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X'PERT REFLECTIVITY

Quick Start Guide

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X'Pert Reflectivity

Quick Start Guide

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This is the third edition of this publication, it is intended for use with version 1.2 of X'Pert Reflectivity software.

ACKNOWLEDGMENTS

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Contents

PANalytical

Chapter 1

Introduction

Contents

X'Pert Reflectivity - Quick Start Guide

Chapter 1. Introduction

1.1 Introduction

This Quick Start Guide is intended to help you to use X'Pert Reflectivity quickly and efficiently. A brief overview of X'Pert Reflectivity is given at the end of this chapter. The next two chapters provide worked examples. These examples have been chosen to demonstrate the most important functionality of X'Pert Reflectivity.

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

1.2 Contents of the Quick Start Guide

The worked examples in this Quick Start Guide are:

Chapter 2: Simulating and Fitting a Simple Structure
The example in this Chapter describes how to create a sample consisting of a substrate and two single layers. Once the sample has been created, the exercise will then go on to show how to perform a simulation and how to fit the sample parameters using both the Segmented fitting and Genetic Algorithm routines.

Chapter 3: Simulating and Fitting Samples with Superlattice Layers
The example in this Chapter describes how to create a new sample and then compare that new sample with the data from a previously measured sample.

Chapter 4: Determining the Thickness of a Layer
The example in this Chapter describes how to open a measured data file and use two different methods of checking the thickness of a layer.

Chapter 5: Simulating and Fitting SiGe on Si
The example in this Chapter describes how to open a measured sample and then fit a simulated graph to that sample.

Chapter 6: Diffuse Scatter
The example in this Chapter describes how to open an ω-scan and find out what Hurst parameter and lateral correlation lengths best suit the sample.

Chapter 7: Checking the Vertical Correlation

The example in this Chapter describes how to open a sample with superlattice structure, perform a simulation of a reciprocal space map, and then change the vertical correlation settings to show the influence on the simulation pattern of the vertical correlation of the roughness between the layers.

Chapter 8: Automating Your Diffraction Measurements/Analyses

This chapter demonstrates two simple examples of automating your analyses either using X'Pert Reflectivity directly from the command line.

1.3 Terms and Conventions Used

This section describes the terms and conventions used in this Quick Start Guide and how they relate to the graphical user interface.

1.3.1 Terms Indicating an Action

Click	Press the left (primary) mouse button and quickly release it.
Check (✔)	Switch an option or an item on or off, usually by clicking on it. Also referred to as a tick mark.
Confirm	In the examples in this Quick Start Guide we terminate most actions by pressing the **OK** button. When the **OK** button is the default button (indicated by a thick shadow) you can press the ***Enter*** key as well.
Double-click	Press the left (primary) mouse button twice (quickly) on an icon, button, item or program.
Drag	Press and hold down the mouse button and move the pointer to move an object or define an area.
Enter	Type in information. This can be either text or numerical data.

Press	A key on the keyboard or a button (using the left mouse button) in a window.
Right-click	Press the right (secondary) mouse button and quickly release it on an item. This opens a context-sensitive pop-up (or: shortcut) menu.
Select	Move the pointer to the option you want and click the left mouse button.
Tick (✔)	Switch an option or an item on or off, usually by clicking on it. Also referred to as a check mark.
Toggle	Switch between parameters or states (for example: On-Off-On, Visible-Invisible-Visible).
	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 proceeded 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 are intended to show you what you will see on your screen when you perform that action. However, if there are any differences, follow what you see on your screen.

1.3.3 Buttons and Fields

Buttons in a dialog frame are indicated by bold text (for example: **Apply** or **Cancel**), or shown as the actual button image (for example: 

). All fields and tabs in a window are shown between “quotation marks”.

1.3.4 Menu Items and Keys

Menu items are shown in italics, for example: *File* - *Open* etc.

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

1.4 The Menu Structure

X'Pert Reflectivity appears as in Figure 1-1 when the software is started and a measured data file is loaded.

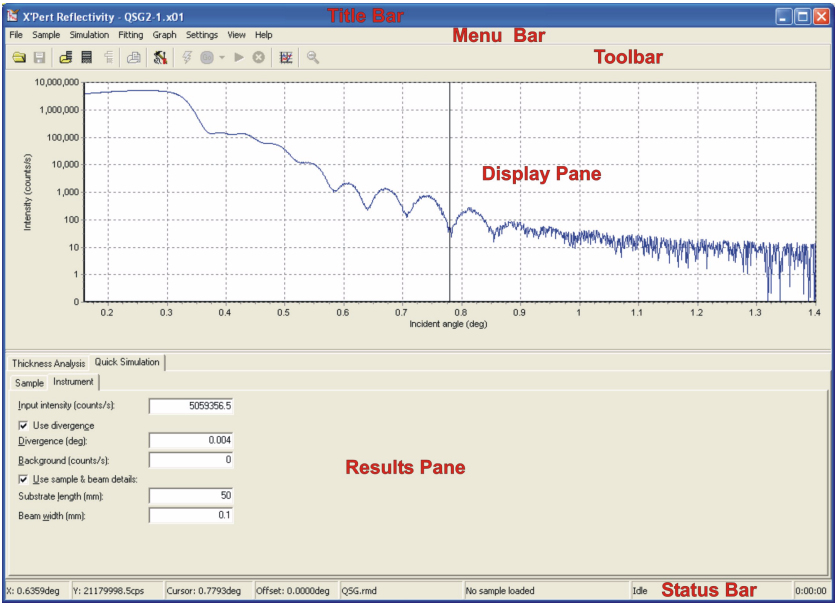

Figure 1.1: The X'Pert Reflectivity Window

The window has a title bar, a menu bar, a toolbar, a display pane, a results pane, and a status line at the bottom. There are eight menu items, they are:

File	To load data, print and so on.
Sample	To open, create and edit samples and material data.
Simulation	To open the simulation setup window and perform a simulation.
Fitting	To select the type of fitting to be performed, open the setup window and perform the fitting. There is also an item to allow you to analyze any errors that may have occurred in the fitting.
Graph	To set the style of the graph that is displayed in the display pane.

Settings To set the program defaults.

View To choose whether the measured data should be displayed as a graph, report or a data file. Also allows the results pane and status bar to be displayed at the top or bottom of the main window, or not at all.

Help To access help information, the release notes and information about this packet.

1.5 Data Files for Use with this Quick Start Guide

Several data files have been supplied with X'Pert Reflectivity Version 1.2 for you to use with this Quick Start Guide. Those files are installed in folder: "C:\Program Files\PANalytical\X'Pert Reflectivity\Examples" and they are:

Used in:	File	Contents
Chapter 2	QSG2-1.x01	Measurement of Fe3O4 on CoO on SrTiO3
Chapter 3	QSG3-1.x01	Measurement of AlAs_GaAs
Chapter 4	QSG4-1.x01	Measurement of SiGe on Si
Chapter 6	QSG6-1.xrdml QSG6-1.sam	Measurement of SiO2 Prepared sample file
Chapter 7	QSG7-1.sam	Prepared sample file
Chapter 8	QSG.rmd Sample 1 for QSG.sam QSG2-1.x01	The materials database created in section 2.2.1. The sample created in section 2.2.2. Measurement of Fe3O4 on CoO on SrTiO3

X'Pert Reflectivity - Quick Start Guide

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Chapter 2

Simulating and Fitting a Simple Structure

Contents

Chapter 2. Simulating and Fitting a Simple Structure

2.1 INTRODUCTION

This exercise will show you how to create a sample consisting of a substrate and two single layers. Once the sample has been created, the exercise will then go on to show how to perform a simulation and how to fit the sample parameters using both the Segmented fitting and Genetic Algorithm routines.

Firstly we'll add three materials to the file containing the material data:

CoO density = 6.45 g/cm^3

Fe_3O_4 density = 5.18 g/cm^3

$SrTiO_3$ density = 5.1 g/cm^3

Then create a sample comprising:

Substrate = $SrTiO_3$ roughness= 1 nm

Layer 1 = CoO thickness = 40 nm roughness = 1 nm

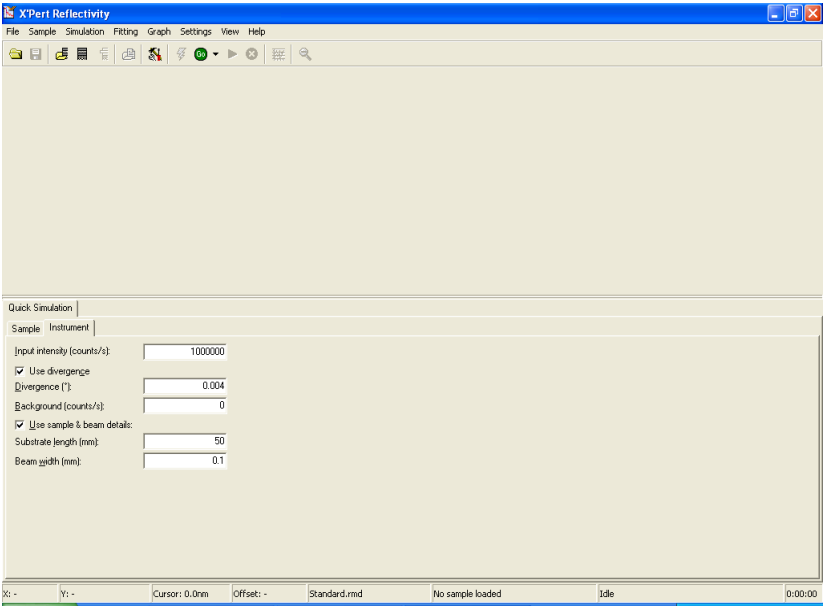
Layer 2 = Fe_3O_4 thickness = 10 nm roughness = 1 nm

Then set up the simulation conditions and perform a simulation, followed by the procedure to set up the fitting parameters and then perform a fit.

2.2 PREPARING THE SAMPLE DATA

- Double-click on the X'Pert Reflectivity Icon 

to start the program.



- If this X'Pert Reflectivity has been used before, go to the next bullet action. If this is the first time that you are using the program: select *Sample - Open Material Data...* from the Menu bar.

  Make sure that the drop-down box "Files of type:" has "Material data files (*.rmd) selected.

  Select "Standard.rmd" and press 

, note that the status bar now shows "Standard.rmd" in the fifth box from the left to show that this is the current database.

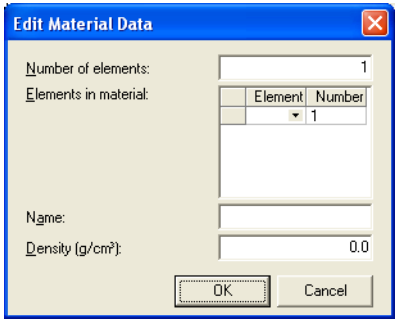
Now we are going to add three new materials into the materials database.

2.2.1 Adding New Materials to the Material Data File

- Select *Sample - Edit Material Data...*

  In the "Material Data" tab, select "DensityOnly".

  Press the Insert Material... button.



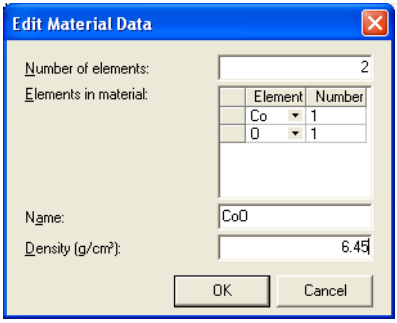
  Enter 2 in the "Number of elements" field.

  Place your cursor in the "Element" box in the "Elements in material" field. A drop-down list of elements appears when you click the mouse button. You can either select the element you require (in this example: Co), or just keep typing the letter "C" until Co appears. Click again and the drop-down list disappears. Now enter the second element (O) by clicking in the second element box, type "O".

  Click in the "Name" field and accept the proposed material name: "CoO".

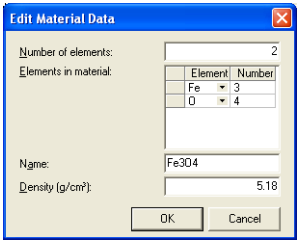
  Click in the "Density" field and enter the material's density: "6.45".

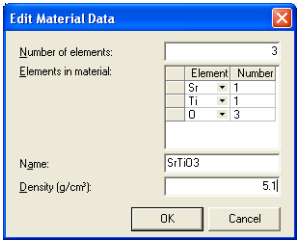
  The completed form should look like this:



Press the OK button and the new material is added in its alphabetical place in the "DensityOnly" branch of the materials database.

- Select "DensityOnly", press the Insert Material... button again and repeat the procedure for the next material: Fe_3O_4 with a density of 5.18 g/cm^3, repeat the procedure for the third material: $SrTiO_3$ with a density of 5.1 g/cm^3 as shown below:



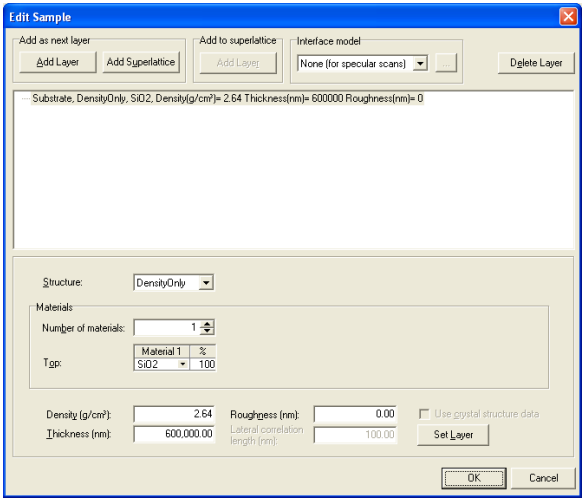


Once you have added all three materials, press the OK button. In the "Save As" window give the materials database the file name "QSG.rmd" and press the Save button.

NOTE: You can set the automatic saving function on or off on the "General" tab of *Settings - Defaults...*

2.2.2 Creating the Sample

- Select *Sample* - *New Sample*.



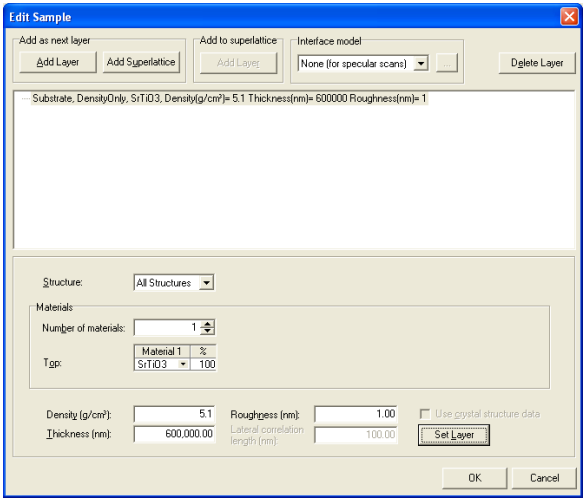
Select “All Structures” (or “DensityOnly”) from the “Structure:” drop-down list.

In the “Materials” frame select “SrTiO3” from the “Material 1” drop-down list.

The “Density (g/cm3):” field should show the density “5.1”.

Enter 1 in the “Roughness (nm):” field.

Press the Set Layer button. This layer is now the substrate.



- Add the next layer:

  In the "Add as next layer" field, press the Add Layer button.

  Select "All Structures" (or "DensityOnly") from the "Structure:" drop-down list.

  In the "Materials" frame select "CoO" from the "Material 1" drop-down list.

  The "Density (g/cm3):" field should show the density "6.45".

  Enter 40 in the "Thickness (nm):" field.

  Enter 1 in the "Roughness (nm):" field.

  Press the Set Layer button. This layer is now Layer 1.

- Add the last layer:

  In the "Add as next layer" field, press the Add Layer button.

  Select "All Structures" (or "DensityOnly") from the "Structure:" drop-down list.

  In the "Materials" frame select "Fe_3O_4" from the "Material 1" drop-down list.

  The "Density (g/cm^3):" field should show the density "5.18".

  Enter 10 in the "Thickness (nm):" field.

  Enter 1 in the "Roughness (nm):" field.

Press the Set Layer button. This is layer is now Layer 2.

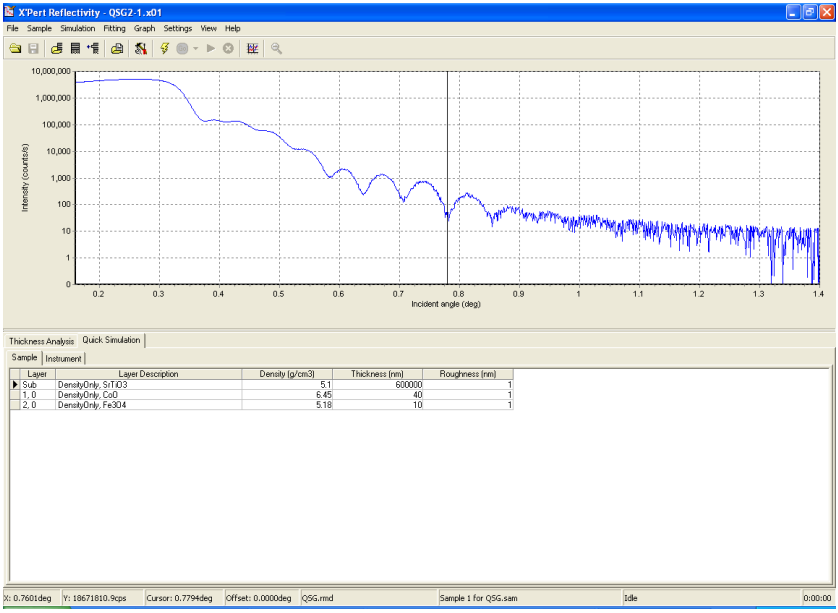
Press the OK button. Depending on your default settings, the sample will be temporarilly stored as “New Sample.sam” which you can save via *Sample - Save Sample...*, or the program opens the “Save As...” window.

Save the sample as “Sample 1 for QSG”.

If you have checked the “Always prompt to save fit settings when sample is saved” in *Settings - Defaults...* a further window offering you the chance to save the settings file will appear. You have not changed the settings file yet, so just press Cancel.

2.3 Setting Up the Simulation

- Open the measured file that you want to simulate by selecting *File - Open Measured Data...* in this example: “../X’Pert Reflectivity/Examples/QSG2-1.x01” a sample containing Fe_3O_4 on CoO on $SrTiO_3$.



- Select *Simulation - Setup....*

  Select the "Specular" radio button.

  Make sure the values are:

  In the "Scan Details" frame:

  "Start (º):"=0.16º

  "End (º):"=1.4º

  Make sure that the "Normalize intensity" box is checked.

  In the "Convolution Details" frame:

  Make sure that the "Use divergence" box is checked.

  "Divergence (º):" = 0.004º

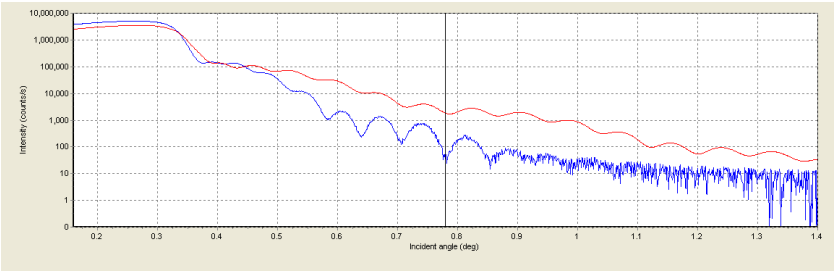
  "Background (counts/s):" = 5

  In the "Sample and Beam Details" frame:

  Make sure that the "Use" box is checked.

  "Substrate length (mm)" = 20

- Press the OK button and a simulation should start (a red line appears on the graph).



2.4 FITTING

2.4.1 Check the Defaults

Before we start the fitting we must make sure that the default settings are as required.

- Select *Settings - Defaults....*

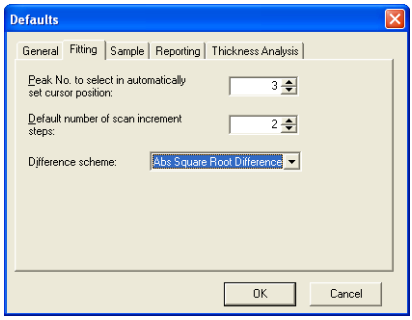
  Select the "Fitting" tab and set the following values:

  "Peak No. to select in automatically set cursor position:" 3

  "Default number of scan increment steps:" 2

  "Difference scheme:" Abs Square Root Difference

- The tab should look like the example shown below:

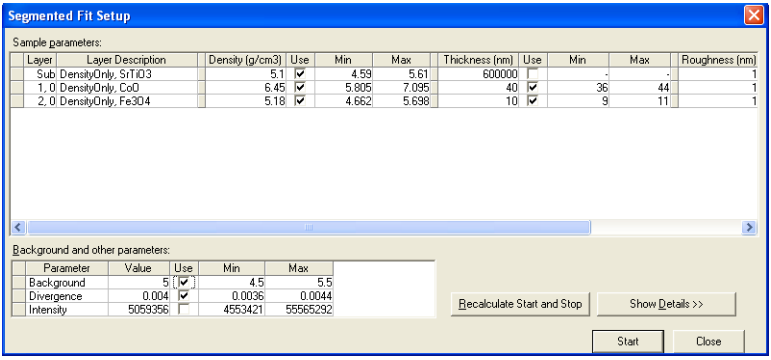


Press the OK button.

2.4.2 Start the Segmented Fitting

In this part of the exercise we are going to tell the program which fitting parameters to use and move the cursor to the end of the initial fitting scan range.

- Select *Graph - Automatically Set Cursor Position* (or press the button). This will move the cursor to the third peak as found by the peak search algorithm as you set in the defaults.
- Select *Fitting - Segmented Fit....* The "Segmented Fit Setup" window opens to allow you to set the fitting conditions:



In the "Sample parameters:" grid "Density" "Use" column, uncheck all three rows. You can do this one at a time, or clicking on the heading "Use" toggles all of the entries in that column on and off.

Set the "Thickness" and "Roughness" values as follows:

Layer	Parameter	Min	Max
Sub	Roughness	0.5	1.5
1,0	Thickness	10	46
1,0	Roughness	0.5	2.5
2,0	Thickness	5	15
2,0	Roughness	0.5	2.5

In the "Background and other parameters:" table set the values as follows:

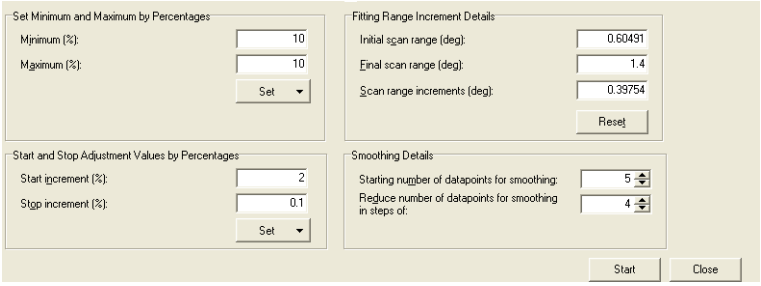
Parameter	Max
Background	8
Divergence	0.008

In the "Sample parameters:" grid, select the substrate and both the layers. You can do this by placing the cursor in the grey box at the left end of one of the rows, clicking, pressing ***Shift***, moving the cursor to the grey box at the left end of the next row, clicking again

and so on. Or you can do it by clicking in the left-hand top grey box (just to the left of the word Layer) and clicking to select all three rows.

Press the Recalculate Start and Stop button.

Press the Show Details >> button.



Press the Start button and the fitting starts. Watch the red line, it should stay close to the blue line, if it doesn't, as in this example, the fitting parameters should be changed. For example: increase the minimum and maximum ranges, or try another fitting method (*Genetic Algorithm...* or *Combined Fitting Mode...*). If you accepted the defaults, you will be asked "Fitting has finished. Update sample now?", click No as we are not satisfied with the result and will try to improve it.

2.4.3 Fitting - If the Sample Parameters are a Long Way Out

If the layer values of the initial file were a long way out you would most likely find that the Segmented Fitting does not return a good result. In this case you should try another fitting method, for example the Genetic Algorithm, or the Combined Fitting Mode.

To demonstrate this we will first edit the sample so this is not as well matched.

- Select *Sample - Edit Sample*.

  Select Layer:1, change the "Thickness" value to 10, press Set Layer.

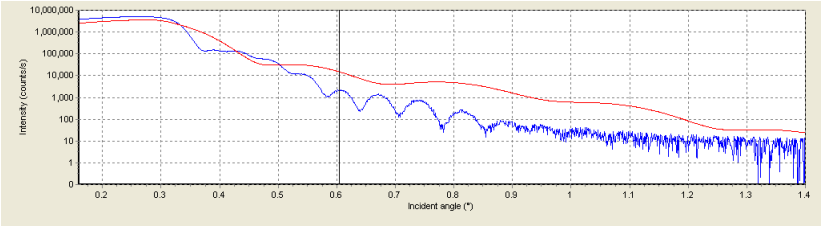
Select Layer:2, change the "Thickness" value to 5, press Set Layer.

Press OK.

Save the new sample data as "Sample 2 for QSG".

If you have checked the "Always prompt to save fit settings when sample is saved" in *Settings - Defaults...* a further window offering you the chance to save the settings file will appear. You have not changed the settings file yet, so just press Cancel.

- Select *Simulation - Simulate* (or press the button).



This is obviously no better, so we will use the Segmented Fit to see if the result improves.

- Select *Fitting - Segmented Fit* .... The "Segmented Fit Setup" window opens to allow you to set the fitting conditions:

  In the "Sample parameters:" grid "Density" "Use" column, uncheck all three rows.

  In the "Sample parameters:" table set the "Thickness" and "Roughness" values as follows:

Layer	Parameter	Min	Max
Sub	Roughness	0.5	1.5
1,0	Thickness	9	50
1,0	Roughness	0.5	2.5
2,0	Thickness	4.5	15
2,0	Roughness	0.5	2.5

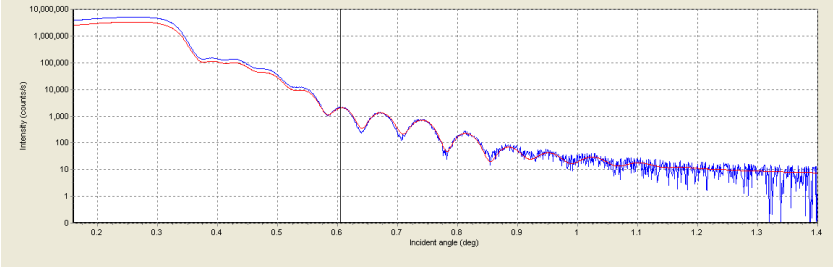
In the “Background and other parameters:” table set the values as follows:

Parameter	Max
Background	8
Divergence	0.008

In the “Sample parameters:” pane, select the substrate and both the layers and press the Recalculate Start and Stop button.

In the “Fitting Range Increment Details” pane, press Reset.

Press the Start button and the fitting starts.



You can see that this result has improved, but we can still try another fitting method to see if we can improve it.

Click No in the “Fitting has finished. Update sample now?” window.

2.4.4 Fitting - Using the Genetic Algorithm

- Select *Fitting - Genetic Algorithm...* (another fitting method).

In the "Density" "Use" column, uncheck all three rows.

In the "Sample parameters:" table set the "Thickness" and "Roughness" values as follows:

Layer	Parameter	Min	Max
Sub	Roughness	0.5	1.5
1,0	Thickness	9	50
1,0	Roughness	0.5	2.5
2,0	Thickness	4.5	15
2,0	Roughness	0.5	2.5

Press the GA Parameters button and set the following values.

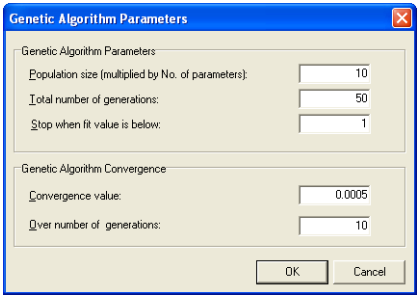
Set "Population size (multiplied by No. of parameters):" to 10

Set "Total number of generations:" to 50

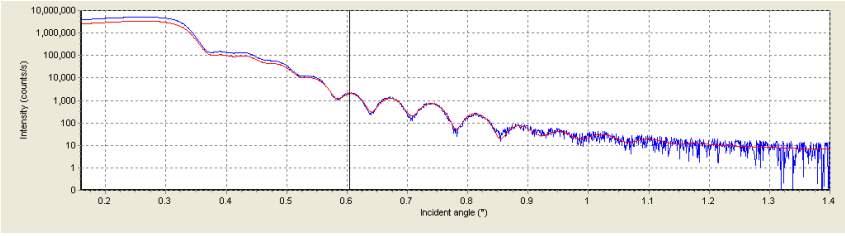
Set "Stop when fit value is below:" to 1

Set "Convergence value:" to 0.0005

Set "Over number of generations:" to 10



Press OK and then on the "GA Setup" window, again press Start.

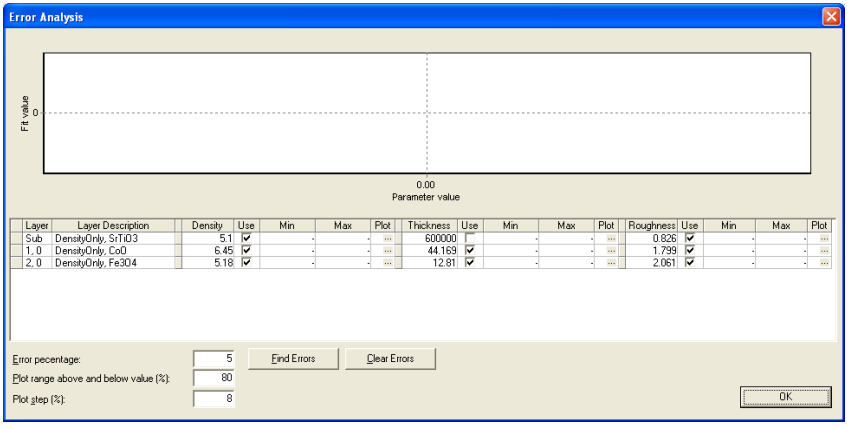


As you can see, this time it is a good fit. Update the sample and save it as "Sample 3 for QSG.sam".

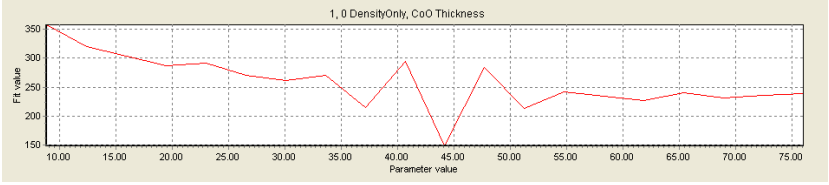
2.5 Error Analysis

You can check the confidence of the results by looking at the Error Analysis.

- Select *Fitting - Error Analysis...*.



Press Find Errors. On the table in the "Error Analysis" window you can see the results of the error analysis. If you want to see more information about a particular analysis press the relevant ... button. In this example we pressed the "Layer 1 - Thickness" ... button:

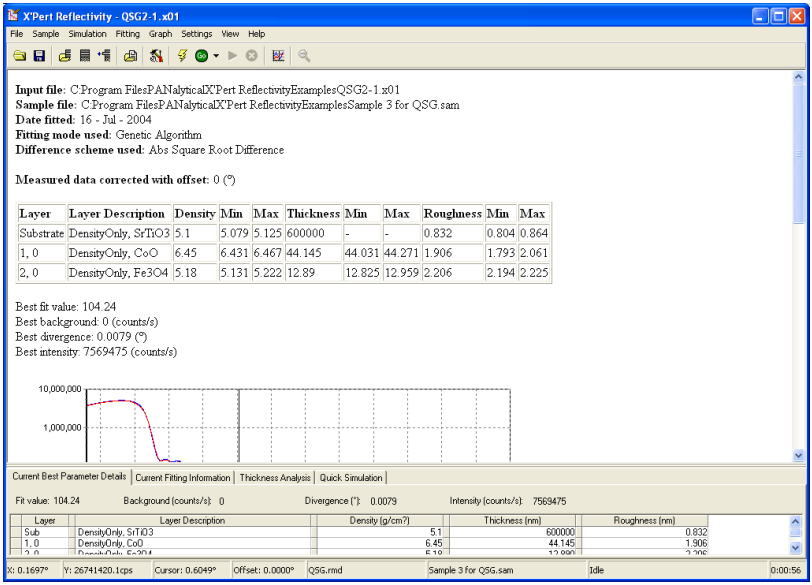


Press OK to close the "Error Analysis" window.

2.6 CREATE REPORT

You can create a report of the simulation you just performed.

- Select *View - Report (HTML)* and a report will be generated using the HTML Template and Style sheet defined in the "reporting" tab of "Defaults".



You have completed the first example exercise, close the program by selecting *File - Exit*.

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Chapter 3

Simulating and Fitting Samples with Superlattice Layers

Contents

X'Pert Reflectivity - Quick Start Guide

Chapter 3. Simulating and Fitting Samples with Superlattice Layers

3.1 Introduction

This exercise will show you how to create a new sample and then compare that new sample with the data from a previously measured sample.

3.2 Preparing the Program

- Double-click on the X'Pert Reflectivity Icon 

to start the program.

  You can set the program up with defaults to make the program react in ways that are suitable to you. In this example we are going to create a new sample we will set the system up to always ask if we want to save at the end of a sequence.

- Select *Settings - Defaults...*

  On the "General" tab make sure that the boxes:

  "Always prompt to save material data file when edited",

  "Always prompt to save sample when edited", and

  "Always prompt to update sample at end of fitting"

  are checked (✔) and that

  "Always prompt to save fit settings when sample is saved"

  is not checked (☐).

- Press OK.

3.3 Preparing the Material Data

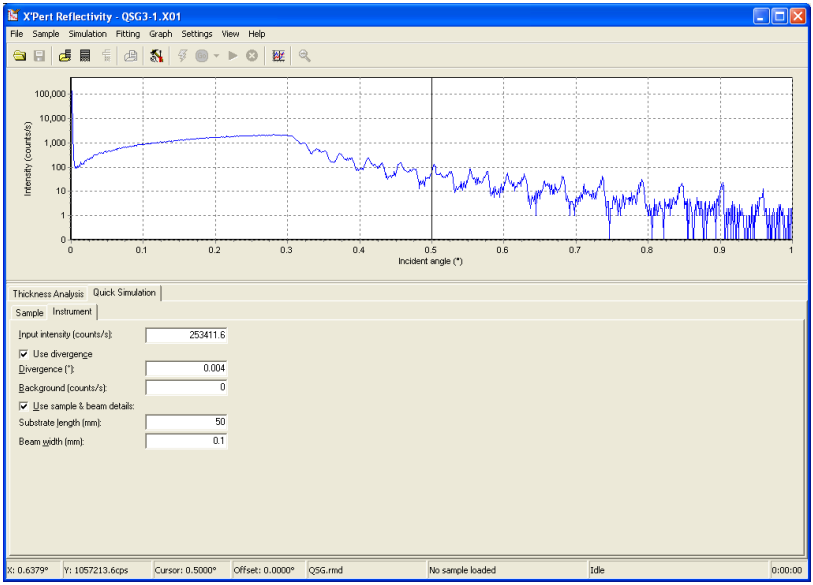
- Ensure that you have the required materials data file open:

  Sample - Open Material Data...

  Browse until you find the correct file: "QSG.rmd" that you created in Chapter 2, and press Open.

3.4 LOADING DATA

- Select *File - Open Measured Data...*, select "QSG3-1.X01" a measurement of AlAs_GaAs and press Open.



If you did not start this exercise by opening X'Pert Reflectivity (in other words, it was still open from the previous example) it could be that the red simulated data is displayed on the graph. If it is, select *File - Close - Simulated Data*.

3.5 CREATING A SAMPLE

- Select *Sample - New Sample...* (or press the button).
- Set the substrate as follows:

  Select “ZincBlende: from the “Structure:” drop-down list.

  In the “Site A” frame, select “Ga” from the “Element: 1:” drop-down list.

  In the “Site B” frame, select “As” from the “Element: 1:” drop-down list.

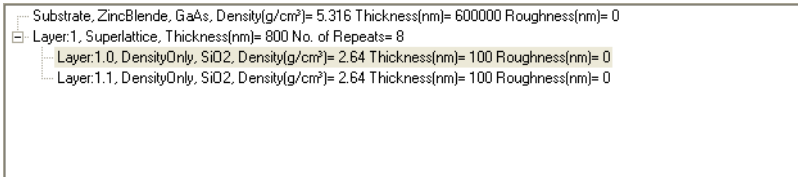
  Make sure that the “Use crystal structure data” box is checked (✔).

  Press Set Layer.
- Add the superlattices as follows:

  In the “Add as next layer” frame press Add Superlattice.

  Set the “Number of repeats:” to 8.

  Press Set Layer.
- In the “Add to superlattice” frame press Add Layer.



Select the first layer (1.0) as shown above and make the following entries:

“Structure:”	ZincBlende	
“Site A:	“Number of elements:”	1
	“Element: 1:”	Al
“Site B:	“Number of elements:”	1
	“Element: 1:”	As

"Thickness (nm):" 85

"Roughness (nm):" 0.8

Make sure that the "Use crystal structure data" box is checked (a).

Press Set Layer.

- Click on the second layer (1.1):

  Make the following entries:

  "Structure:" ZincBlende

  "Site A: "Number of elements:" 1

  "Element: 1:" Ga

  "Site B: "Number of elements:" 1

  "Element: 1:" As

  "Thickness (nm):" 80

  "Roughness (nm):"0.8

  Make sure that the "Use crystal structure data" box is checked (✔).

  Press Set Layer.

- Press OK and save the new sample as "Sample 4 for QSG.sam".

3.6 Setting the Simulation Parameters

- Select *Simulation - Setup...*.

  Accept the offered values except:

  Ensure that the "Specular" radio button is selected

  In the "Scan Details" frame:

  "Input intensity (counts/s):" = 100000

  Ensure that the "Normalize intensity" box is **not** checked.

  In the "Convolution Details" frame:

  Make sure that the "Use divergence" box is checked (✔).

"Divergence (°):" = 0.001°

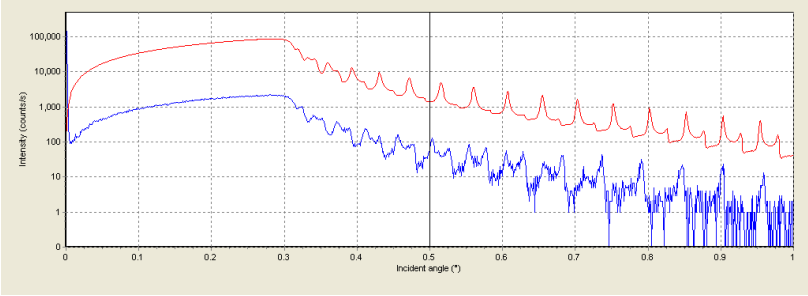
"Background (counts/s):" = 0.5

In the "Sample and Beam Details" frame:

Make sure that the "Use" box is checked (✔).

"Substrate length (mm)"=2

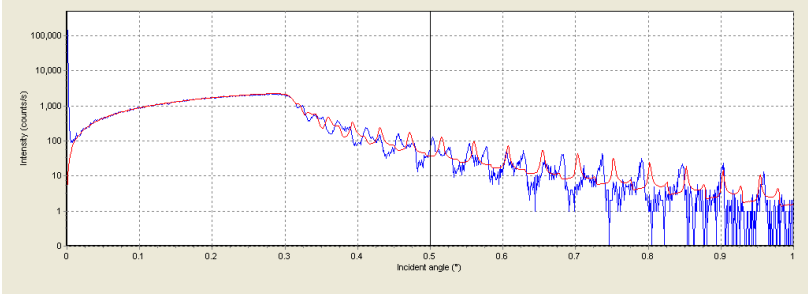
Press the OK button and a simulation should start (a red line appears on the graph).



As you can see there is a discrepancy between the measured data and the simulated data. In this example we can cure this in either of two ways:

Method 1:

- Select *Simulation - Setup...*, check (✔) the "Normalize intensity" box and press OK again.



Before you can try the second method you must revert to the "initial" situation:

- Select Simulate - Setup

  In the "Scan Details" frame:

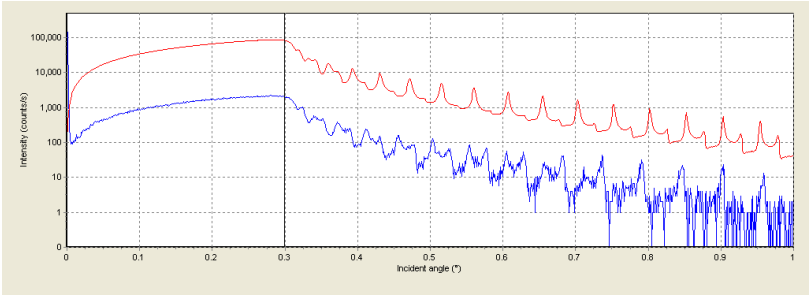
  "Input intensity (counts/s):"=100000

  Ensure that the "Normalize intensity" box is **not** checked.

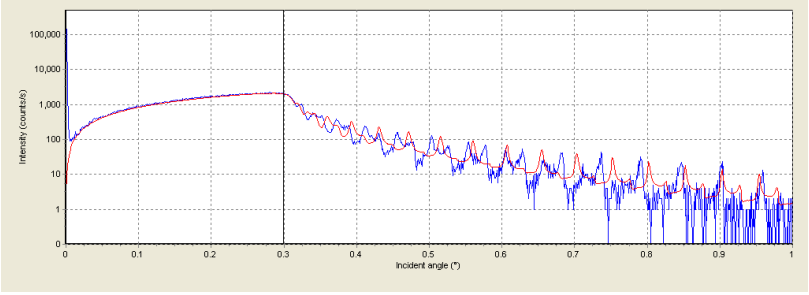
  Press OK.

Method 2:

- Manually move the cursor to the maximum point on the measured (blue) curve.



Select *Graph - Normalize Intensity at Cursor Position*.



3.7 FITTING

Make sure that you have the correct defaults for this example:

Select *Settings - Defaults...* The entries on the "Fitting tab" should be:

Peak No. to select in automatically set cursor position:	3
Default number of scan increment steps:	3
Difference scheme:	Abs Square Root Difference

Press OK.

- Select *Graph - Automatically Set Cursor Position* (or press the  button). This will move the cursor to the third peak as found by the peak search algorithm, as you just set in the defaults.
- Select *Fitting - Segmented Fit...*

  In the "Sample parameters:" table set the "Roughness" values as follows:

Min	Max
0.1	0.5
0.5	1.2
0.5	1.2

  In the "Background and other parameters:" table set the values as follows:

  "Background" uncheck the "Use" box.

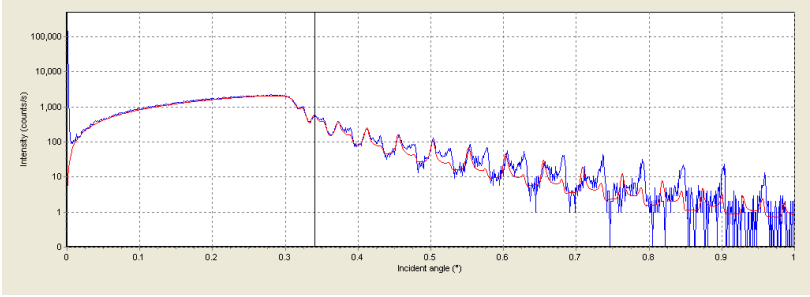
  "Divergence" Min 0.0002 Max 0.0011

  Highlight the substrate and the two superlattice layers, press the Recalculate Start and Stop button.

  Press the Show Details >> button.

  In the "Fitting Range Increment Details" pane, press Reset.

  Press the Start button to start the fitting.



In this example we are going to improve the result by increasing the percentages for all of the settings.

- Select *Fitting - Segmented Fit...*

  Highlight the substrate and the two superlattice layers.

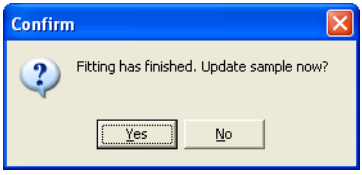
  In the "Set Minimum and Maximum by Percentages" frame set:

  Minimum (%):20

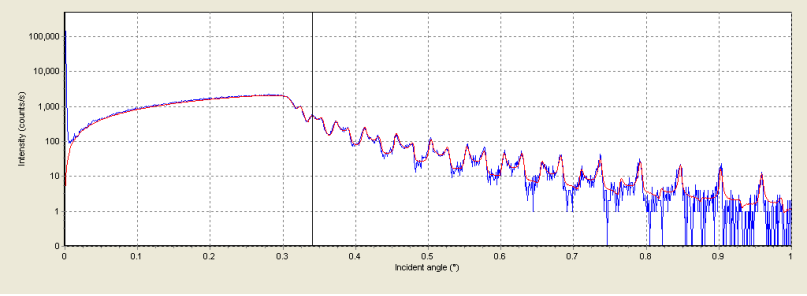
  Maximum (%):20

  Press the Set button and choose "Set the selected layer's thickness min and max".

  Press the Start button and the fitting starts again.



  If you are happy with the result you can update the current sample by clicking the Yes button and saving it as "Sample 5 for QSG.sam".



If you wish to you could then create a report via *View - Report (HTML)*.

X'Pert Reflectivity - Quick Start Guide

PANalytical

Chapter 4

Determining the Thickness of a Layer

Contents

Chapter 4. Determining the Thickness of a Layer

4.1 Introduction

This exercise will open a measured data file and use two different methods of checking the thickness of the layer of SiGe in a Si substrate.

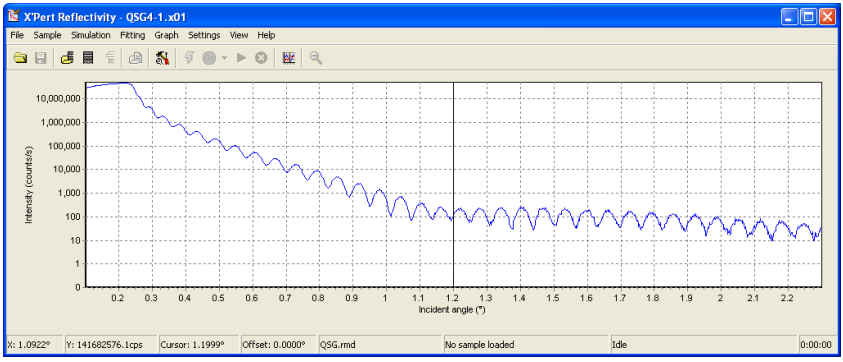
4.2 Starting the Program

- Double-click on the X'Pert Reflectivity Icon 

to start the program.

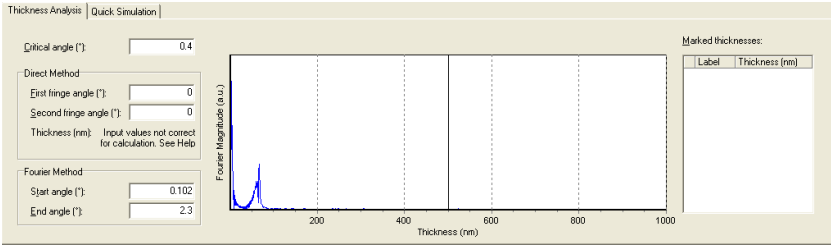
4.3 Loading Data

- Select *File - Open Measured Data...*, select "QSG4-1.x01" and press Open.



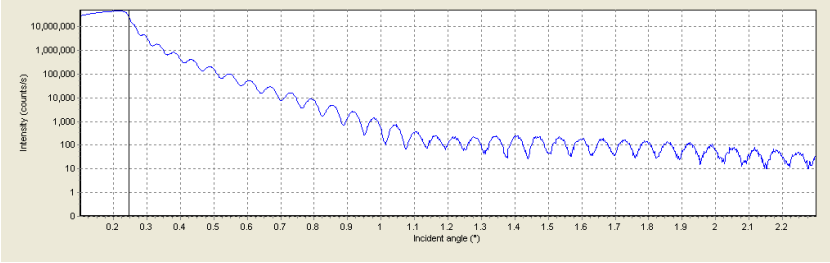
4.4 USING THE FOURIER METHOD

- Select the "Thickness Analysis" tab on the lower half of your X'Pert Reflectivity window.

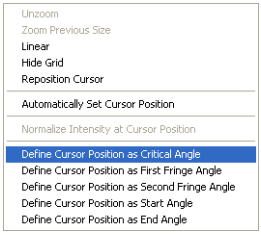


You can see two frames in the tab: "Direct Method" and "Fourier Method", in this section we will show you how to use the Fourier Method to determine the thickness of the SiGe layer.

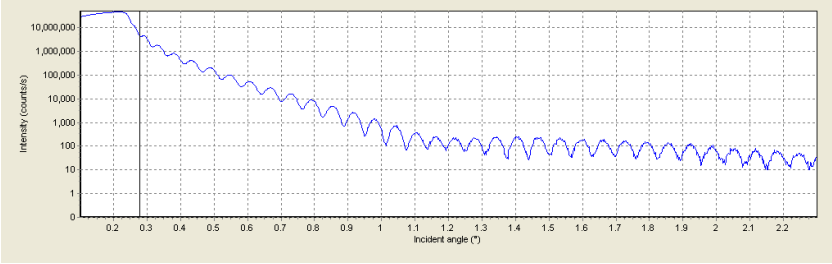
- Move your mouse pointer over the cursor on the main scan and drag (hold down the left mouse button) the cursor to the critical angle.



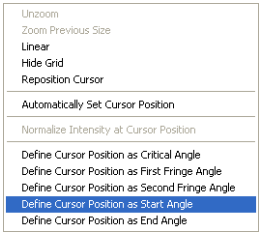
- Click the right mouse button and define this position as "Define Cursor Position as Critical Angle".



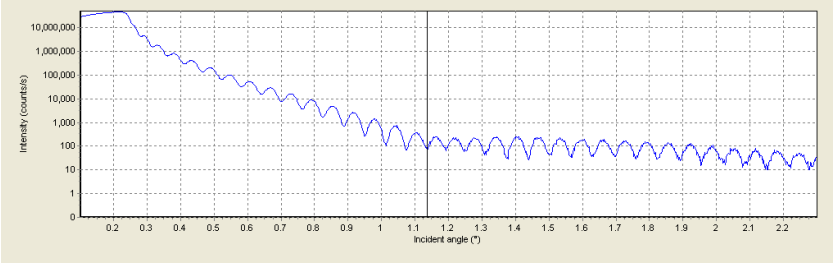
- Now drag the cursor to where the fringing starts. This point is not too critical and you can select either the peak or the valley.



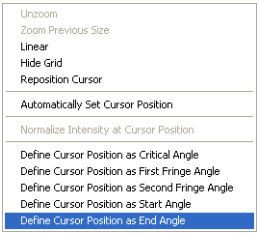
- Click the right mouse button and define this position as “Define Cursor Position as Start Angle”.



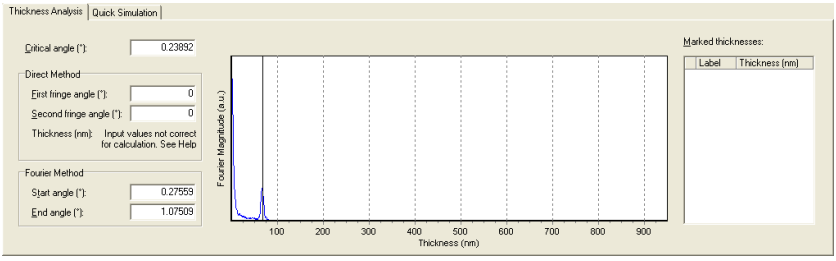
- Now drag the cursor to where the noise starts to become apparent (1.0751° in this example).



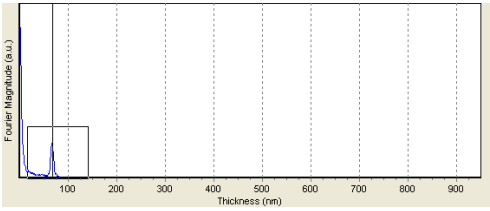
- Click the right mouse button and define this position as “Define Cursor Position as End Angle”.

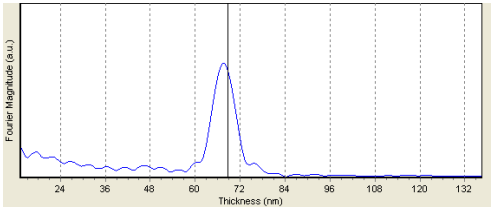


- Now go to the scan window in the "Thickness Analysis" tab and move the cursor to the peak (at about 65 nm).

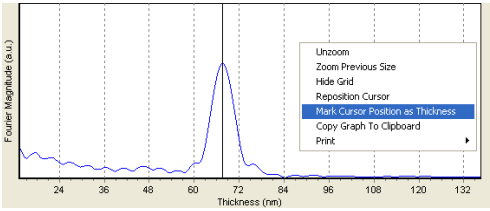


- Zoom in on the peak to enable you to set the cursor more accurately on the peak.

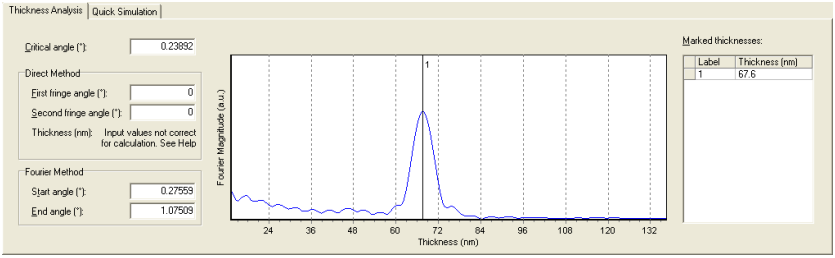




- Place your mouse pointer on the cursor (the line), click the right mouse button and select “Mark Cursor Position as Thickness”.



Now you can see the result in the “Marked thicknesses:” table.



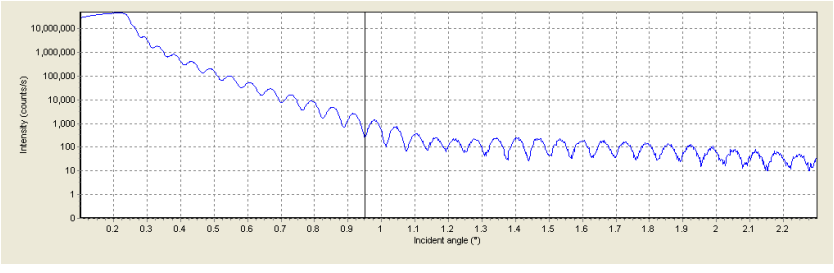
In this experiment the thickness is measured at 67.6 nm.

Now we will try another method of measuring the thickness and compare the results.

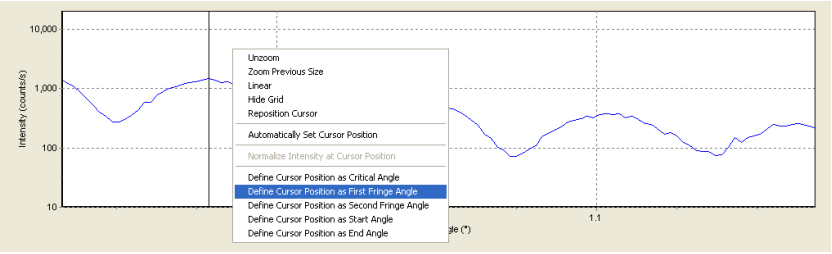
4.5 Using the Direct Method

In this method we are going to measure the distance between two fringes to ascertain the thickness of the layer.

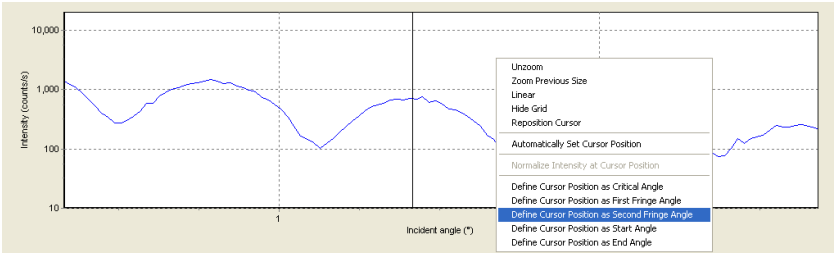
- On the main scan, zoom into an area with clearly defined peaks or valleys.



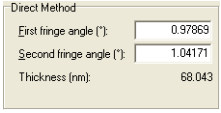
- Move the cursor to a peak or valley. Click the right mouse button and define this position as "Define Cursor Position as First Fringe Angle".



- Now move the cursor to the next peak or valley. Click the right mouse button and define this position as "Define Cursor Position as Second Fringe Angle".



Now you can see the result in the "Direct Method" frame.



In this experiment the thickness is measured at 68.043 nm.

The results were very close in both methods, and it shows that the thickness is just about 68 nm. We can use this information about the thickness in the next chapter.

PANalytical

Chapter 5

Simulating and Fitting SiGe on Si

Contents

5.1 Introduction

This exercise will show you how to create a new sample and then compare that new sample with the data from a previously measured sample.

5.2 Preparing the Program

- Double-click on the X'Pert Reflectivity Icon 

to start the program.

  You can set the program up with defaults to make the program react in ways that are suitable to you. In this example we are going to create a new sample and we will set the system up to always ask if we want to save at the end of a sequence.

- Select *Settings - Defaults...*

  On the "General" tab make sure that the boxes:

  "Always prompt to save material data file when edited",

  "Always prompt to save sample when edited", and

  "Always prompt to update sample at end of fitting"

  are checked (✔) and that

  "Always prompt to save fit settings when sample is saved"

  is not checked (☐).

  Press OK.

5.3 Preparing the Material Data

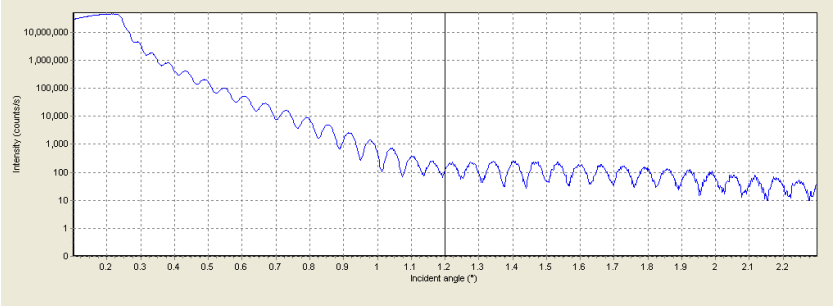
- Select *Sample - Open Material Data...*.

  Browse until you find the required materials data file file: "QSG.rmd"

  and press Open.

5.4 Loading Data

- Select *File - Open Measured Data...*, select "QSG4-1.x01" and press Open.



If you did not start this exercise by opening X'Pert Reflectivity (in other words, it was still open from the previous example) it could be that the red simulated data is displayed on the graph. If it is, select *File - Close - Simulated Data*.

5.5 Creating a Sample

- Select *Sample - New Sample...* (or press the button).
- Set the substrate:

  Select "Diamond: from the "Structure:" drop-down list.

  In the "Materials" frame, select "Si" from the "Material 1:" drop-down list.

  Make sure that the "Use crystal structure data" box is checked (✔).

  Set the "Roughness (nm):" to 0.5 nm.

  Press Set Layer.

- Add Layer 1:

  In the "Add as next layer" frame press Add Layer.

  Select "Diamond: from the "Structure:" drop-down list.

In the “Materials” frame:

Enter “2” into the “Number of materials:” box.

Select “Si” from the “Material 1:” drop-down list and enter 84 for the “%”.

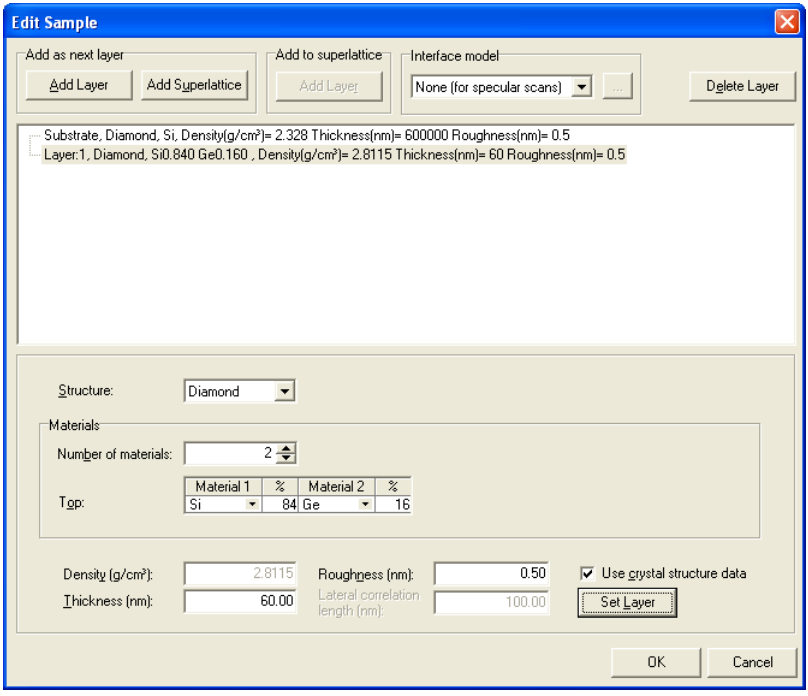
Select “Ge” from the “Material 2:” drop-down list and check that the program has made the “%” 16.

Set the “Thickness (nm):” to 60 nm.

Set the “Roughness (nm):” to 0.5 nm.

Make sure that the “Use crystal structure data” box is checked (✔).

Press Set Layer.



Press OK and save the sample as “Sample 6 for QSG.sam”.

5.6 Setting the Simulation Parameters

- Press the (Simulation Setup) button.

  Accept the offered values except:

  In the "Scan Details" frame:

  Ensure that the "Normalize intensity" box is checked.

  In the "Convolution Details" frame:

  Ensure that the "Use divergence" box is checked.

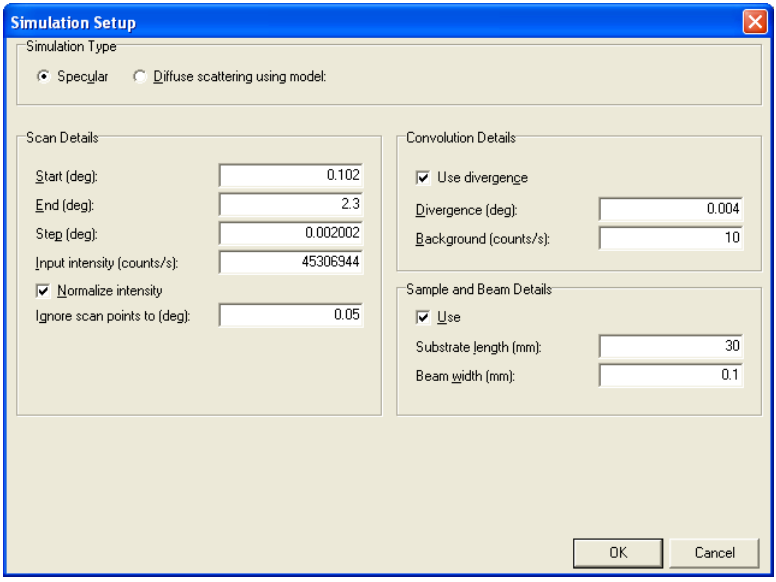
  "Divergence (°):" = 0.004

  "Background (counts/s):"= 10

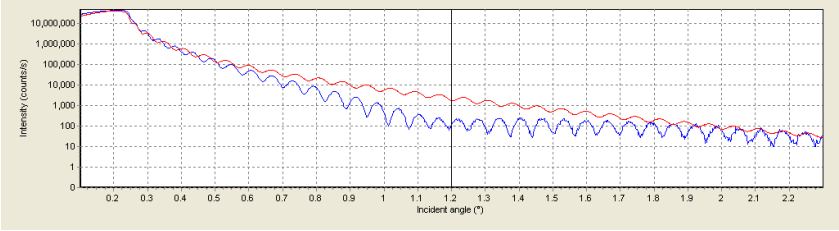
  In the "Sample and Beam Details" frame:

  Ensure that the "Use" box is checked.

  "Substrate length (mm)" = 30



- Press the button and a simulation should start (a red line appears on the graph).



5.7 Fitting the Simulated Graph

- Make sure that you have the correct defaults for this example: select *Settings* - *Defaults...* The entries on the "Fitting tab" should be:

Peak No. to select in automatically set cursor position:	3
Default number of scan increment steps:	2
Difference scheme:	Abs Square Root Difference

Now make the first attempt to make a fit.

- Select *Graph* - *Automatically Set Cursor Position* (or press the button). This will move the cursor to the third peak as found by the peak search algorithm as you set in the defaults.
- Select *Fitting* - *Segmented Fit...*

  In the "Sample parameters:" table set the "Roughness" values for the substrate and the "Thickness" and "Roughness" values for layer 1 as follows:

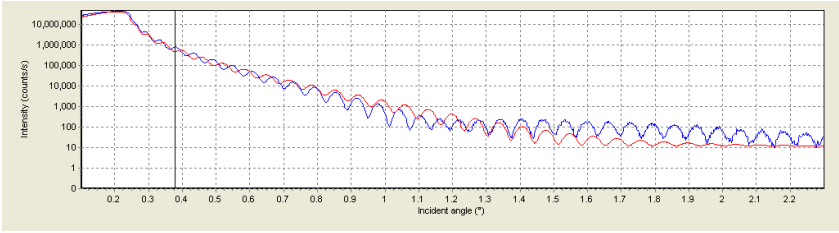
Layer	Parameter	Value	Min	Max
Sub	Roughness	0.5	0.1	1
1	Thickness	60	50	70
1	Roughness	0.5	0.1	1

In the "Background and other parameters:" table set the values as follows:

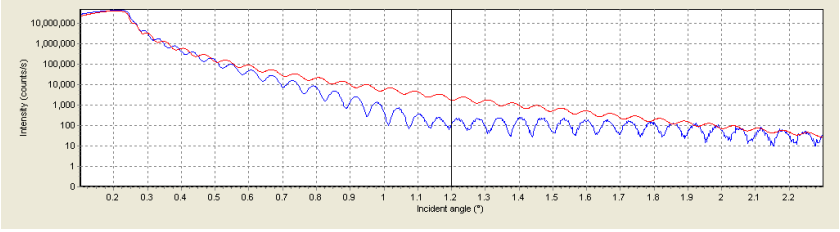
Parameter	Value	Min	Max
Background	11	9	13
Divergence	0.004	0.001	0.01

Highlight the substrate and the layer, press the Recalculate Start and Stop button.

- Press the Start button to start the fitting.



This isn't a perfect fit. If we compare it with the initial simulation:



We can see that there is a slight low frequency modulation on the measured data, which we do not see on the simulated data, which would suggest that another layer is present. This layer would be thin, maybe 1 to 2 nm, as the frequency of the modulation is low (remembering that the higher the frequency of the fringes, the thicker the layers are). So maybe during the growth process a thin oxide layer was formed on top of the grown layer. So lets go back and add a thin Silicon Oxide layer to our sample:

Do not save the sample (press No).

- Select Sample - Edit Sample... (or press the button).
- Add Layer 2:

  Highlight Layer 1.

  In the "Add as next layer" frame press Add Layer.

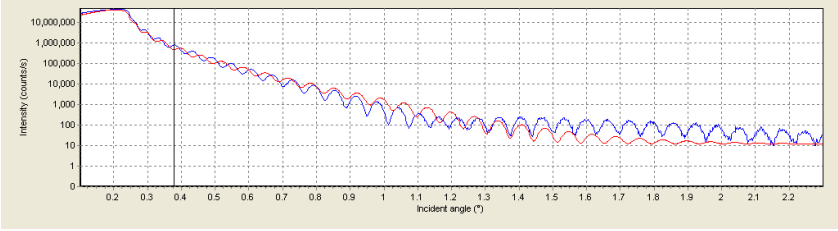
  Set the "Thickness (nm):" to 2 nm.

  Set the "Roughness (nm):" to 1 nm.

  Press Set Layer.

  Press and save the sample as "Sample 6 for QSG.sam" (Yes).

  Press .



This looks like a better starting point than before, so let's see if we can fit this:

- Press the button again to make sure that the cursor is in the right position, then select the menu item *Fitting* - *Segmented Fit...* and enter the parameters as follows:

  In the "Sample parameters:" table set:

  the "Roughness" values for the substrate,

  the "Thickness" and "Roughness" values for layer 1 and

  the "Density", "Thickness" and "Roughness" values for layer 2

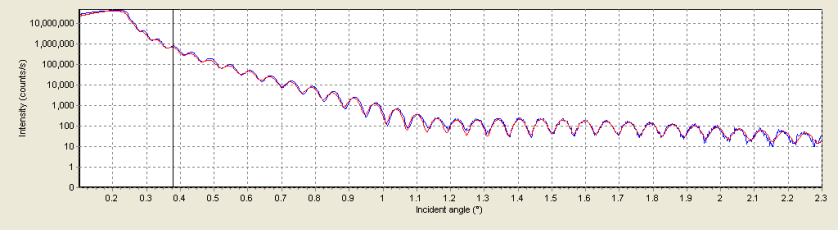
Layer	Parameter	Value	Min	Max
Sub	Roughness	0.5	0.1	1
1	Thickness	60	50	70
1	Roughness	0.5	0.1	1
2	Density	2.64	1.5	2.64
2	Thickness	2	1	3
2	Roughness	1	0.1	2

In the "Background and other parameters:" table set the values as follows:

Parameter	Value	Min	Max
Background	11	9	13
Divergence	0.004	0.001	0.01

Highlight the substrate and the two layers, press the Recalculate Start and Stop button.

- Press the Start button to start the fitting. The result should be an almost perfect fit:



- Save the sample as "Sample 7 for QSG.sam".

PANalytical

Chapter 6

Diffuse Scatter

Contents

6.1 Introduction

This exercise will open an ω-scan and find out what Hurst parameter and lateral correlation lengths best suit the sample.

6.2 Starting the Program

- Double-click on the X'Pert Reflectivity Icon 

to start the program.

6.3 Preparing the Material Data

In this example we are going to open a sample that was delivered together with X'Pert Reflectivity. However, before we do that we must first prepare the Materials Database so that it includes the material in the sample.

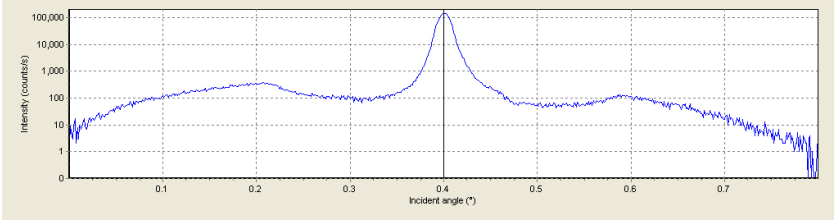
- Make sure that you have the QSG.rmd database open (the current database is shown in the fifth box from the left on the lower status bar). If you do not, select *Sample - Open Material Data...*, choose "QSG.rmd" and press

  Open

6.4 Loading Data

- Select *File - Open Measured Data...*, select "QSG6-1.xrdml" and press

  Open



6.5 Prepare the Simulation Setup

- Press the (Simulation Setup) button.

Select the "Diffuse scattering using model:" radio button.

Select "DWBA" as the model.

In the "Scan Details" frame:

"Scan type:" = Omega

"Start (°):" = 0.0004 (obtained from measured scan)

"End (°):" = 0.7996 (obtained from measured scan)

"Step (°):" = 0.0012 (obtained from measured scan)

"2Theta (°):" = 0.8 (obtained from measured scan)

"Input intensity (counts/sec):" = 38200000

In the "Convolution Details" frame:

"Divergence (°):" = 0.005

"Background (counts/s):" = 1

Make sure that the "Rescale scan after convolution" box is not checked

In the "Sample and Instrument Details" frame:

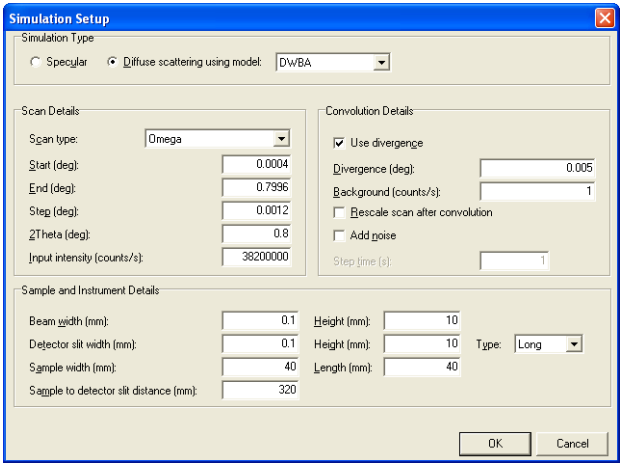
"Beam width (mm):" = 0.1

"Detector slit width (mm):" = 0.1

"Sample width (mm):" = 40

"Length (mm):" = 40

"Sample to detector slit distance (mm):" = 320



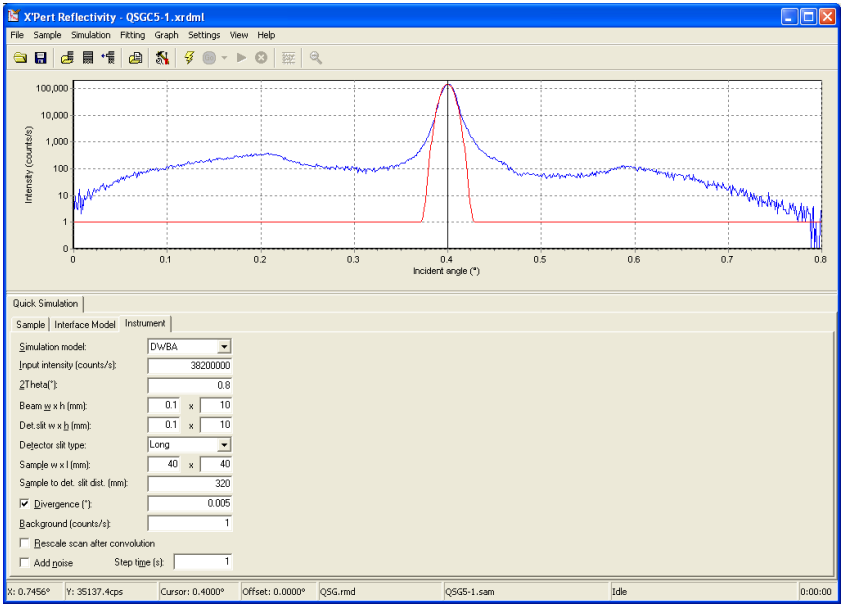
- Press OK.

6.6 Open a Sample

- Select *Sample - Open Sample...* (or press the button), choose "QSG6-1.sam" and press Open.

6.7 Perform the First Simulation

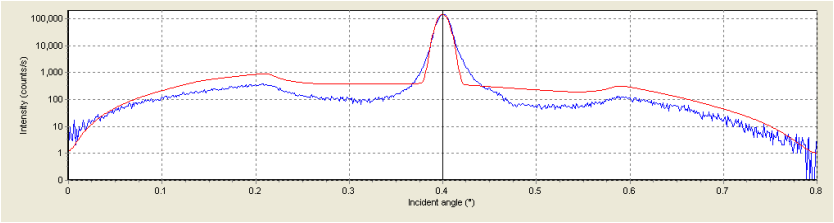
- Now select *Simulation* - *Simulate*, or press F2, or press  and look at the result of the simulation.



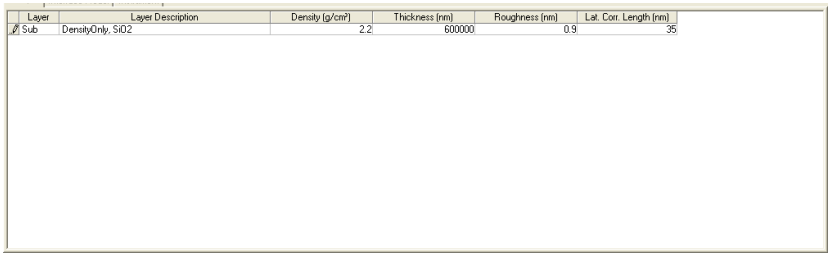
6.8 Fitting the Simulated Graph

The thickness and roughness of the sample have already been ascertained during the "Specular" fitting; we are now concerned with the correlation length of the sample and the "Hurst" parameter.

- In the "Quick Simulation" pane, click on the "Sample" tab. Make an assumption of the "Lat. Corr. Length (nm)", in this example we shall try 70 for the substrate.
- Click on the "Interface Model" tab and in the "Fractal Parameters" frame, set the "Hurst parameter:" to 0.2.
- Now press F2 or  and look at the result of the simulation.

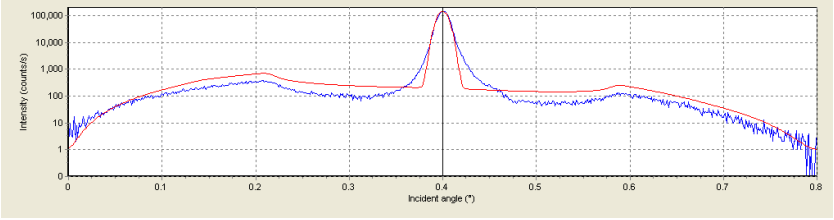


As a first step in fitting this simulation, it can be seen that the lateral correlation length was too big. To decrease the intensity level of the diffuse scattering you can decrease the lateral correlation length, so change it to 35.



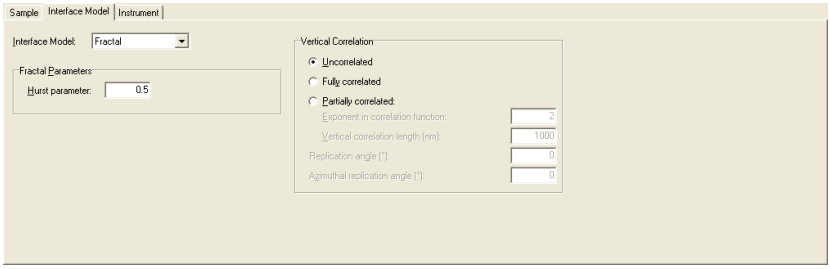
Layer	Layer Description	Density (g/cm³)	Thickness (nm)	Roughness (nm)	Lat. Corr. Length (nm)
Sub	DensityOnly, SiO2	2.2	600000	0.9	35

and press  .

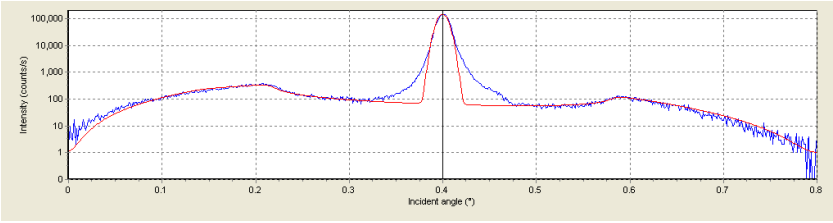


This is a big improvement, but it is still not as good as we would like, so this time we shall try adjusting the Hurst parameter.

- Click on the “Interface Model” tab and in the “Fractal Parameters” frame, set the “Hurst parameter:” to 0.5.



- Now press F2 or  and look at the result of the simulation,



and the result is just about right.

This exercise has shown us that a good simulation can be obtained with a correlation length of 35 nm and a Hurst Parameter of 0.5.

PANalytical

Chapter 7

Checking the Vertical Correlation

Contents

Chapter 7. Checking the Vertical Correlation

7.1 Introduction

This exercise will show an example of a sample with a superlattice structure comprising 10 periods of GaAs/AlAs with an interface roughness of 0.5 nm and a lateral correlation of 200 nm. We will then perform a simulation of a reciprocal space map using the settings contained in a settings file which is also delivered together with the program. Finally we will change the vertical correlation settings to show the influence on the simulation pattern of the vertical correlation of the roughness between the layers.

7.2 Starting the Program

- Double-click on the X'Pert Reflectivity Icon 

to start the program.

7.3 Loading the Sample and Setting Up the Simulation

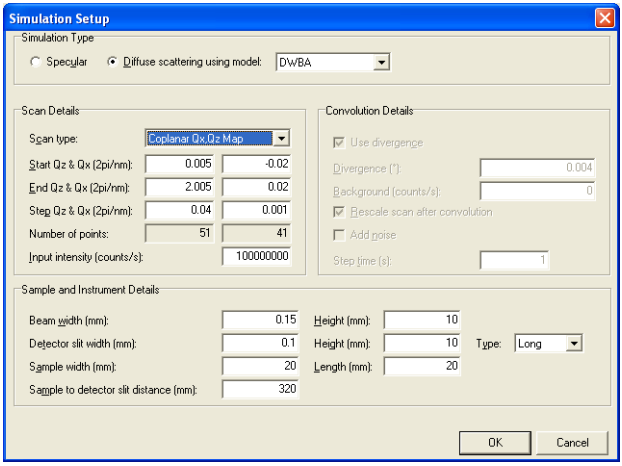
- Select *Sample* - *Open Sample*... (or press the  button), choose "QSG7-1.sam" and press 

.
- Select *Simulate* - *Setup*...

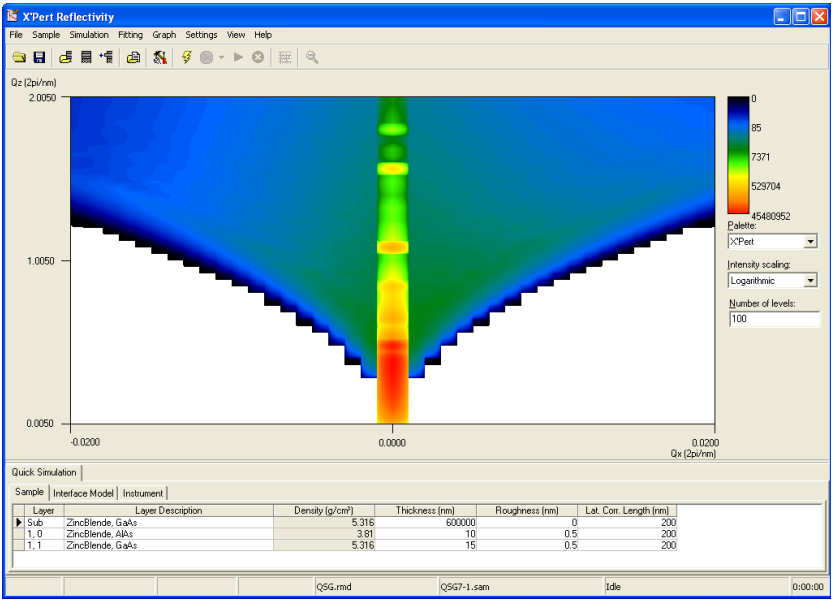
  Click on the "Diffuse scattering using model:" radio button and accept the default model "DWBA" (Distorted Wave Born Approximation).

  Choose "Coplanar Qx,Qz Map" for the "Scan type:" because we need to simulate a map in order to see the effects of vertical correlation.

  Accept the rest of the defaults.



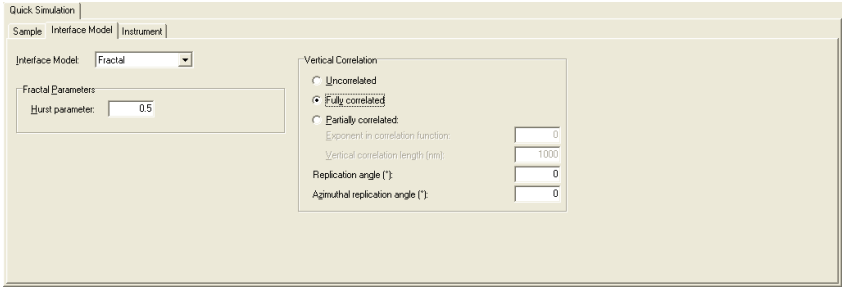
Press OK.



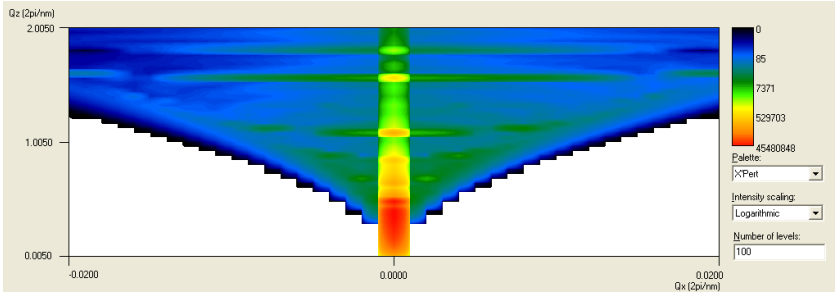
This simulation shows a reciprocal space map of the periodic structure.

7.4 Influence of the Vertical Correlation

- In the “Quick Simulation” pane (the lower half of your screen) open the “Interface Model” tab and click on the “Fully correlated:” radio button.



Now when you select *Simulation* - *Simulate*, or press F2, or press and look at the result of the simulation (it takes a few seconds, you can watch the progress in the status bar):



The most pronounced feature due to the correlation of roughness of the interfaces is the concentration of the intensity on the equidistantly placed RDS sheets (the horizontal green lines in this example) in the reciprocal space map. The presence of these RDS sheets indicates that there is a vertical correlation between the roughness of the interfaces.

This is a fairly “normal” example of how you can quickly get an impression of these effects, you could if wanted go on to study them in more detail by choosing a smaller step size in Simulation - Setup. However, this results in the simulation taking more time to do. If you find that it’s taking too long, you can always use the button to stop the simulation.

PANalytical

Chapter 8

Automating Your Reflectivity Measurements/Analyses

Contents

Chapter 8. Automating Your Reflectivity Measurements/ Analyses

8.1 Introduction

It is possible to automate your analyses either by using the Automatic Processing Program (APP) supplied as an add-on with the X'Pert Data Collector, Version 2.2, or by using X'Pert Reflectivity directly from the command line (for example: by defining a shortcut).

This chapter demonstrates two simple examples using the command line. It is also possible to use scripts. This is explained in the APP help file.

The first example shows how to automatically print out your scan data immediately after it has been measured using the X'Pert Data Collector.

The second example shows how to start a segmented fitting and when that has finished, to save the result as "seg report.html" to the current folder and print that report on your default printer.

8.2 Automatic Printing of Scan Data using the APP

Assume that you are working with the X'Pert Data Collector and you have created an absolute scan program called Program Refl QSG as User-1. To print out the scan 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:

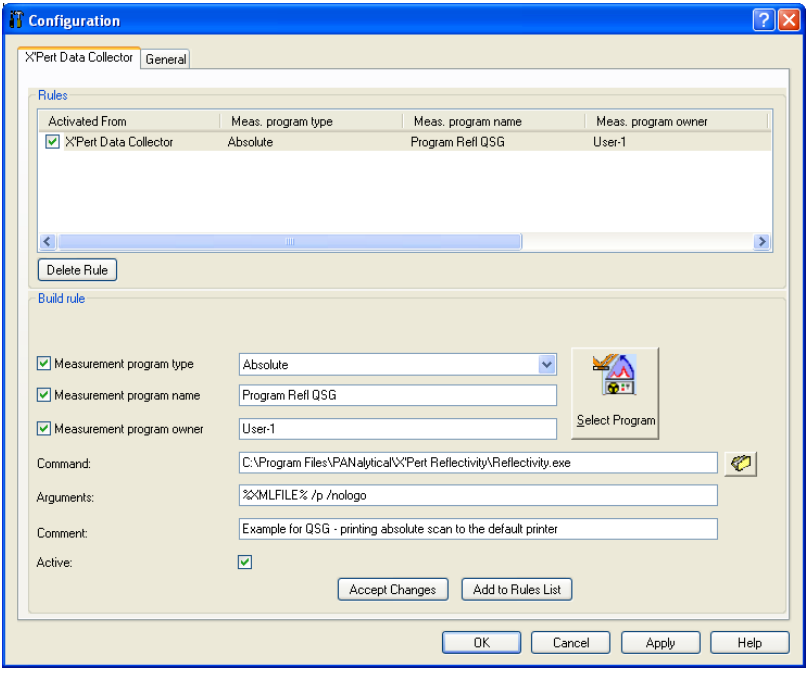
  Check all of the "Measurement program ..." check boxes.

  Enter the details of the X'Pert Data Collector program and your user name.
- In the "Command" field enter the path name for running X'Pert Reflectivity: "C:\Program Files\PANalytical\X'Pert Reflectivity\Reflectivity.exe".
- In the "Arguments" field enter %XMLFILE% /p where:

  %XMLFILE% is used to indicate the measured file

  /p indicates that the scan must be printed.

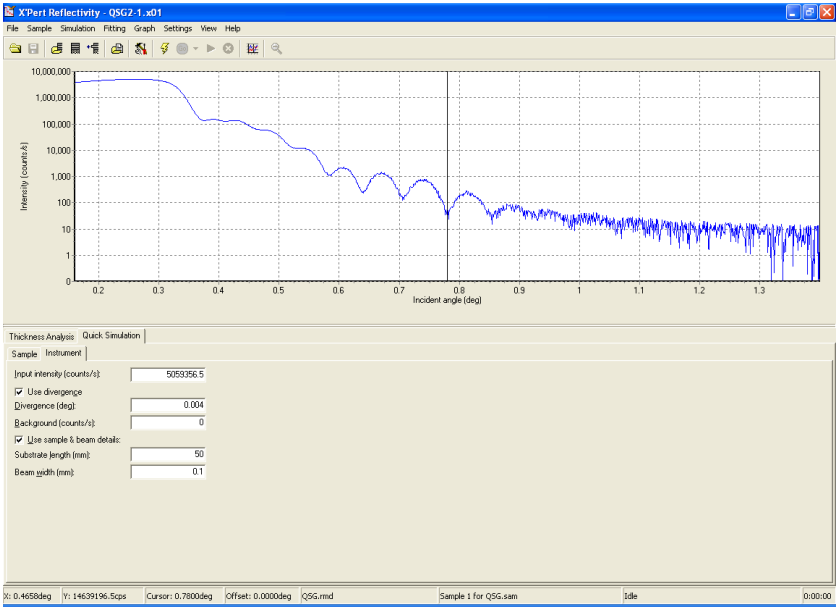
- Activate the rule you have just saved by checking the "Active:" check box.
- Click on the **Add to Rules List** button.
- Click **OK**.



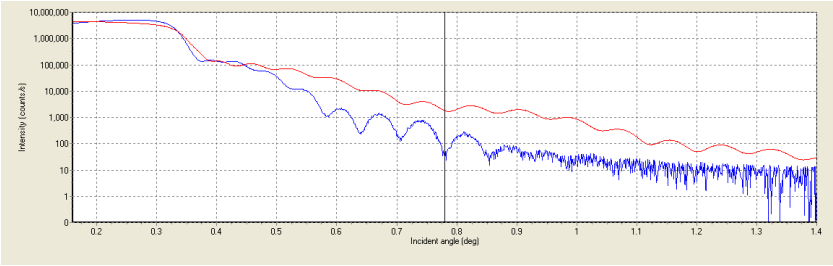
- Return to the X'Pert Data Collector, start data collecting, and when the scan has been completed it will be printed out.

8.3 Automatic Fitting of Scan Data using a Command Line

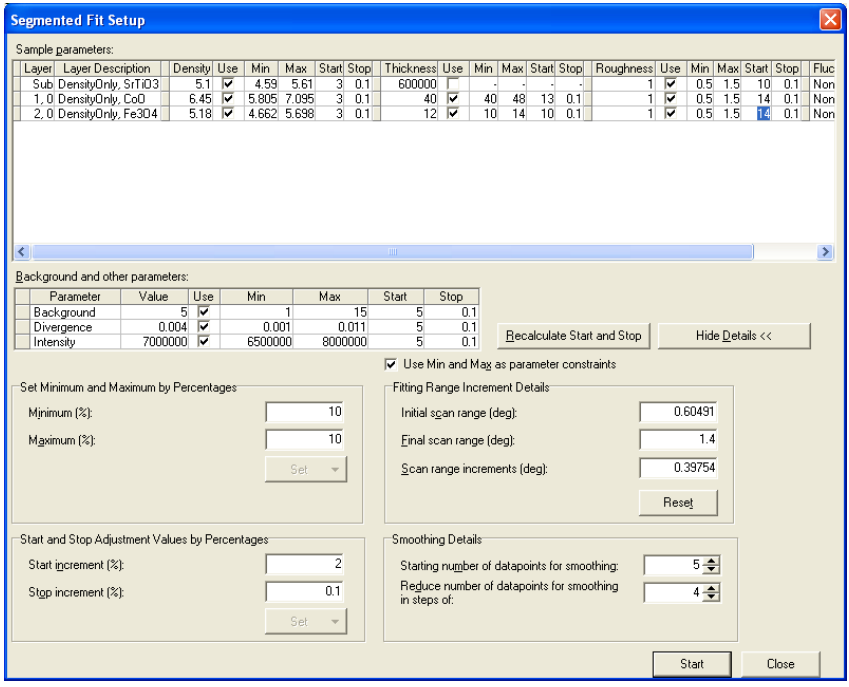
- If it is not already running, start X'Pert Reflectivity.
- Select *Sample - Open Material Data...*, select "QSG.rmd" that we created in section 2.2.1 and press the Open button.
- Select *Sample - Open Sample...*, select "Sample 1 for QSG.sam" that we created in section 2.2.2 and press the Open button.
- Select *File - Open Measured Data...*, select "QSG2-1.x01" from the "Examples" folder and press the Open button.



- Select *Simulation - Simulate*, or press the button.



- Select *Fitting - Segmented Fit...*, and make sure that the "Segmented Fit Setup" contents are as shown in the following screen grab:



- When you are satisfied that all of the entries are correct press the Close button.

- Select *File - Save Settings...*, and save these settings as “Sample 1 for QSG.set”.
- Select *Settings - Defaults...*, click on the “fittings tab, make sure that “Abs Square Root Difference” is selected as the “Difference scheme:” and press OK.
- Now close X’Pert Reflectivity to ensure that the “Difference scheme:” is written to the .ini file.
- Open an editing tool, for example: Notepad, and create the following batch file:

```
reflectivity.exe "Examples\Sample 1 for
QSG.sam" "Examples\QSG2-1.x01"
"Examples\Sample 1 for QSG.set" "qsg.rmd" /
fit:seg:"fitted sample.sam", "seg
fitted.set", "seg fitted scan.x00" /s:"seg
report.html" /p /html /nologo
```

NOTE: You will need to update the file paths if you did not install X’Pert Reflectivity in the default folder.

- Save this as “run.bat”.
- Run the batch program by selecting ***Start*** *- Run - CMD*.
- Change the directory to the directory where the batch file is, in this example: “cd C:\Program Files\PANalytical\X'Pert Reflectivity”.
- Enter the command “run” and the batch will runs. When it has completed the task, the report will be saved to the current folder and printed on your default directory.

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