in X'Pert Texture: Pole Figure View, ODF View and Corrections View. Views enable you to display, manipulate and report a range of texture/correction data. These views contain three tabs: “Organizer”, “Options” and “Gallery”. You use the “Organizer” and “Options” tabs to define what data is displayed, how many graphs and how they will be displayed on the “Gallery” tab. In addition, the “Gallery” tab is used to enhance the data display by enabling the addition of text/angle labels, zoom/rotate actions, axes and Roe/Bunge co-ordinates. You can display a graph on a View window even if you have not created an ODF Project.

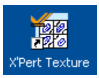
See Chapter 2 of the X’Pert Texture User's Guide for detailed information on the file formats that can be used with X'Pert Texture.

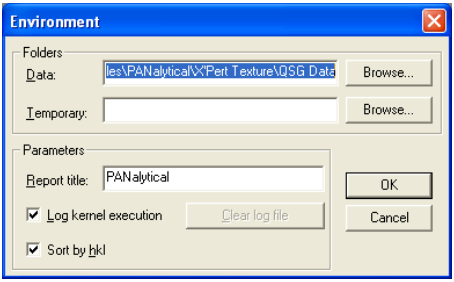
2.3 GETTING STARTED

Now you have read and understood the concepts you can go on to customize X'Pert Texture for use.

2.3.1 Customizing X'Pert Texture

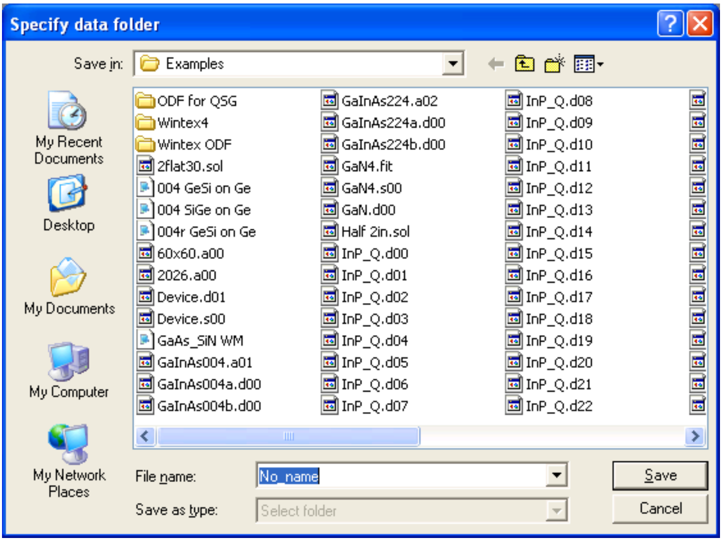
This section tells you how to set-up the Environment options that are accessed via the *Options* menu.

- Start X’Pert Texture by double-clicking on the  icon.
- Select *Environment...* from the *Options* menu.



This window enables you to set the options for the location of data files and what settings must be loaded when X'Pert Texture starts. To define your environment settings, proceed as follows:

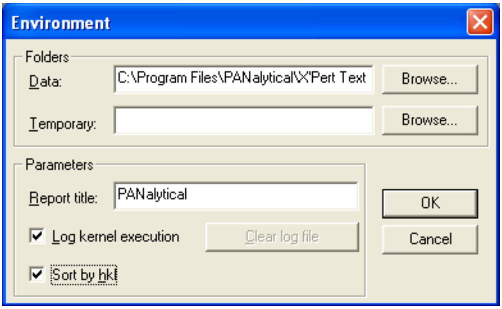
- Click on the Browse... to display a "Specify data folder" window.



- Create a new folder for your data to be stored in:

  Press the button, name the newly created folder "QSG Data" press Open and then Save.

- Enter your own title in the "Report title:".



- Check the "Log kernel execution" to save the execution history of the X'Pert Texture kernel in a LOG file and attach it to the report.
- Check the "Sort by hkl" to sort items in the ODF Project window by hkl.
- Press OK to save all of the options you have just set and close the window.

2.3.2 Analysis Strategies

Decide if you want to observe previously obtained data or perform a full ODF analysis.

Create or open the relevant view as described in section 2.3.2.1.

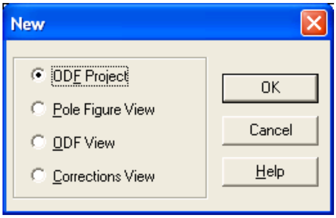
OR

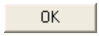
Create or open an ODF Project and perform a full ODF analysis as described in section 2.3.2.2.

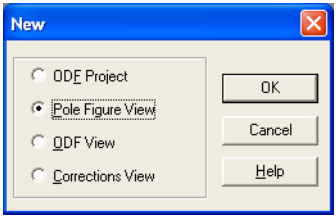
2.3.2.1 Graphical Views

To display and inspect previously obtained data, proceed as follows:

- Select *File - New...*



- Select the “Pole Figure View” radio button and press .

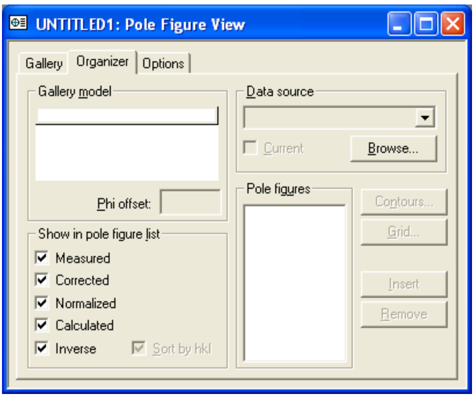


The resulting “Pole Figure View” window has three tabs:

The “Gallery” tab where you can manipulate the graphs.

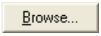
The “Organizer” tab where you define what is to be displayed.

The “Options” tab to define how the graphics are projected.

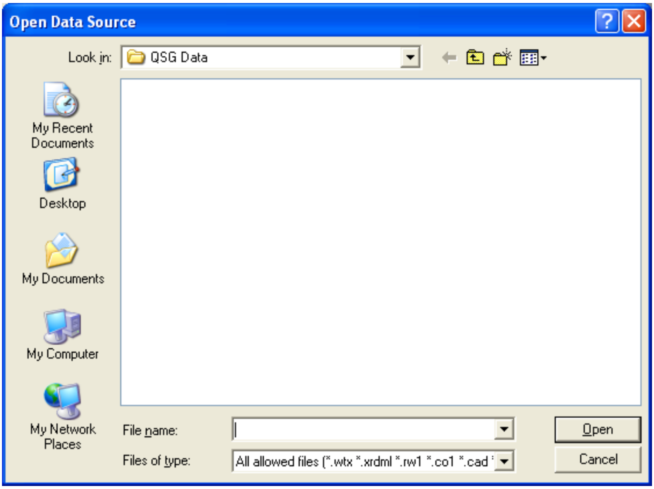


You can swap between tabs and modify settings to improve your results prior to printing, examples of this are shown in Chapter 3 onwards.

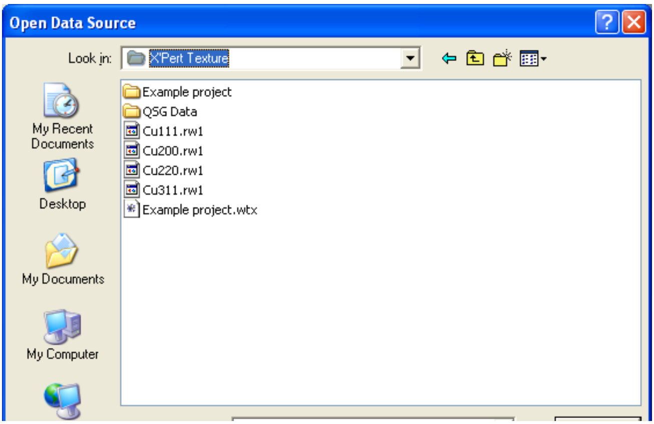
Select the input data on the Organizer tab, as follows:

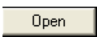
- Click on 

and the "Open Data Source" window is displayed.



- Press the  button to go up one level.

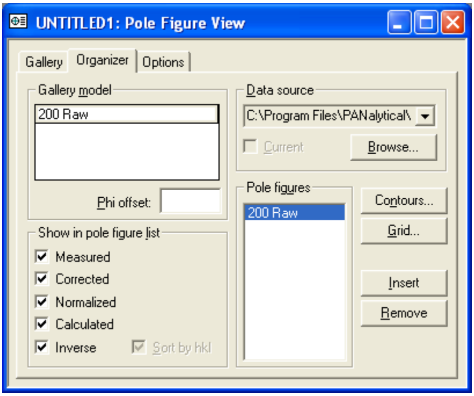


- Select "Cu200.rw1" from the folder: "\Program Files\PANalytical\X'Pert Texture", and then click on the 

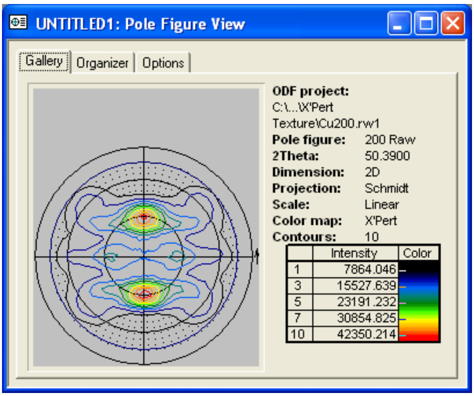
button.

On the "Pole Figure View" window, the path and file name is displayed in the "Data source" field and "200 Raw" is displayed in the "Pole figure" list.

- Click on "200 Raw" and then the Insert button, or double-click on "200 Raw" to place the pole figure in the "Gallery model" list.



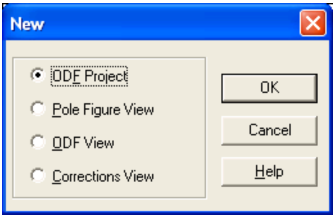
- Click on the "Gallery" tab to see the pole figure displayed in 2D.



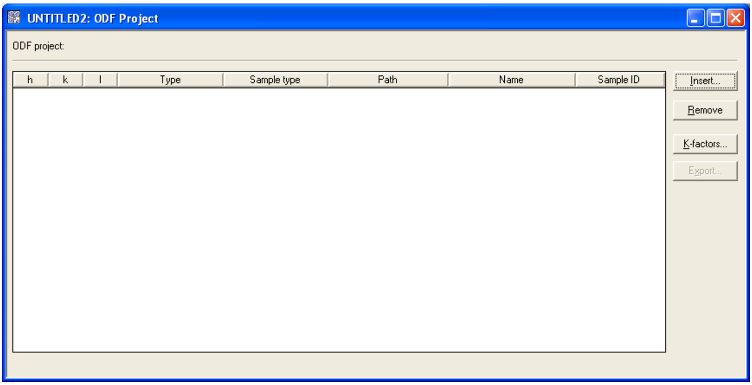
2.3.2.2 ODF Analysis

Proceed as follows to set up an ODF project and perform a full ODF analysis:

- Select *File - New...*

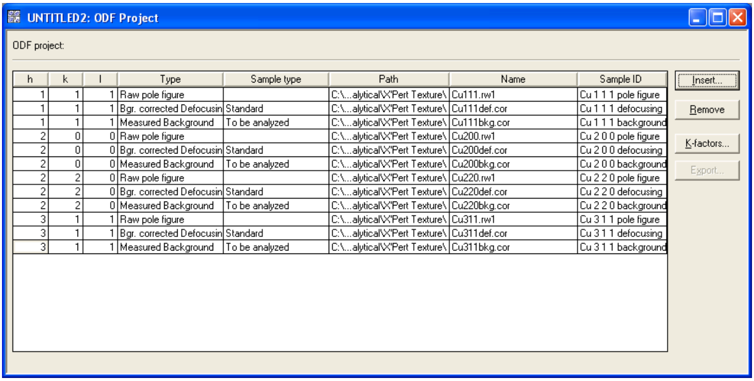


- Select the "ODF Project" radio button and press OK.



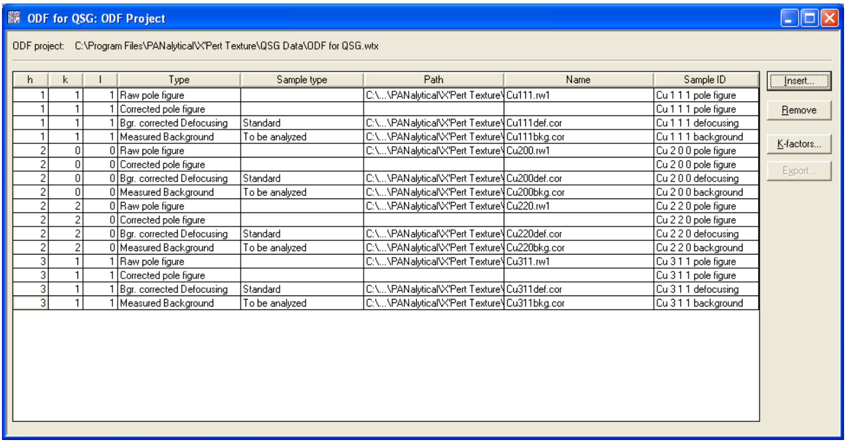
Now you need to import all of the files that you need in order to perform an ODF analysis.

- Press Insert (if necessary browse until you open the directory ...\X'Pert Texture), select all of the files (Cu111.rw1, Cu111bkg.cor, Cu111def.cor, Cu200.rw1, Cu200bkg.cor, Cu200def.cor, Cu220.rw1, Cu220bkg.cor, Cu220def.cor, Cu311.rw1, Cu311bkg.cor, Cu311def.cor) and press Open.



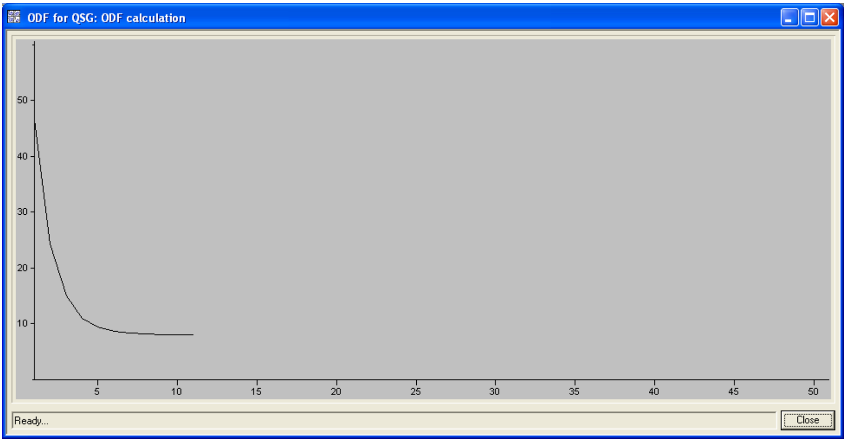
h	k	l	Type	Sample type	Path	Name	Sample ID
1	1	1	Raw pole figure		C:\...alytical\X'Pert Texture\	Cu111.rw1	Cu 1 1 1 pole figure
1	1	1	Bgr. corrected Defocusin	Standard	C:\...alytical\X'Pert Texture\	Cu111def.cor	Cu 1 1 1 defocusing
1	1	1	Measured Background	To be analyzed	C:\...alytical\X'Pert Texture\	Cu111bkg.cor	Cu 1 1 1 background
2	0	0	Raw pole figure		C:\...alytical\X'Pert Texture\	Cu200.rw1	Cu 2 0 0 pole figure
2	0	0	Bgr. corrected Defocusin	Standard	C:\...alytical\X'Pert Texture\	Cu200def.cor	Cu 2 0 0 defocusing
2	0	0	Measured Background	To be analyzed	C:\...alytical\X'Pert Texture\	Cu200bkg.cor	Cu 2 0 0 background
2	2	0	Raw pole figure		C:\...alytical\X'Pert Texture\	Cu220.rw1	Cu 2 2 0 pole figure
2	2	0	Bgr. corrected Defocusin	Standard	C:\...alytical\X'Pert Texture\	Cu220def.cor	Cu 2 2 0 defocusing
2	2	0	Measured Background	To be analyzed	C:\...alytical\X'Pert Texture\	Cu220bkg.cor	Cu 2 2 0 background
3	1	1	Raw pole figure		C:\...alytical\X'Pert Texture\	Cu311.rw1	Cu 3 1 1 pole figure
3	1	1	Bgr. corrected Defocusin	Standard	C:\...alytical\X'Pert Texture\	Cu311def.cor	Cu 3 1 1 defocusing
3	1	1	Measured Background	To be analyzed	C:\...alytical\X'Pert Texture\	Cu311bkg.cor	Cu 3 1 1 background

- Save the file *File - Save*, give it the file name “ODF for QSG” and press Save.
- Select *Actions - Corrections*, accept the defaults by pressing OK and the corrected pole figures are added to the list.



h	k	l	Type	Sample type	Path	Name	Sample ID
1	1	1	Raw pole figure		C:\...\PANalytical\X'Pert Texture\	Cu111.rw1	Cu 1 1 1 pole figure
1	1	1	Corrected pole figure				Cu 1 1 1 pole figure
1	1	1	Bgr. corrected Defocusing	Standard	C:\...\PANalytical\X'Pert Texture\	Cu111def.cor	Cu 1 1 1 defocusing
1	1	1	Measured Background	To be analyzed	C:\...\PANalytical\X'Pert Texture\	Cu111bkg.cor	Cu 1 1 1 background
2	0	0	Raw pole figure		C:\...\PANalytical\X'Pert Texture\	Cu200.rw1	Cu 2 0 0 pole figure
2	0	0	Corrected pole figure				Cu 2 0 0 pole figure
2	0	0	Bgr. corrected Defocusing	Standard	C:\...\PANalytical\X'Pert Texture\	Cu200def.cor	Cu 2 0 0 defocusing
2	0	0	Measured Background	To be analyzed	C:\...\PANalytical\X'Pert Texture\	Cu200bkg.cor	Cu 2 0 0 background
2	2	0	Raw pole figure		C:\...\PANalytical\X'Pert Texture\	Cu220.rw1	Cu 2 2 0 pole figure
2	2	0	Corrected pole figure				Cu 2 2 0 pole figure
2	2	0	Bgr. corrected Defocusing	Standard	C:\...\PANalytical\X'Pert Texture\	Cu220def.cor	Cu 2 2 0 defocusing
2	2	0	Measured Background	To be analyzed	C:\...\PANalytical\X'Pert Texture\	Cu220bkg.cor	Cu 2 2 0 background
3	1	1	Raw pole figure		C:\...\PANalytical\X'Pert Texture\	Cu311.rw1	Cu 3 1 1 pole figure
3	1	1	Corrected pole figure				Cu 3 1 1 pole figure
3	1	1	Bgr. corrected Defocusing	Standard	C:\...\PANalytical\X'Pert Texture\	Cu311def.cor	Cu 3 1 1 defocusing
3	1	1	Measured Background	To be analyzed	C:\...\PANalytical\X'Pert Texture\	Cu311bkg.cor	Cu 3 1 1 background

- Select *Actions - Calculate ODF...*, accept the defaults by pressing OK.



- Press Close to return to the ODF project where a new entry “ODF data” has been added to the list.

You can report or export results in several ways, depending on your requirements. These are all described in Chapter 7.

CHAPTER 3

VIEWING GRAPHS

Contents

3.1 INTRODUCTION

In this chapter, we will answer the following questions about 1D and 2D graphs:

- How do I get a graph displayed on screen?

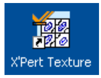
- How can I make it bigger?

- How can I add labels?

In order to do this we will use the file “Cu111.rw1”.

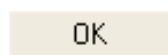
3.2 GETTING GRAPHS ON-SCREEN

The fastest way of displaying a graph is to select a data file in a format usable by X'Pert Texture such as *.rw1. A full list of the supported file formats is given in Chapter 2 of the X’Pert Texture User's Guide.

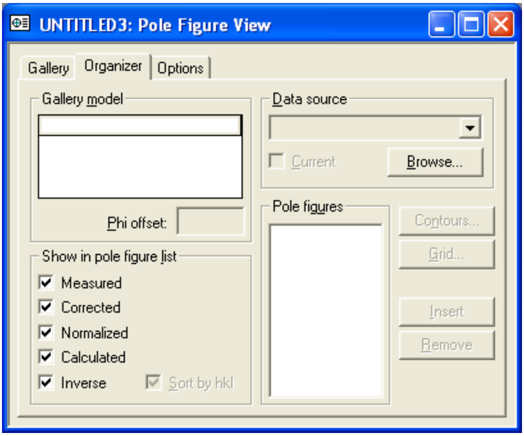
- Start X'Pert Texture by double-clicking on its icon 

, or by selecting *Start/All Programs/PANalytical X’Pert Texture/X’Pert Texture*.
- Click on the tool bar button 

  Or

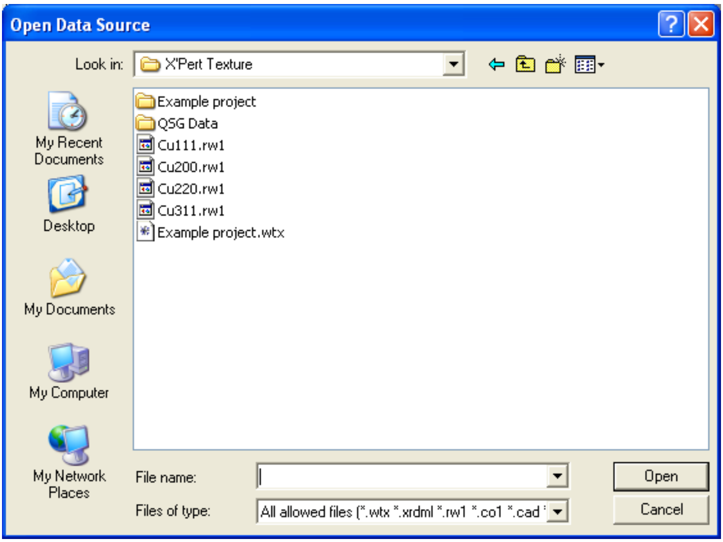
  Select *File - New* to display the “New” window, click on the “Pole Figure View” radio button and then press 

.



Select the input data on the Organizer tab, as follows:

- Click on Browse... and the "Open Data Source" window is displayed.

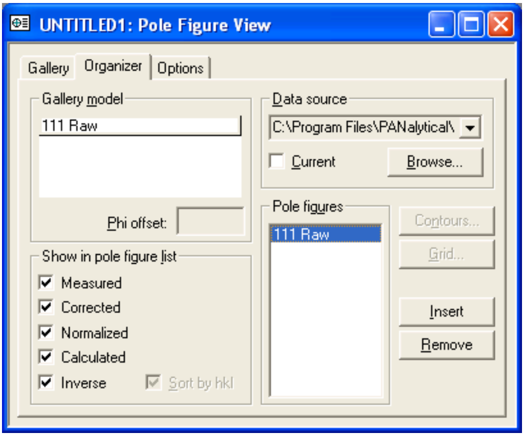


- Browse to "\Program Files\PANalytical\X'Pert Texture" and then select "Cu111.rw1" from the folder, and then click on the Open button.

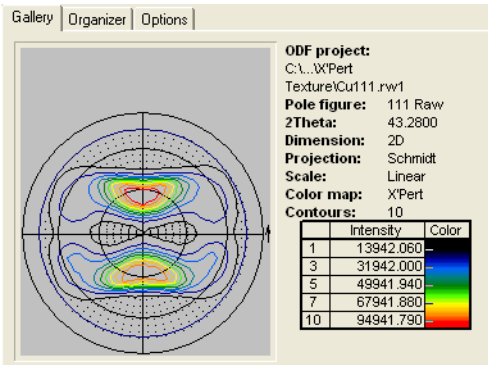
On the “Pole Figure View” window, the path and file name is displayed in the “Data source” field and “111 Raw” is displayed in the “Pole figure” list.

- Click on “111 Raw” and then the 

button, or double-click on “111 Raw” to place the pole figure in the “Gallery model” list.



- Click on the “Gallery” tab to see the pole figure displayed in 2D.



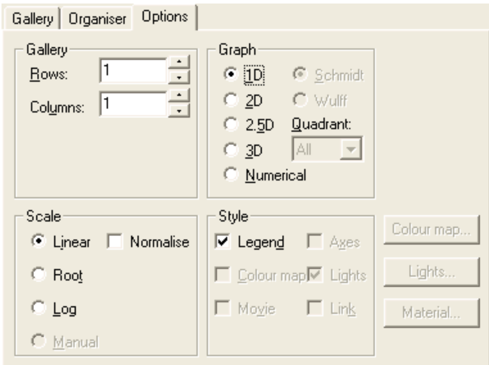
3.3 HANDLING 1D/2D GRAPHS

Now that you have a graph displayed on-screen, you can go on and perform several graphical operations such as switching between dimensions, projections, zooming, scrolling and labelling (text/angles) graphs.

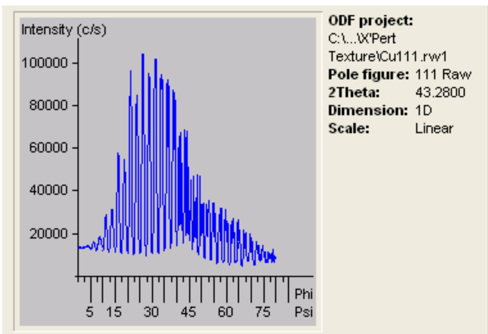
3.3.1 Switching Between Projections

To look at other graphical dimensions, proceed as follows:

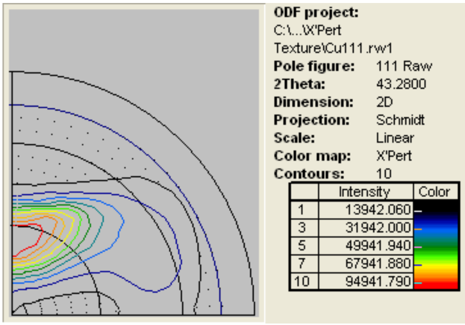
- Click on the "Options" tab.
- Select the type of dimension you want by clicking on the relevant radio button. In this example, select 1D from the "Graph" frame.



- Switch to the "Gallery" tab to see the 1D view of the graph.



If you select 2D on the “Options” tab you can also select the number of the quadrant to be displayed. For the following figure, we selected quadrant 1 and then switched to the “Gallery” tab.



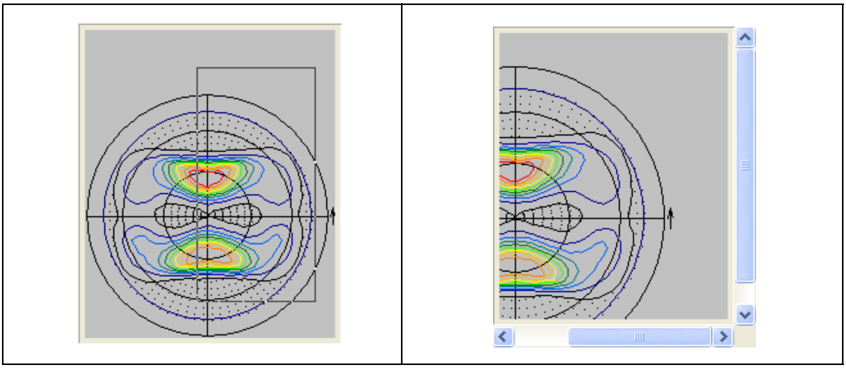
Note: The 2.5D and 3D graphics dimensions are described in Chapter 4 of this Quick Start Guide.

3.3.2 Zooming & Scrolling Graphs

Zooming is the best way of more closely inspecting areas of interest on any of the graphics displayed. The Zoom function operates differently depending on the graphics dimensions you are in. In the next example, we selected all quadrants on the “Options” tab and then clicked on the “Gallery” tab.

To zoom a 1D or 2D graph, proceed as follows:

- Drag the mouse while holding down the left mouse button to draw a rectangle around the area you want to enlarge (see left figure below). When you release the mouse button, the area is enlarged as illustrated on the right figure below.

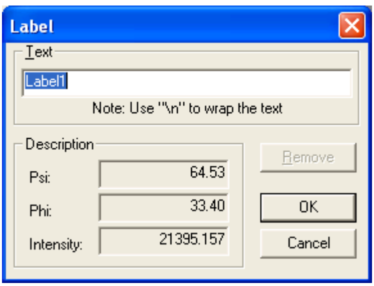


When you enlarge an area on a graph, you can display more of the hidden graph using the scroll bars (see above right figure) or by holding down the ***Ctrl*** key plus the left mouse button and dragging the mouse. Double-clicking in the zoomed area restores the graph to its original size.

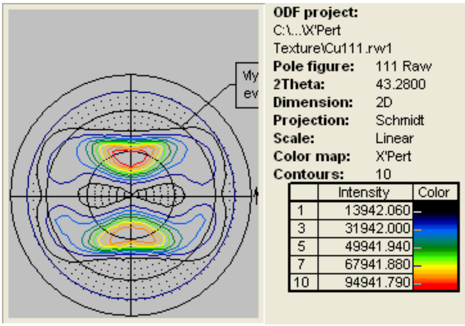
3.3.3 Adding Text Labels to Graphs

You can add text labels to your 1D and 2D graphs as follows:

- Use the *Actions - Label* option or click on the tool bar button **L** to enter the "Label" mode.
- Point at the position to be labelled and with the right mouse button depressed drag to the point where you want the text. When you release the mouse button, the Label window is displayed.

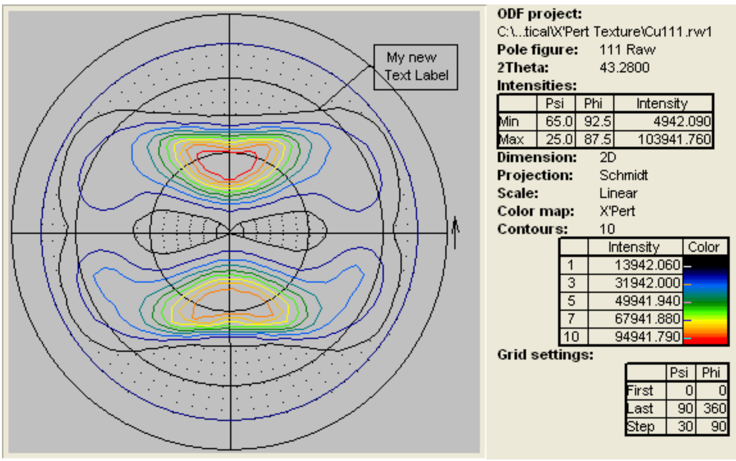


- Enter your text. In the figure, we entered "My New \n Text Label".
- Click OK.



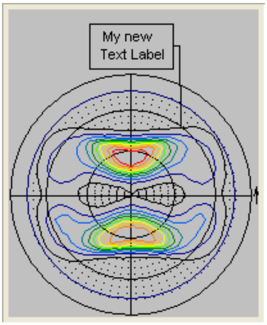
If, as in this example, the label is not completely visible in the window, there are two actions you can take to make it visible:

- Make the complete "Pole Figure View" window larger by grabbing one of the corners and holding the left mouse button down while dragging the window to the required size.



Or:

- By dragging the text box to a new location. Do this by dragging the connecting line with the right mouse button depressed.



Double-clicking the right mouse button with the cursor over the label enables you to either modify or delete the label.

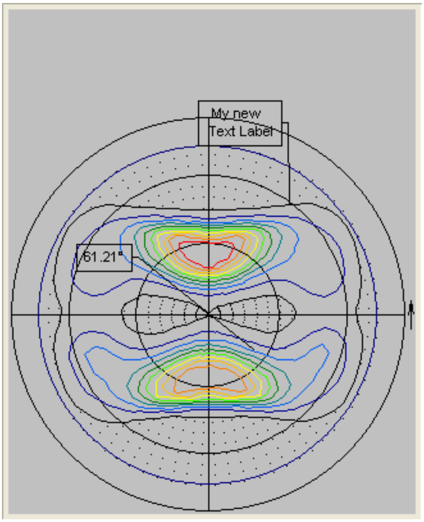
Note: The Label option cannot be used in 2.5D or 3D graphics dimensions. However, labels entered in 1D or 2D remain visible on the graph.

3.3.4 Adding Angle Labels To Graphs

The angular distances between points on a pole figure graph can be calculated and displayed as a label.

- Select 1D or 2D graph on the "Options" tab and then go to the "Gallery" tab. In the following figure we selected 2D.
- Select *Actions - Angle*, or click on the tool bar button A to enter the "Angle" mode.
- Point at the first position on the graph and with the right mouse button depressed drag to the second point.

When you release the mouse button, a label showing the angle between the two specified points, measured on the great circle that connects them, is displayed. The angle α_{AB} is set between the directions (ψ_A, φ_A) and (ψ_B, φ_B).



You can change the position of either point by dragging with the right mouse button depressed.

You can delete the angle by double-clicking the right mouse button when the cursor is on the angle label. Then click Remove.

Note: The "Angle" option is not available in the 2.5D and 3D graphics dimensions. However, angles entered in 1D or 2D remain visible on the graph.

You can now go on with the examples in Chapter 4 or close your graph/view and save it as "View 111.v_p".

CHAPTER 4

ENHANCED DISPLAY

Contents

4.1 INTRODUCTION

In this chapter, we will answer the following questions about 2.5D and 3D graphs:

- What does “Enhanced Display” mean?
- How do I get a 3D graph displayed on screen?
- How can I make it bigger?
- How can I rotate it?
- How can I change the look of the graph?
- How can I enhance the 3D effect?

We will use the file saved at the end of Chapter 3 (View 111.v_p). If you used the proposed defaults during installation, the file is stored in the “C:\Program Files\PANalytical\X'Pert Texture” folder.

4.1.1 What Does Enhanced Display Mean?

The 2D contour map is the traditional way of displaying three dimensional pole figure data: the projection of the data.

2.5D and 3D graphics dimensions present it spatially as a 3-dimensional body:

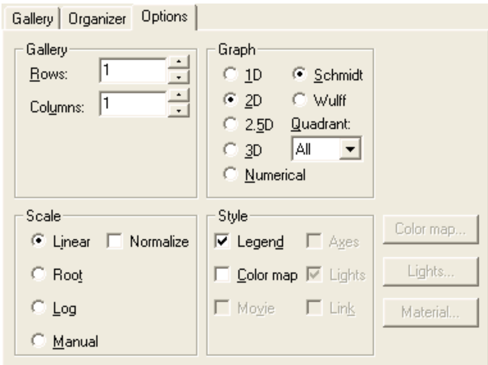
> 2.5D is somewhat reminiscent of the traditional 2D pole figure in that the intensities are vertically extruded from the pole figure.
>
> 3D is the most realistic representation of pole figures and ODFs because the data is displayed in “true” 3D. This enables you to view the data in any plane and enhance how it is displayed using the “Movie” option.

4.2 GETTING GRAPHS ON-SCREEN

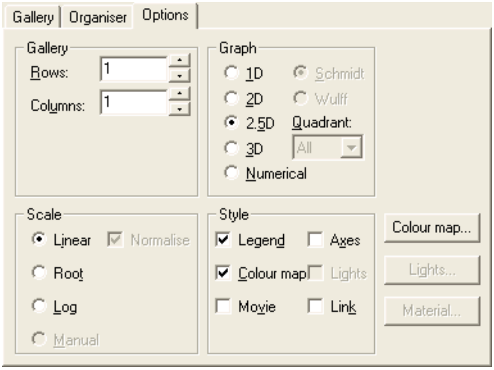
If you do not have the graph from Chapter 3 open, click on the toolbar button and select the file you want to view from the "Open" window.

By default all of the allowed file types are displayed. Use the drop-down list for "Files of type:" ( ) to display other file types. In this example, we selected the file "View 111.v_p" from the folder "C:\Program Files\PANalytical\X'Pert Texture" and then clicked on OK.

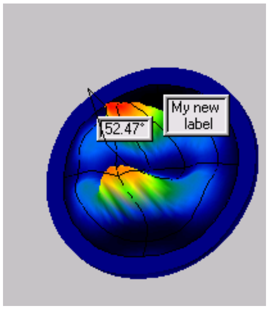
- Click on the "Options" tab.



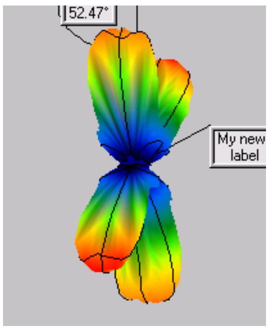
- Select the graphics dimension you want by clicking on the relevant radio button. In this example: select "2.5D" from the "Graph" frame, and "Color map" from the "Style" frame (if "Lights" are checked, you will have to un-check it to make "Color map" available).



- Switch to the "Gallery" tab.



- Switch to the "Options" tab, select "3D" from the "Graph" frame, and switch back to the "Gallery" tab.



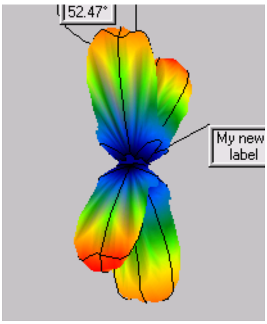
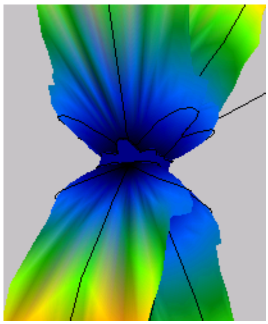
4.3 HANDLING 2.5D/3D GRAPHS

Now that you have a graph displayed on-screen, you can go on and perform several graphical operations such as zooming, rotating and defining lights/materials for graphs.

4.3.1 Zooming & Rotating Graphs

To zoom 2.5D or 3D graphs on the "Gallery" tab, proceed as follows:

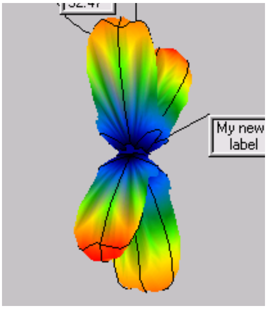
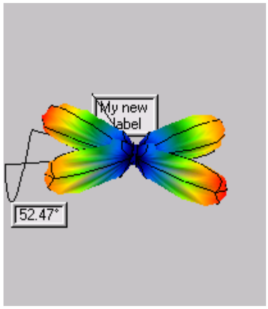
- Hold down the left mouse button and drag the cursor down towards the bottom of the graph to zoom the image. When you release the mouse button the zoom is stopped.
- Hold down the left mouse button and drag the cursor up towards the top of the graph to unzoom the image.

	
Unzoomed 3D Pole Figure	**Zoomed Pole Figure**

Note: Zooming 2.5D or 3D graphs is performed on the center of the "object", not on a selected part.

To rotate 2.5D or 3D graphs on the "Gallery" tab, proceed as follows:

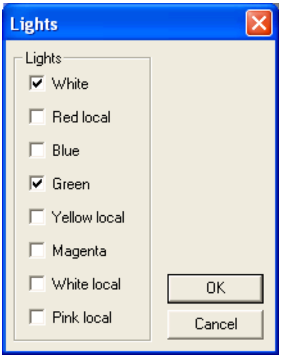
- Hold down the right mouse button and drag the cursor. The direction of rotation is defined by the motion of the "vector" between the center of the figure and the cursor.

	
Unrotated 3D Pole Figure	**The same Pole Figure rotated**

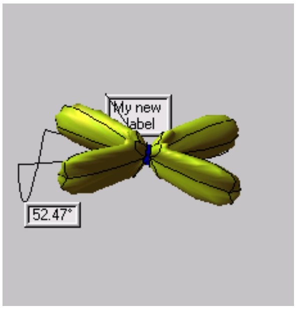
4.3.2 Defining Lights & Materials

The Lights-Material model is a tool which provides enhanced 3D rendering. It displays a 2.5D or 3D shape as a solid body with the surface reflectivity typical for the selected material. This is illuminated by several light sources. By default, the Lights & Materials are enabled when you switch to 2.5D or 3D mode. However, if they are not, proceed as follows on the "Options" tab:

- Uncheck the "Color map" (if it is checked).
- Check the "Lights" check box and click on [Lights...].
- Select the lights model you want, in this example "White" and "Green", and click on [OK]. Then click on [Material...], select the material you want, in this example "Shiny Gold" and click on [OK].



- Use the settings shown above and then click on the “Gallery” tab. The 3D graph will look like the representation below:



CHAPTER 5

MANIPULATING GRAPHS IN THE GALLERY

Contents

5.1 INTRODUCTION

In this Chapter, we will answer the following questions about 2.5D and 3D graphs:

- How do I display multiple graphs?
- How can I apply all my changes simultaneously?

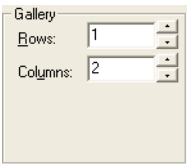
In this Chapter we will use the files “View 111.v_p” and “Cu200.rw1”. If you used the proposed defaults during installation, the files are stored in the “C:\Program Files\PANalytical\X'Pert Texture” folder.

If you do not have a graph open, click on the toolbar button and select the file you want to view from the “Open” window. By default all of the allowed file types are displayed. Use the “List Files Of Type” to display other file types. In this example, select the file “View 111.v_p” from the folder “C:\Program Files\PANalytical\X'Pert Texture” and then click on OK .

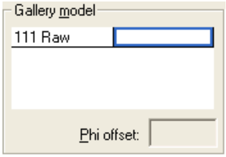
5.2 DISPLAYING MULTIPLE GRAPHS

To add more than one file to the gallery model grid, proceed as follows.

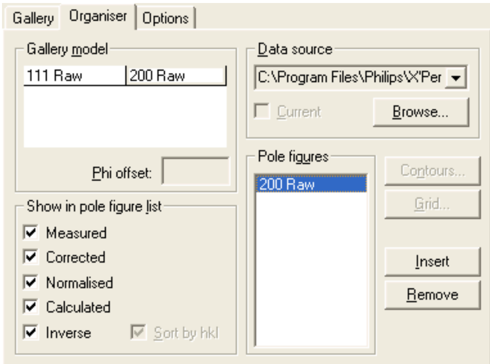
- Switch to the “Options” tab.
- Set “Rows” to 1 and “Columns” to 2.



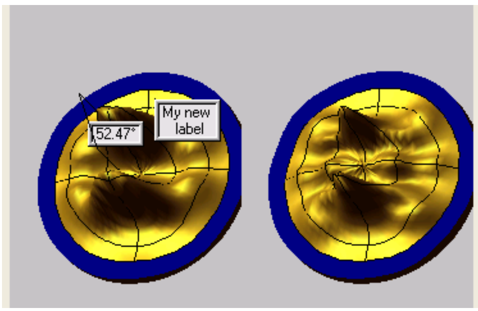
- Click on the “Organizer” tab.
- Click on Browse... .
- Select the “Cu200.rw1” file.
- Click on the second column in the “Gallery model” frame.



- Click on "200 Raw" in the "Pole figures" frame and then either click on  or double-click on the object.



- Click on the "2.5D" radio button in the "Graph" frame on the "Options" tab.
- Switch to the "Gallery" tab and the displayed graph should look like:



5.2.1 Applying Actions Simultaneously to All Graphs

You can zoom or rotate all the 2.5D/3D figures in the Gallery at once. To use this feature, proceed as follows:

- Click on the “Options” tab and check the “Link” check box in the “Style” frame.
- Go to a “Gallery” tab and perform a zoom and/or rotate on one of the graphs and note that all the graphs in the Gallery are manipulated simultaneously.

Note: The “Link” option can be used together with the “Movie” option.

CHAPTER 6

ANALYZING TEXTURE DATA

Contents

6.1 INTRODUCTION

In this Chapter, we are going to set-up an ODF Project, calculate the Orientation Distribution Function and a Pole Figure. Then observe the ODF in 2D and 3D graphics.

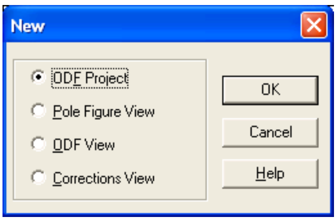
Typically, texture calculations comprise the following steps:

- Create an ODF Project, then insert your experimental pole figures and correction files.
- Perform correction of the raw pole figures. The corrected pole figures are added to the ODF Project object list (not done in this example).
- Calculate the ODF. The resulting data is added to the list.
- Calculate pole figures or inverse pole figures from the ODF. All new objects are added to the list.

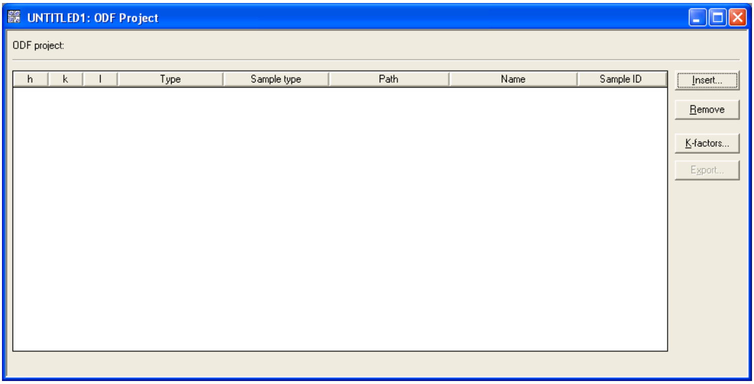
6.2 SETTING UP AN ODF PROJECT

To create an ODF project, proceed as follows:

- Select *File - New*, the "New" window is displayed.



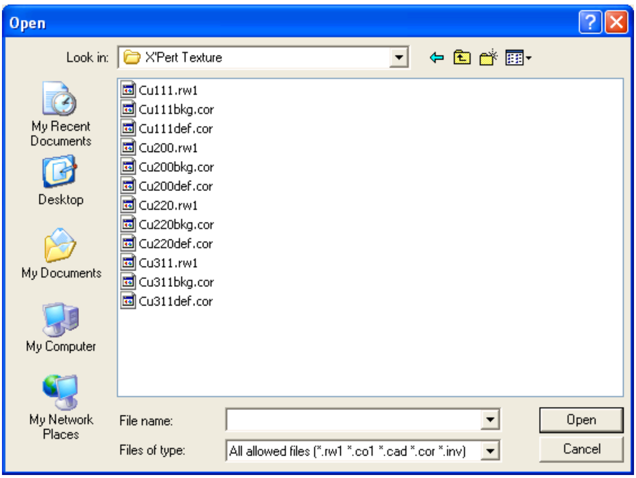
- Click on the "ODF Project" radio button and then on OK. The ODF Project window is displayed.



On this window, you specify which files are used in the calculations and stored together as an ODF project. In addition, all the calculated data you create is displayed on this window.

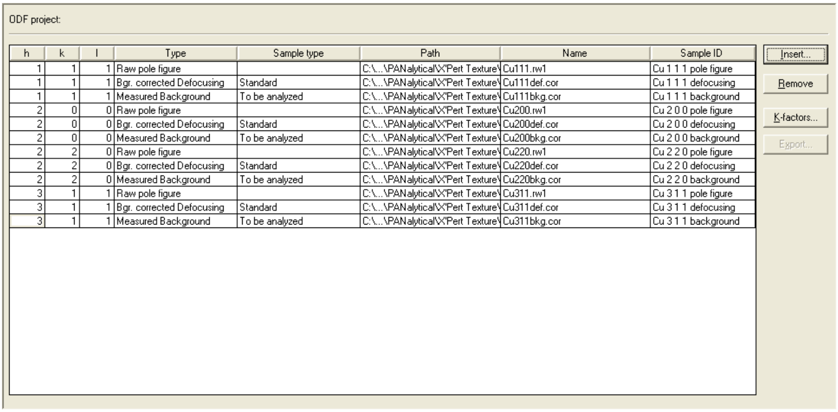
6.2.1 Adding Files

- Click on Insert, select the files you want to analyze from the "Open" window and click Open.



Refer to Chapter 2 of the User's Guide for detailed information on the file formats you can use.

- In this example: select "Cu111.rw1", "Cu111bkg.cor", "Cu111def.cor", "Cu200.rw1", "Cu200bkg.cor", "Cu200def.cor", "Cu220.rw1", "Cu220bkg.cor", "Cu220def.cor", "Cu311.rw1", "Cu311bkg.cor" and "Cu311def.cor". The ODF Project window should now look as follows:



ODF project:

h	k	l	Type	Sample type	Path	Name	Sample ID
1	1	1	Raw pole figure		C:\...\PANalytical\X'Pert Texture\	Cu111.rw1	Cu 1 1 1 pole figure
1	1	1	Bgr. corrected Defocusing	Standard	C:\...\PANalytical\X'Pert Texture\	Cu111def.cor	Cu 1 1 1 defocusing
1	1	1	Measured Background	To be analyzed	C:\...\PANalytical\X'Pert Texture\	Cu111bkg.cor	Cu 1 1 1 background
2	0	0	Raw pole figure		C:\...\PANalytical\X'Pert Texture\	Cu200.rw1	Cu 2 0 0 pole figure
2	0	0	Bgr. corrected Defocusing	Standard	C:\...\PANalytical\X'Pert Texture\	Cu200def.cor	Cu 2 0 0 defocusing
2	0	0	Measured Background	To be analyzed	C:\...\PANalytical\X'Pert Texture\	Cu200bkg.cor	Cu 2 0 0 background
2	2	0	Raw pole figure		C:\...\PANalytical\X'Pert Texture\	Cu220.rw1	Cu 2 2 0 pole figure
2	2	0	Bgr. corrected Defocusing	Standard	C:\...\PANalytical\X'Pert Texture\	Cu220def.cor	Cu 2 2 0 defocusing
2	2	0	Measured Background	To be analyzed	C:\...\PANalytical\X'Pert Texture\	Cu220bkg.cor	Cu 2 2 0 background
3	1	1	Raw pole figure		C:\...\PANalytical\X'Pert Texture\	Cu311.rw1	Cu 3 1 1 pole figure
3	1	1	Bgr. corrected Defocusing	Standard	C:\...\PANalytical\X'Pert Texture\	Cu311def.cor	Cu 3 1 1 defocusing
3	1	1	Measured Background	To be analyzed	C:\...\PANalytical\X'Pert Texture\	Cu311bkg.cor	Cu 3 1 1 background

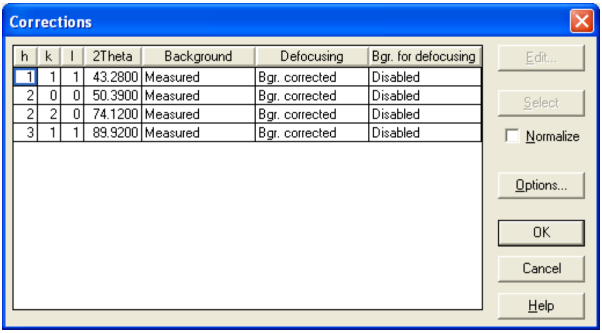
Insert...
Remove
K-factors...
Export...

- Save the ODF project by selecting *File - Save* and giving it the name "ODF rolled copper".

6.2.2 Performing Corrections

The next action is to correct the raw pole figure data for background intensities and defocusing affects.

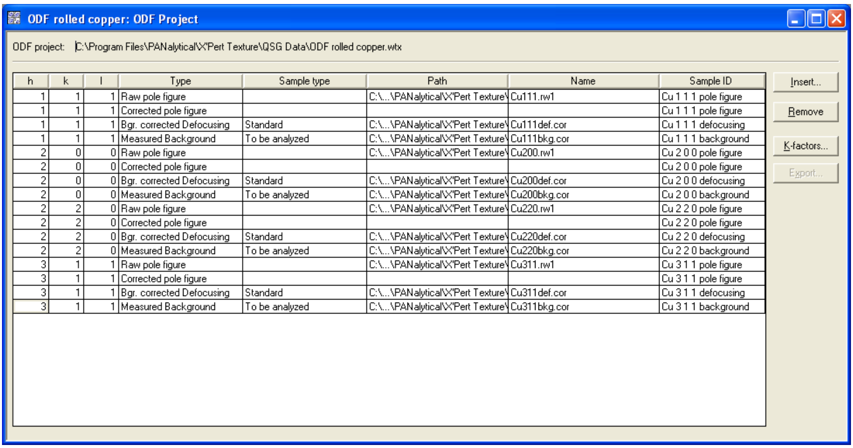
- Select Actions - Corrections, the "Corrections" window is displayed.



By default the available correction data from the ODF project are shown in the “Background”, “Defocusing” and “Bgr. for defocusing” columns. In this example we are going to use the background corrected defocusing data. You can select other correction methods by pressing the Select button.

- Press the OK button and the corrections are performed.

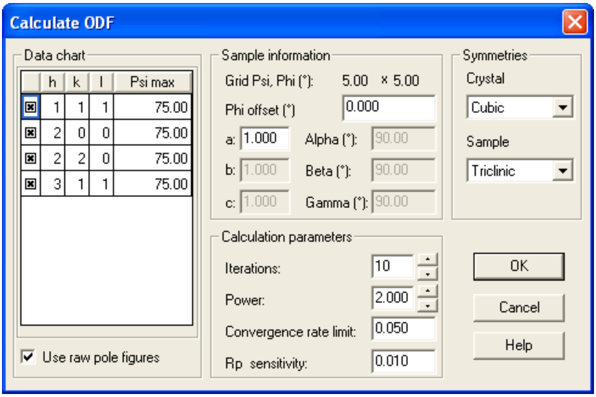
The corrected pole figures are added to the list in the ODF project.



6.2.3 Calculating ODF

Now we will calculate the ODF from the measured (raw) Pole Figures.

- Select *Actions - Calculate ODF* and the "Calculate ODF" window is displayed.
- Make sure that the "Use raw pole figures" check box is not checked in order to use the corrected pole figure data for the ODF calculation.



- In the "Data chart" frame, make sure that all of the pole figures are selected for use in the ODF calculation (the ⊠ is shown in the left-hand column of the table).

The "h" "k" "l" fields indicate the Miller indices of pole figures. "Psi max" is the maximum value of Psi available or allowed for use in ODF calculation. In this example, we selected pole figures 111, 200, 220 and 311, Psi max = 75º.

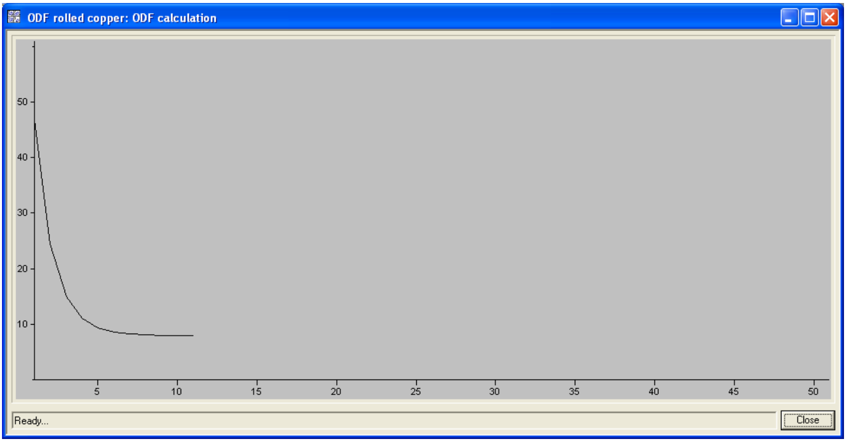
- Select "Cubic" from the "Crystal" drop-down list in the "Symmetries" frame and "Orthorhombic" from the "Sample" drop-down list in the "Symmetries" frame.
- Click on the "Iterations" to define the maximum number of iterations that will be applied during the ODF calculation. In this example, we selected the proposed default value (10).
- Click on the "Power" to define the exponent in the equation for the calculation of the sum of differences between measured and calculated pole figures. In this example, we used the proposed default value (2.000).

The Convergence rate limit defines the minimum value of the convergence criterion (Rp), when the ODF calculation will be stopped. We used proposed default value (0.050) in this example.

The Rp sensitivity defines the minimum value of the changes of the convergence criterion Rp, when the calculations will be stopped, we used the proposed default values in this example (0.010).

- Press OK.

The ODF calculation starts, displaying the window with the progress indicator.



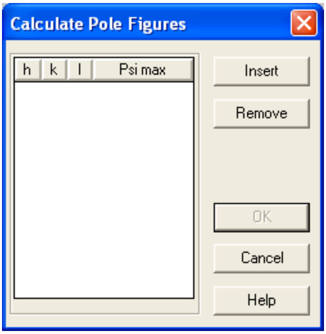
- Close the ODF Calculation window (Close) when the calculations have finished (the progress indicator shows “Ready...”).

The ODF data is added to the project.

6.2.4 Calculating Pole Figures

Now we will calculate a 311 Pole Figure from the ODF.

- Select *Actions - Calculate Pole Figures...* The “Calculate Pole Figures” window is displayed. This is only active when the ODF data is available in the ODF project.



On this window, you can specify the parameters that are necessary for the calculation of pole figures from the ODF.

- Click on Insert to insert a new row in the grid. This is necessary before you can enter the hkl values for the pole figure.
- Enter "3", "1", "1".

The Psi max column defines the maximum value of Psi to be used during the calculation.

Note: Normally, pole figures are calculated up to 90°. Alternatively, use the same values as in the measured pole figures (used for the ODF calculations) to simplify comparison.

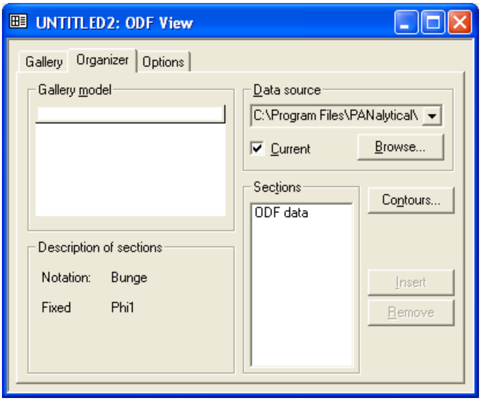
- Click on OK. Note that there no graph, however, you can watch the progress of the calculation on the progress indicator.
- When the calculations have finished (the progress indicator shows "Ready...") close the "Pole figure calculation" window ().

After the Pole Figure is calculated, it is included in the ODF Project as internal file.

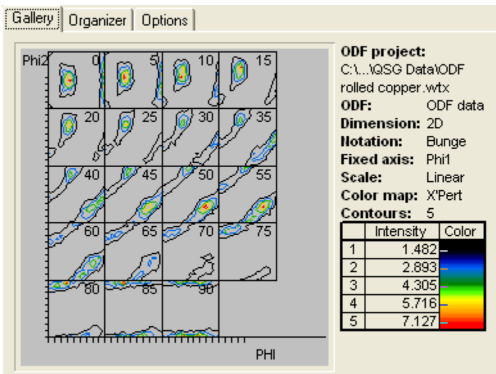
6.3 ANALYZING ODF DATA

- Make sure that the ODF Project (“ODF rolled copper”) is open.
- Select *File - New* and select “ODF View”, or click on the tool bar.

The ODF View window is displayed with the current project in the “Data Source” field and “ODF data” in the “Sections” list.



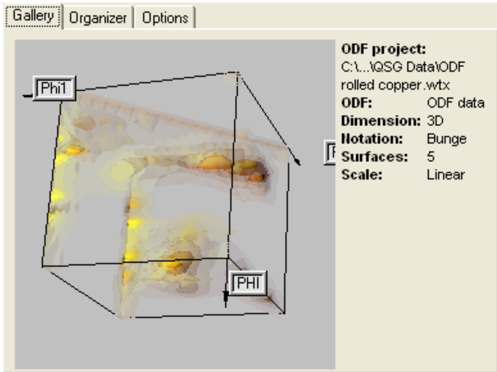
- Click on “ODF data” in the “Sections” frame and press Insert.
- Click on the “Gallery” tab.



The 2D graph of the ODF is displayed.

- Go to the "Options" tab and select the "3D Iso-surfaces" radio button in the "Graph" frame.
- Click on the "Gallery" tab again.

The 3-dimensional graph of the ODF just calculated is displayed.

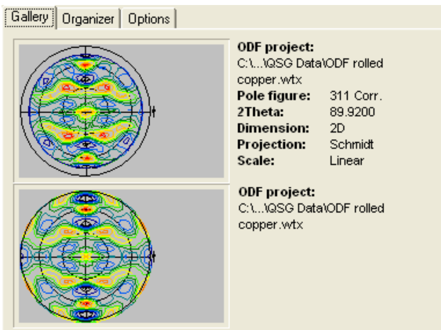


6.4 COMPARING POLE FIGURES

With the ODF Project “ODF rolled copper” open, proceed as follows:

- Select *File - New*, select “Pole Figure View” or click on the toolbar button.
- Click on the “Organizer” tab, check the “Current” check box and the “Data source” will display “.\ODF rolled copper.wtx”, (the current project).
- Go to the “Options” tab and select 2 rows, 1 column in the “Gallery” frame.
- Select the “Linear” radio button in the “Scale” frame and check the “Normalize” check box.
- Go to the “Organizer” tab, click on “311 Corr.” in the “Pole figures” list and then Insert.
- Click on the second row in the “Gallery model” frame, click on “311 Calc.” in the “Pole figures” list and then Insert.
- Click on the “Gallery” tab.

The corrected and calculated 311 pole figures can now be compared. The maxima are at the same places in both pole figures. The relative intensities differ significantly. The corrected pole figures were used for calculation of the ODF from which the calculated pole figure was derived.



- Save the view. We saved this version as “2PFs.v_p”.

CHAPTER 7

PROCESSING GRAPHICS & TABLES

Contents

7.1 INTRODUCTION

In this Chapter, we will illustrate how to export files for importing into other texture or Windows applications. Print Setting up, Print Preview and Printing are described in Chapter 10 of X'Pert Texture User's Guide.

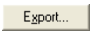
7.2 EXPORTING DATA

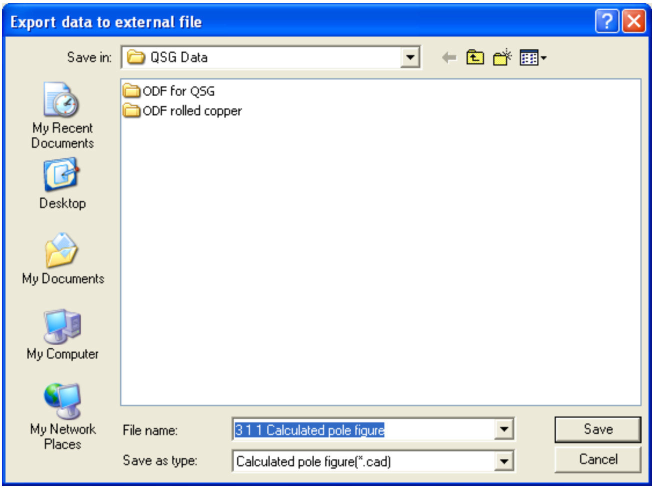
Two types of information are available for further use in X'Pert Texture: numerical and graphical. This information can be stored in X'Pert Texture format or it can be exported into formats used by other applications.

7.2.1 Export To External Files

The results of texture calculations (ODF, pole figures, inverse pole figures, corrections) are available in the form of internal files.

To export pole figures (calculated, corrected or inverse) or correction data into PC-Texture format data, proceed as follows:

- Switch to or open an ODF Project.
- Click on the object (pole figure, inverse pole figure or correction curve), to be exported. In our example, we selected "311 calculated pole figure".
- Click on . The "Export data to external file" window is displayed.



- Enter the name of the file the data will be exported to. The default proposed was "3 1 1 Calculated pole figure".

Note: The default export directory is defined as described in the section on setting the Environment options.

- Click on Save. The data is exported in PANalytical *.cad format.

Notes: a. To convert *.rw1, *.co1 or *.cor file to other formats, use the PHILCONV program. Inverse (*.inv) and calculated (*.cad) pole figures can be converted as *.rw1 files if you change their file extensions to rw1.

b. The export function is not available for ODF. Use export via the Clipboard for ODF (see next section).

7.3 USING THE CLIPBOARD

Any graphical or numeric data displayed on the “Gallery” tab of a View window can be copied to the Windows Clipboard and then pasted into other Windows applications.

To do this, proceed as follows:

- Create the required data in the Gallery. In this example, we opened 2PFs.v_p and then switched to the “Gallery” tab.
- Maximize the “Gallery” window to enhance the print quality.
- For graphics, click on the graph you want to place on the Clipboard. For numerical tables, mark the area of the text you want to export.
- Select *Edit - Copy* or click on  on the tool bar. The information is placed on the Clipboard.

To paste the contents of the Clipboard into another Windows application, use the Paste option in the application. To paste the contents of the Clipboard with a conversion of the format, use the Paste Special option.

For example: numerical data from X'Pert Texture can be pasted in Microsoft Word as formatted or unformatted text. Graphics can be pasted in Word in picture format (recommended) or as a bit map. A bit map can also be pasted in other applications, such as Paint(brush).

CHAPTER 8

AUTOMATING VIEWING OF POLE FIGURES

Contents

8.1 INTRODUCTION

It is possible to automate viewing of pole figures either by using the Automatic Processing Program (APP) supplied as an add-on with the X'Pert Data Collector, Version 2.0 (or later), or by using X'Pert Texture directly from the command line (for example: by defining a shortcut).

This chapter demonstrates a simple example using a script. This is explained in the APP help file.

8.2 AUTOMATIC VIEWING OF POLE FIGURES USING THE APP

Assume that you are working with the X'Pert Data Collector and you have created a texture program called Program 1. To print out the texture data immediately after it has been collected:

- Start the X'Pert Data Collector.
- Use the right mouse button to click on the “APP” icon in the system tray at the right-hand end of the Windows taskbar.
- Select *Configure*.
- In the “Build Rule” frame enter the details of the X'Pert Data Collector program type “Texture”.
- In the “Command” field enter the path name for running X'Pert Texture: “C:\Program Files\PANalytical\X'Pert Texture\Wintex.exe”.
- In the “Arguments” field enter %XMLFILE% /2ndcopy /p /nologo

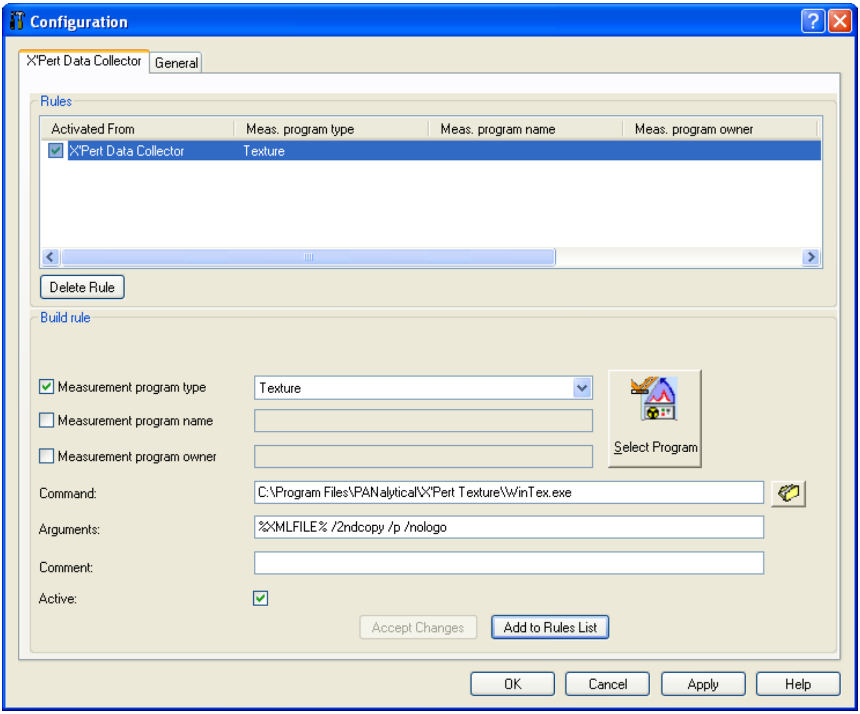
  where: %XMLFILE% is used to indicate the measured file

  /2ndcopy indicates that a second copy of X’Pert Texture be opened

  /p indicates that the scan must be printed

  /nologo indicates that the X'Pert Texture startup screen will be suppressed.

- Activate the rule you have just saved by ticking the “Active:” check box.
- Click on the Add to Rules List button.



- Press OK to save and close the “Configuration” window.
- Return to the X'Pert Data Collector, start data collecting, and when the texture measurement has been completed it will be printed out.

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