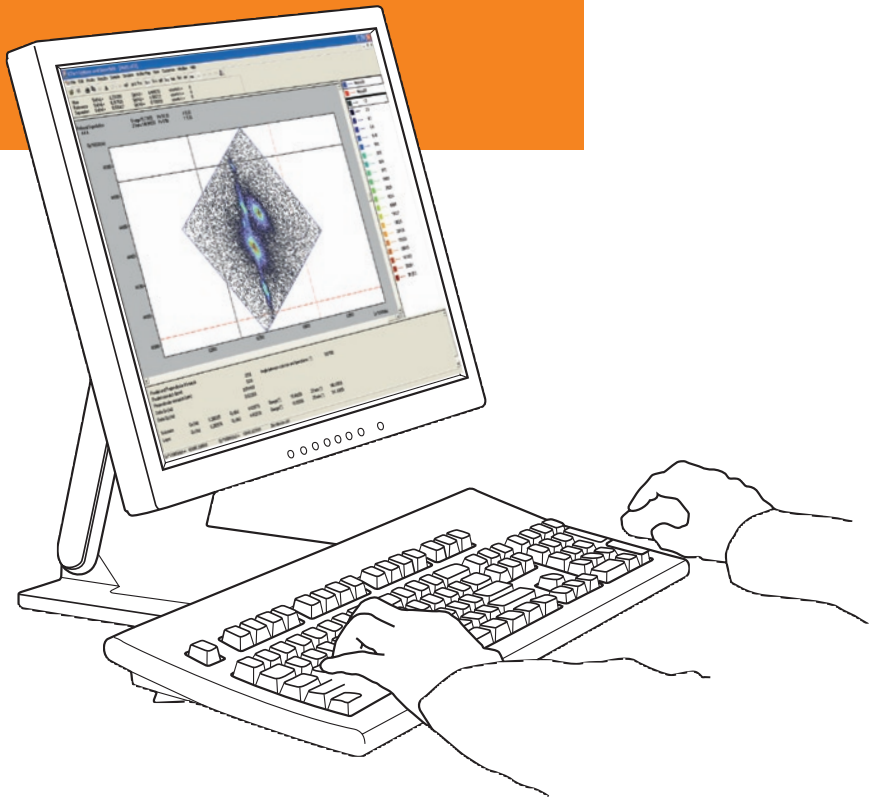


X'PERT EPITAXY AND SMOOTHFIT

Quick Start Guide



X'Pert Epitaxy

Quick Start Guide

EDITION NOTICE: Seventh Edition, January 2007

This is the Seventh Edition of this publication, it is intended for use with version 4.2 of the X'Pert Epitaxy software.

ACKNOWLEDGMENTS

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Chapter 1. Introduction

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X'Pert Epitaxy Quick Start Guide

1.1 Introduction

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

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: Measuring Composition and Thickness from a Rocking Curve

This Chapter describes how to use X'Pert Epitaxy to plot a rocking curve and to determine layer thicknesses and compositions from marked peak positions in rocking curves from cubic semiconductor samples.

Chapter 3: Using Graphics with Area Scans

This Chapter describes how to load and display area data and mark peaks for area scans. In addition the procedures for extracting single scans from a area scan or projecting a area scan as a single scan are described. The examples used in this chapter are FeRAMs (Ferroelectric Random Access Memory) samples.

Chapter 4: Creating a Wafer Map from a Set of Rocking Curves

This Chapter details how to use the X'Pert Epitaxy Wafer Map function to create maps showing the variation in a sample parameter (e.g. substrate peak width or layer mismatch) as a function of position on the wafer from a set of rocking curves.

Chapter 5: Creating Sample Files

This Chapter describes how to create sample files for samples with more than one layer. These files are required when using the automatic fit functionality. Layer linking is described. The chapter is divided into three independent sections - one for each of the major sample types supported: SiGe alloy structures, III-V alloy structures and hexagonal nitride materials.

Chapter 6: Making Simulations and Using Automatic Fitting

This Chapter describes how to use X'Pert Epitaxy to simulate a rocking curve and how to use automatic fitting.

Chapter 7: Determining Composition & Relaxation from Rocking Curves

This Chapter details how use determine layer composition and relaxation for semiconductor samples from a set of rocking curves.

Chapter 8: Determining Composition and Relaxation from Maps

This Chapter details shown how to determine layer composition and relaxation for semiconductor samples from a set of reciprocal pace maps.





Chapter 9: Automating Your Diffraction Measurements

This Chapter describes how automatic analysis can be initiated by creating a new epitaxy icon and associating a specific sample file, measured file and results menu item.

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

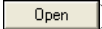
Click	Press the left (primary) mouse button and quickly release it.
Check (✓)	Switch an option or an item on or off, usually by clicking on it. Also referred to as a tick mark.
Confirm	In the examples in this Quick Start Guide we terminate most actions by pressing the  button. When the  button is the default button (indicated by a thick shadow) you can press the <i>Enter</i> 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 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 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 window frame are indicated by bold text (for example: **Apply** or **Cancel**), or shown as the actual button image (for example: ). All fields 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 Epitaxy appears as in Figure 1-1 when the software is started and a single scan is loaded.

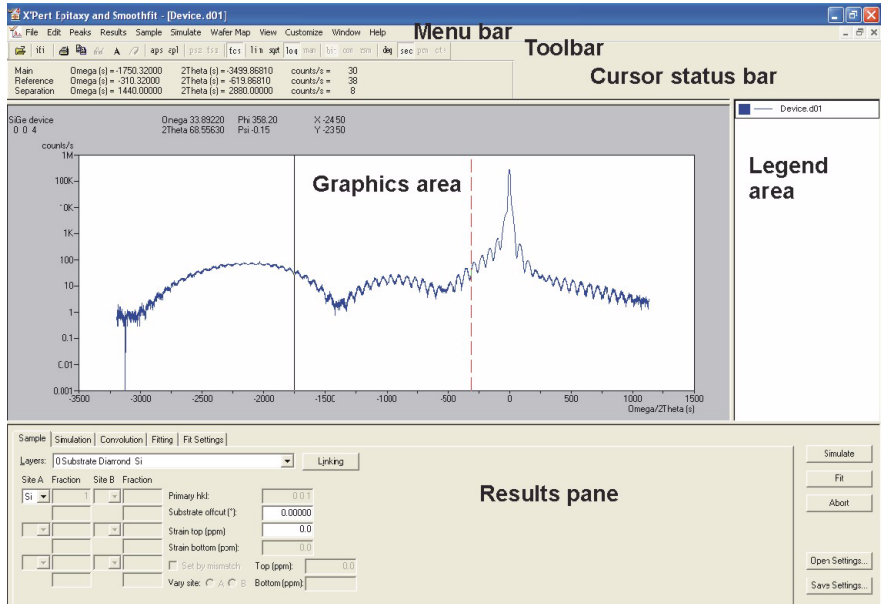


Figure 1-1: The X'Pert Epitaxy Window on Start-up

The window has a toolbar under the title bar and a status line at the bottom. There are eleven menu items, three of which appear after scan data has been loaded:

- | | |
|---------|---|
| File | For loading data, printing and so on. |
| Edit | For adding and removing text. For changing the number of single scans in a window. |
| Peaks | For selecting and labelling peaks. For sending peaks to the Orientation Matrix Refinement list. |
| Results | For making calculations from peak positions. |

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Sample	For creating sample files for <i>Simulate\Results</i> menu.
Simulate	For simulating rocking curves (X'Pert Epitaxy) and automatic fitting (X'Pert Smoothfit).
Wafer Map	For creating maps from an array of rocking curves.
View	For changing the appearance of the window and the plots of the data.
Customize	For setting up defaults.
Windows	For selecting between windows containing plotted scans, including cascading and tiling.
Help	For accessing help information.

A new child window is opened every time data files are opened using *File - Open*. The menu items available depend on the type of data displayed. The three child window types are for single scans (as shown in Figure 1-1), area scans and wafer maps.

1.4.1 Layout of Plots

As shown in Figure 1-1 the plotted data has a legend area to the right and a header area. The single and area scan windows also have a results pane. This header, legend area and the results pane can be toggled off from the *View* menu.

The relative sizes of the results pane, plot area and legend area can be changed by dragging on the splitter bars. When the areas are too small to accommodate the available information, scroll bars appear.

1.4.2 Changing the Appearance of Plots

Intensity scaling and angular scaling are chosen using the *View* menu.

It is also possible to offset single scans horizontally and vertically.

It is possible to change between contours and bit maps for area scans, and there is a choice of plotting in the full available area or having equal angular scaling on both the axes.

It is possible to change between displaying contours, or values, or both for wafer maps.

Many of the *View* menu options are also available on the toolbar and in pop-up menus (accessed by clicking right mouse button when the mouse pointer is in the graphics area).

Zoomed areas are defined by dragging the mouse.

Text can be added within the plot area.

1.4.3 Marking Peaks

If you wish to analyse single scan data using X'Pert Epitaxy the peaks must first be found and labeled. This can be done both automatically and manually using the *Peaks* menu. This menu is also used for labeling the peaks. There is a semi-automatic peak find facility for area scans.

1.4.4 Customizing X'Pert Epitaxy

A wide range of default parameters can be set using the *Customize* menu:

- default folders

- options for displaying single scans

- options for displaying area scans

- options for displaying wafer maps

- screen and printer palettes

- default single scan peak search and label parameters for single scans

- default intensity levels for area scans

- default scaling for plots in reciprocal lattice units

- default substrate and layer combinations for sample files

- default convolution parameters for simulated scans

- default fitting parameters for automatic fitting

1.5 Data Files for Use with this Quick Start Guide

Several data files have been supplied with X'Pert Epitaxy Version 4 for you to use with this Quick Start Guide. Those files are installed in folder: "C:\Program Files\PANalytical\X'Pert Epitaxy\Examples" and they are:

Used in:	Data File
Chapter 2	004 GeSi on Ge.xrdbl
Chapter 3	SBTN fibre.a00, 2026.a00, 60x60.a00
Chapter 4	GaAs_SiN WM.xrdbl, 2flat30.sol, Inp_Q.d00 to Inp_Q.d35, InP_Q.s00, Half 2in.sol
Chapter 6	Q on InP.s00 SiGe.d00, SiGe4.s00, SiGe4.fit, SiGe grad.x00, SiGe grad4.s00, SiGe4.s00, SiGe4.fit GaN.d00, GaN4.s00, GaN4.fit
Chapter 7	GaInAs004a.d00, GaInAs224a.d00, GaInAs004b.d00, GaInAs224b.d00
Chapter 8	Map004a.a00, Map444a.a00, Map004b.a00, Map444b.a00

Chapter 1. Introduction

Other data supplied with X'Pert Epitaxy, also installed in folder: “C:\Program Files\PANalytical\X'Pert Epitaxy\Examples” are:

Single scans:	
Opt0.d00, Opt90.d00, Opt180.d00, Opt270.d00	use with Results - Substrate Offset
004 GeSi on Ge.xrdbl, 004r GeSi on Ge.xrdbl	use with Results - Mismatch (symm) - sample used in Chapter 2 of Quick Start Guide
Device.d01, Device.s00	a good quality rocking curve with sample file for analysis and automatic fitting
OR333Si.d02, OR513Si.d02, OR531Si.d02	use with Results - Orientation Matrix Refinement

Area scans:	
GaInAs004.a01, GaInAs224.a02 - 004 and 224 from a partially relaxed layer of gallium indium arsenide on (001) GaAs	use for calculating relaxation and com- positor
Multi.a01, Multi.a02 - 004 and 444 maps from a partially relaxed superlattice on (001) GaAs	GaAs use for calculating relaxation and superlattice period

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Chapter 2. Measuring Composition and Thickness from a Rocking Curve

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Chapter 2. Measuring Composition and Thickness from a Rocking Curve

2.1 Introduction

In this example we will show you how to use X'Pert Epitaxy to display a rocking curve from a single crystal substrate with a heteroepitaxial layer, and determine the composition and thickness of the layer.

The example provided is an 004 rocking curve from a (001) germanium substrate with a strained heteroepitaxial layer of germanium silicon recorded using a PANalytical X'Pert Pro MRD. The scan file "004 GeSi on Ge.xrdbl" is an $\omega/2\theta$ scan which was recorded using a mirror plus a Ge 220 four crystal monochromator as primary optics modules and a receiving slit as secondary optics module. This file is put in the folder "C:\Program Files\PANalytical\X'Pert Epitaxy\Examples" during the installation of X'Pert Epitaxy.

The procedure for analyzing a rocking curve will be described in six parts:

1. Setting the default sample.
2. Setting up default peak finding and labeling.
3. Displaying the scan file.
4. Determining the layer composition and thickness.
5. Printing out the results.
6. Preparation for working on similar samples.

2.2 The Procedure

- Start X'Pert Epitaxy

2.2.1 Setting the Default Sample

Now we will set the default sample:

- Select *Customize - Defaults*.
- Click on the "Sample Data" Tab.
- Use the drop-down list box to set the "Default substrate structure:" to Diamond.

First set the substrate:

- In the tree view highlight the Diamond Substrate.
- In the Site A frame:
 - Enter 1 for the "No. of Elements".
 - Use the drop-down list box to select Ge as the Site A Element.

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- Enter 0 0 4 (0<space>0<space>4) for the “Simulations HKL”.
- Enter 0 0 1 for the “Primary HKL”.
- Enter 600 for the “Thickness”.
- Enter 0.0 for the “Offcut angle”.
- Use the drop-down list box to set the “Layer Structure” to diamond.

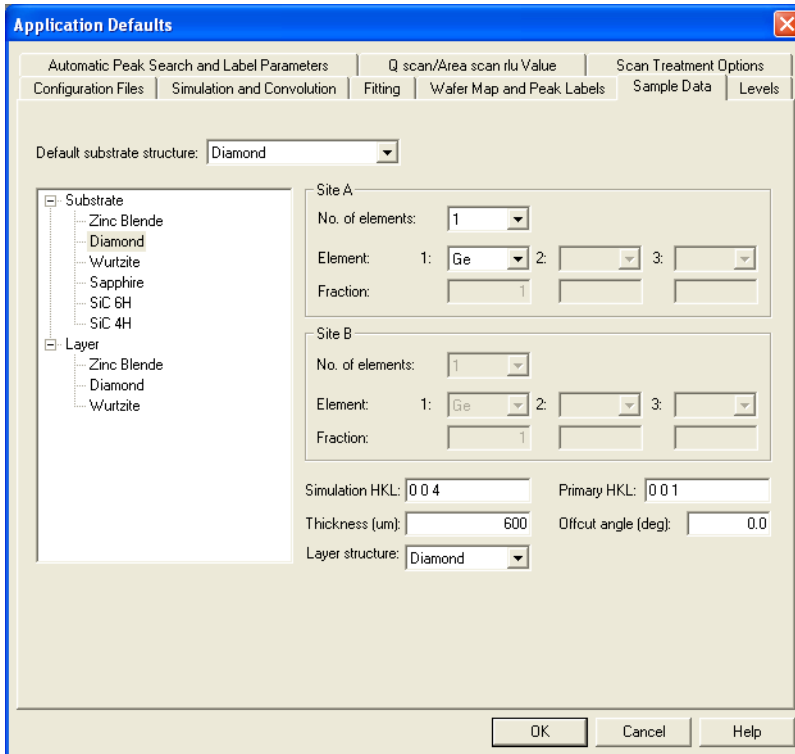


Figure 2-1: The Default “Sample data” tab set for a Ge (001) Substrate

Chapter 2. Measuring Composition and Thickness from a Rocking Curve

Now set the layer:

- In the tree view highlight the “Diamond Layer”.
- Use the drop-down list box to set the “No of Elements” to 2 in the Site A Frame.
- Use the drop-down list box to set “Element 1” to Ge.
- Use the drop-down list box to set “Element 2” to Si.
- Enter 0 0 4 for the “Simulations HKL”.
- Enter 0.1 for the “Thickness”.

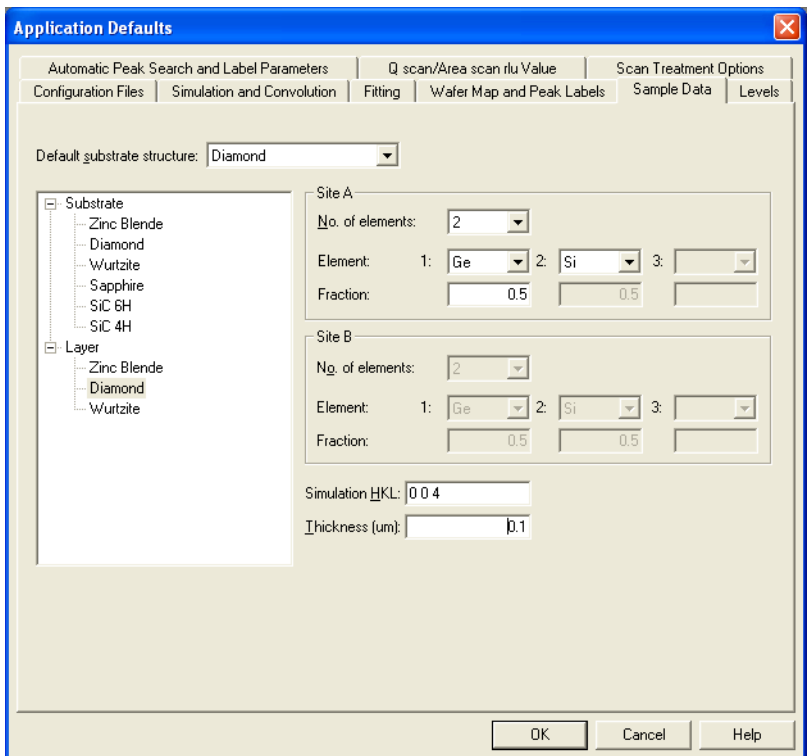



Figure 2-2: The Default “Sample data” tab set for a GeSi Layer

- Click  to save default settings.

2.2.2 Setting the Default Peak Labelling

Set up peak labeling for the layer and substrate peaks and two thickness fringes:

- Select *Customize - Defaults*.
- Select the “Automatic Peak Search and Label Parameters” tab.
- Set up the parameters as shown in Figure 2-3 in the “Peak search parameters” frame, the “Label Parameters” frame and the “Automatic Peak Marking on Opening” frame.

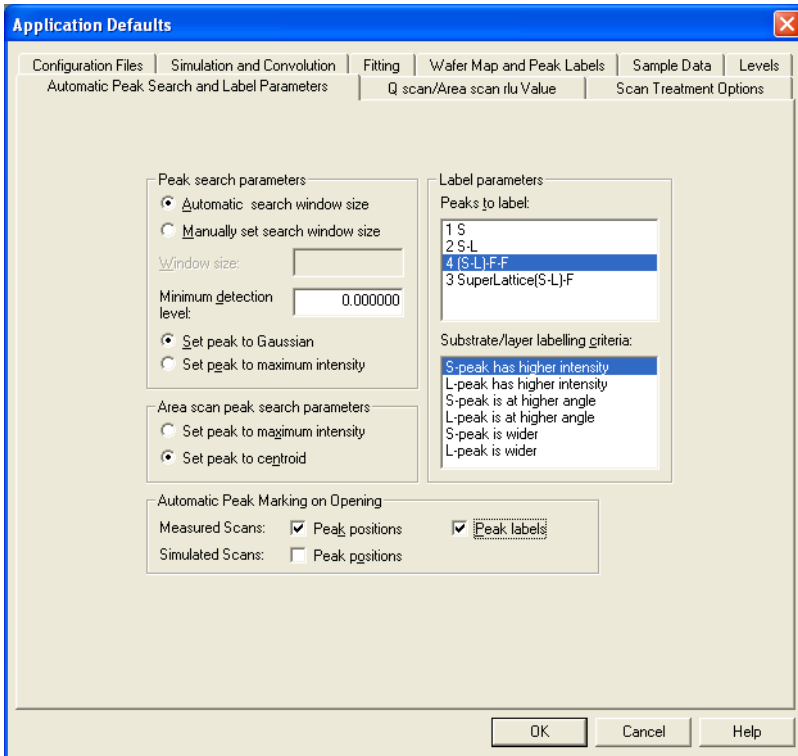


Figure 2-3: The “Automatic Peak Search And Label Parameters” tab

- Click . From now on, as a measured scan is loaded, peak positions will be marked with vertical lines and the substrate and layer peaks will be marked S and L respectively, two thickness fringes will be labeled F.

Chapter 2. Measuring Composition and Thickness from a Rocking Curve

2.2.3 Displaying the Measured Data

First we set the default single scan options:

- Select *Customize - Single Scan Options*.
- In the “Default - X - scaling type” pane select the “Relative seconds plot” radio button if you wish to plot in seconds, or “Degree plot” radio button if you wish to plot in degrees.
- In the “Default Y-scaling type” pane select the “Logarithmic” radio button.
- Click to close the window.

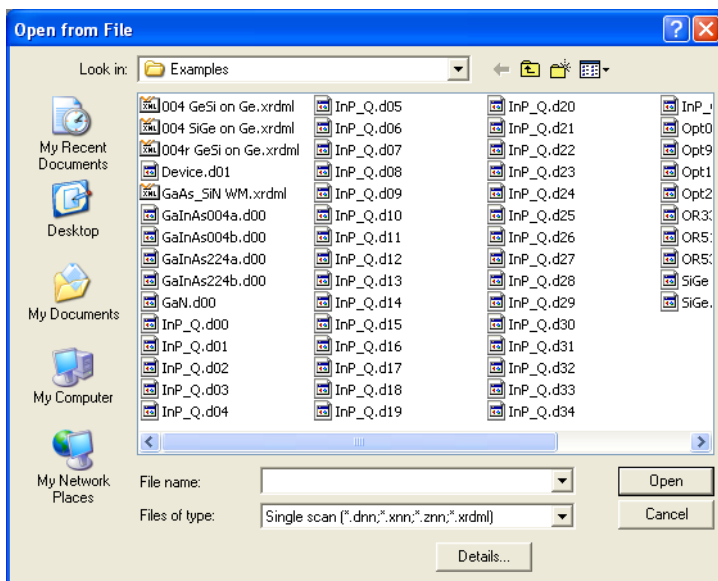


Figure 2-4: The Open from File Window

Now we will open the measured file

- Select *File - Open*, the window shown in Figure 2-4 will appear.
- Select “004 GeSi on Ge.xrdml” (you may have to change the folder to: C:\Program Files\PANalytical\X'Pert Epitaxy\Examples) so that it appears in the “File name” field.

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- Click .

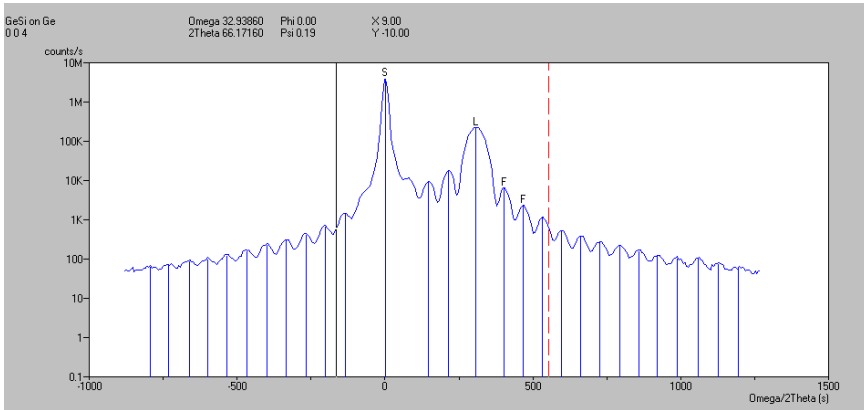


Figure 2-5: The Graphics Area after Opening the Scan

The scan data appears as shown in Figure 2-5 in a single scan graphics window (relative seconds version illustrated). The position information above the plot is the scan center read from the file header, the file name is shown in the legend area on the right. If these areas are missing toggle them ON in the *View* menu.

Quick ways to manipulate your screen plots:

- To zoom in on the plot, drag with the mouse to define the required area. Use the toolbar button **psz** to go back to the previous zoomed size, or **fsz** for the full size plot. When the plot is zoomed, horizontal and vertical scroll bars are available for moving around the entire area of the plotted data.
- You can use the toolbar buttons marked **lin** and **log** to change between linear and logarithmic intensity scaling.
- You can use the toolbar buttons marked **deg** and **sec** to change between scaling in degrees and relative seconds.

Chapter 2. Measuring Composition and Thickness from a Rocking Curve

2.2.4 Determining the Layer Composition and Thickness

We are now ready to find the layer composition and thickness.

- Select *Results - Results Summary*.
- If only part of the results pane is visible at the bottom of the screen drag the splitter bar between the results pane and the graphics area upwards.

The calculated results are shown in the results pane at the bottom of Figure 2-6.

Results Summary				
Name	Omega (°)	2Theta (°)	FWHM (°)	Intensity (cps)
Substrate: Ge	32.88484	66.06408	0.00448	4000793.50000
Layer: GeSi	32.97017	66.23473	0.01695	226346.45313
<input type="checkbox"/> Calculate the site B composition				
Relaxed mismatch (ppm):	-2281	Strained mismatch (ppm):	-1303	
Relaxed composition:	Ge0.949025i0.05098			
Strained composition:	Ge0.970975i0.02903			
Thickness (um):	0.299249			
<input type="text" value="1, None, Diamond, thick = 0.100000 um, Ge0.55i0.5"/>				

Figure 2-6: The Results Pane

The layer and substrate peak positions, intensities and half widths are given together with values of the layer thickness. Two values for the mismatch and composition are supplied - one assumes the layer is fully relaxed and the other assumes that the layer is fully strained. As the thickness fringes are very clear the layer appears to be fully strained, thus the fully strained value is the correct value for this sample.

The procedure described above, is one of two possible ways of finding the composition and mismatch for a cubic sample. Further information about interpreting single scans, including the equations used, is given the X'Pert Epitaxy Help File. The layer thickness can be found more accurately by marking all the fringes on the right-hand side of the layer peak - see the help topic "Labeling Multiple Peaks".

2.2.5 Printing the Results

If you wish to print out the graphics plus results:

- Select *File - Print*.
- Click on **Properties** to change the paper or print quality as required.
- Click to print.

2.2.6 Preparation for Working on Similar Samples

If this sample was the first of many similar samples to be measured you could save the sample file and the .INI file to automate the analysis of further samples (see Chapter 9).

Save the sample details as a sample file:

- Click the right mouse button when the mouse pointer is inside the results pane to bring up the pop-up menu.
- Display the pop-up menu from the results pane.
- Click on *Update Layer*.
- In the Update window select the “Strained Values” radio button.
- Click the button.
- Click to update the layer thickness - the layer details have now been changed in the sample file.
- To save this sample file select *Sample - Edit Sample* from the main menu.
- Click on .
- Enter “GeSi on Ge” as the sample file name.
- Click and then to close the “Sample Data” window.

Save all of the default settings in an INI file for future use as follows:

- Select *Customize - Save Defaults As...*
- Enter “ResSum.ini” for the file name.
- Click .

Chapter 9 explains how this INI file can be used to automate analysis.

That is the end of this exercise, close all files and close Epitaxy.

Chapter 3. Using Graphics with Area Scans

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Chapter 3. Using Graphics with Area Scans

3.1 Introduction

In this chapter we will show you how to manipulate area scan data. We will look at three files recorded from materials used for Ferro-electric Random Access Memories (FeRAM).

The first example uses data collected from a sample which has a layer of SBTN ($=\text{SrBi}_2(\text{Ta}_{0.7}\text{Nb}_{0.3})_2\text{O}_9$) on a (100) Si substrate coated with layers of silicon dioxide, titanium and platinum. We will look at how to project a 2Theta-Omega/Psi map as a powder scan.

The second and third examples use data collected from a sample which has an SBT ($=\text{SrBi}_2\text{Ta}_2\text{O}_9$) layer on a strontium titanate ($=\text{SrTiO}_3$) substrate. We will look at how to measure the perpendicular and parallel mismatches between the layer and substrate from a reciprocal space map. We will also look at how to extract small area maps from large maps.

3.2 Example 1 - Projecting an Area Scan

We will learn how to select plot options for a area scan and how to project a scan. The data used is file “FiberSBTN.a00”.

Analysis of this data is described in detail in a paper published by Saito et al: Jpn J Appl, Phys 39, 5489-5495 (2000)

Proceed as follows:

- Start Epitaxy.
- Select *Customize - Area Scan Options*. The window should look like this:

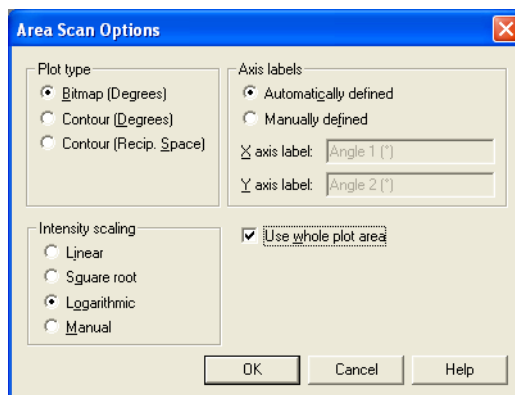


Figure 3-1: Area Scan Options Window

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If the radio button settings are as shown, click . If they are not as shown above, first change the radio button settings to match this example and then click .

- Select *File - Open*.
- Choose “Area Scan” in “Files of type:” drop-down list box.
- Double-click on the file “SBTN fibre.a00” to load that file.
- Select *View* and click on *Plot in Absolute Values* (when it is selected, this menu item has a bullet beside it).

The graphics area should look like this:

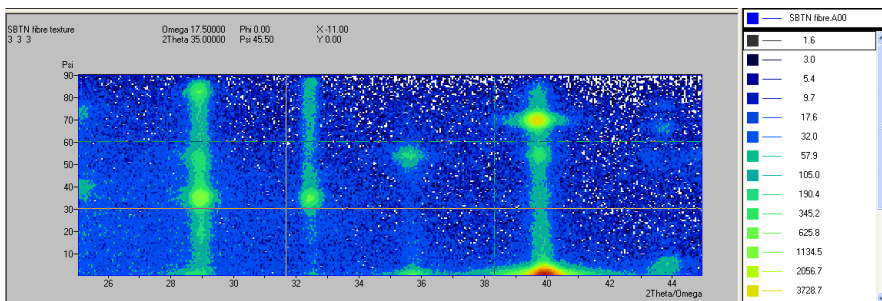


Figure 3-2: “SBTN fibre.a00” plotted in Absolute Degrees

This area map is a set of 2Theta-Omega scans recorded for Psi values between 0 and 90 degrees. The thin film has a fibre texture - the intensity for each reflection is distributed along vertical lines in the plot. By projecting all the intensity onto the horizontal axis we will create a 2Theta-Omega scan which would be recorded from a polycrystalline sample of the same material. This scan can be used to check the phases which are present.

- To project the map: select *Edit - Project to X Axis*.

Now you will either see the projected scan (see Figure 3-3) or you will be asked for a file name. If you provide a file name, or accept the proposed “mm” you can then use *File - Open* to view the scan.

Chapter 3. Using Graphics with Area Scans

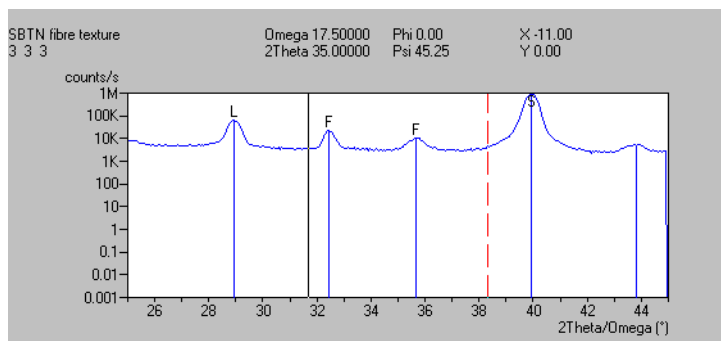


Figure 3-3: Projected Scan with Logarithmic Intensity Scaling

The projected scan should look like Figure 3-3 when plotted using a logarithmic intensity scale.

3.3 Example 2 - Measuring Parallel and Perpendicular Mismatch

In this example we will show you how to mark peaks in an area scan and use the results menu to find the parallel and perpendicular mismatch. The data used is file “2026.a00”. It is a reciprocal space map which of the 2 0 26 reflection from the SBTN layer and the 114 reflection from the (001) strontium titanate substrate.

- Select *Customize - Area Scan Options*.
- In the “Plot type” pane select: Contour (Reciprocal Space).
- Click .
- Open file “2026.a00” (C:\Program Files\PANalytical\X’Pert Epitaxy\Examples)

The data was recorded with low resolution optics so both reflections show the Copper $K\alpha$ doublet. The stronger doublet is from the substrate. We will now mark the peaks from $K\alpha_1$ peaks from the layer and substrate.

- Select *Peaks - Semi Automatic Peak Search*.
- The cursor will appear as a cross in a box.

- Move the cursor near to the $K\alpha_1$ peak for the substrate. Hold the left-hand mouse button and drag to define a rectangle roughly centred on the peak. The plot should appear as follows:

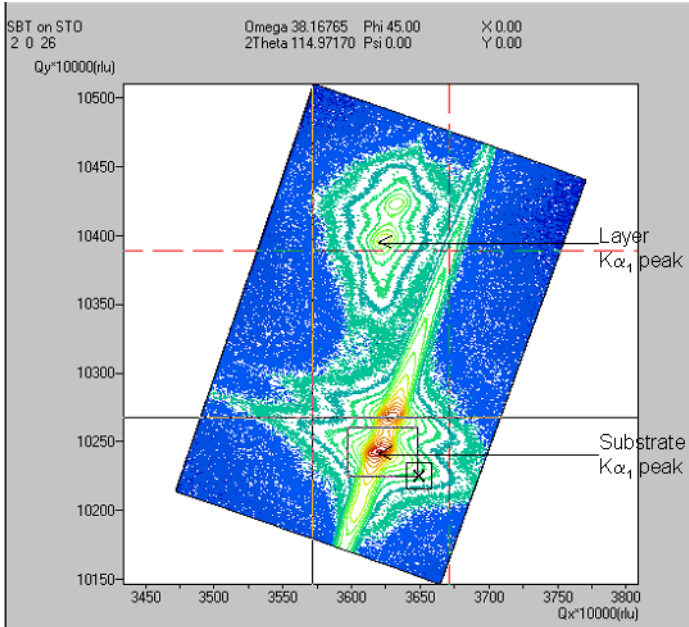


Figure 3-4: Marking the Substrate Peak Position using *Semi Automatic Peak Search*

- Mark the $K\alpha_1$ peak for the layer (the lower peak of the upper pair) in the same way:
- Move the cursor near to the $K\alpha_1$ peak for the layer. Hold the left-hand mouse button and drag to define a rectangle roughly centred on the peak.
- Select *Peaks - Semi Automatic Peak Find* again to change the cursor back to its usual shape.
- Select *Peaks - Automatic Peak Label* and highlight “2S-L” and “S-peak has higher intensity” as shown in Figure 3-5. You can ignore the parameters set on the left-hand side as they are not applicable for area scans.

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If the automatic peak search window does not appear as in Figure 3-5, go to *Customize - Defaults*, select the “Automatic Peak Search and Label Parameters tab” and remove the tick from the “Peak labels” box at the bottom, click the button and return to the previous bullet point.

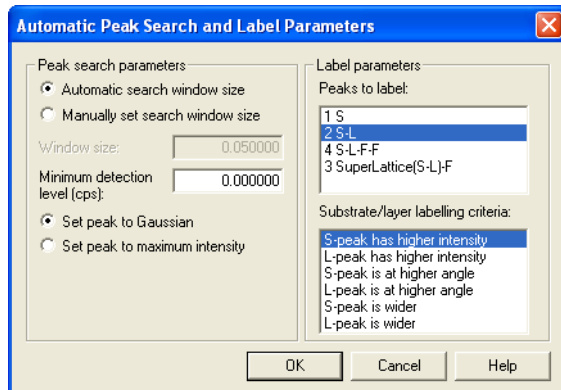


Figure 3-5: Automatic Peak Search Window

- Click .

A small S should appear beside the substrate peak and a small L should appear beside the layer peak.

- Select *Results - Peak Grid*. (If this menu item is not available, first select *View - Results*.)

The peak details should appear below the graphics area. The separator above the grid can be dragged to change the vertical height of the results pane containing the grid.

- Select *Results - Parallel and Perpendicular Mismatch*.

The values for the d-spacing mismatch (fractional differences in d-spacings) parallel & perpendicular to the substrate surface are given as shown in Figure 3-6.

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Parallel and Perpendicular Mismatch								
Parallel mismatch (ppm)				-985	Angle between substrate and layer planes (°)			0.29000
Perpendicular mismatch (ppm)				-14839				
Delta Qx (Å ⁻¹)				0.000275				
Delta Qy (Å ⁻¹)				0.011885				
Substrate:	Qx (Å ⁻¹)	0.278830	Qy (Å ⁻¹)	0.789001	Omega (°)	37.34265	2Theta (°)	113.61170
Layer:	Qx (Å ⁻¹)	0.279105	Qy (Å ⁻¹)	0.800885	Omega (°)	38.79515	2Theta (°)	116.01670

Figure 3-6: d-spacing Mismatch Values

This information can be used to derive the lattice parameters of the layer unit cell assuming the values for the substrate are known.

- Close this example by selecting *File - Close*.

3.4 Example 3 - Extracting Area Scans

We will learn how to extract small area scans from large area scans. The data used is file 60x60.a00. It is a large area reciprocal space map from an SBTN layer on a (001) strontium titanate substrate - the same sample as used in EXAMPLE 2. The data was recorded with low resolution optics so all reflections show the Copper $K\alpha$ doublet. The data extends over 60 degrees in Omega and 60 degrees in 2Theta-Omega.

- Select *Customize - Area Scan Options*.

You will see the window as shown in Figure 3-1. For this example:

- Select “Plot type” as Bitmap.
- Click .
- Select *File - Open*.
- Use the drop-down list box to select file type “Area scan (*.ann, *.ynn)”.
- Find and then double-click on 60x60.a00.

Chapter 3. Using Graphics with Area Scans

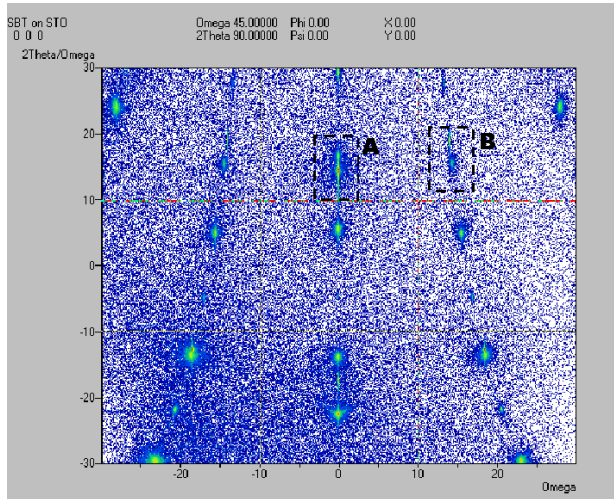


Figure 3-7: Graphics Area

Figure 3-7 shows the graphics area. The two areas indicated by A and B are the two areas which we will extract as maps.

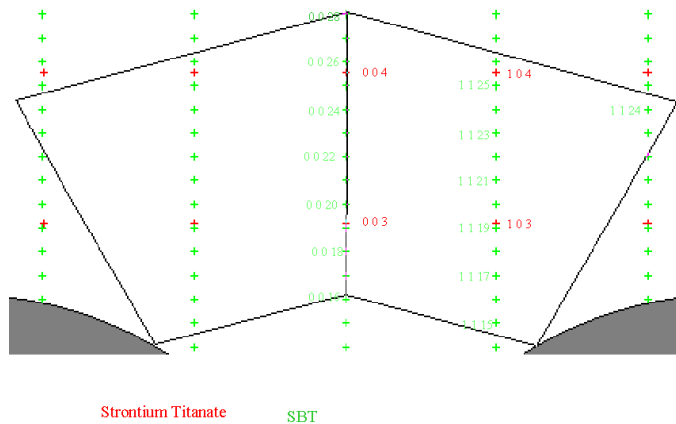


Figure 3-8: Reciprocal Space Area Included in this Scan

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Figure 3-8 shows the area of reciprocal space included in this scan. This figure is an annotated version of the reciprocal space map from X'Pert Data Collector. The red crosses are reflections from the strontium titanate substrate. The green crosses are reflections from the layer. The hkl values are shown for allowed reflections. The four hkl values outlined in black are the reflections included in areas A and B of Figure 3-7.

To extract the two small maps:

- Using Figure 3-7 as a guide, zoom into area A.

The two reflections should appear as in Figure 3-9. When you are satisfied that you have the correct area:

- Select *Edit - Extract Area Scan*.

The graphics screen will redraw to show the full map with the extracted map shown with a red outline. It is automatically named 60x60.a01.

- Repeat the last two steps to extract area B (it should appear as in Figure 3-10 and then with a green outline).
- Select *File -Save - All Scans* to save the two small scans (60x60.a01 and 60x60.a02).

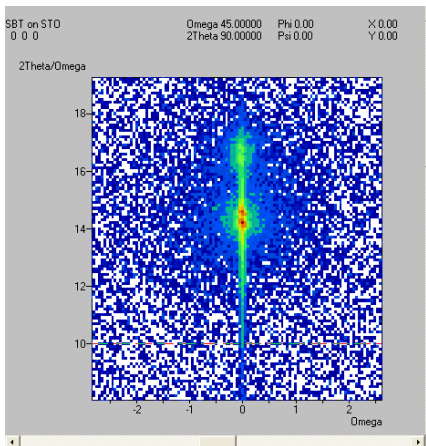


Figure 3-9: Area A

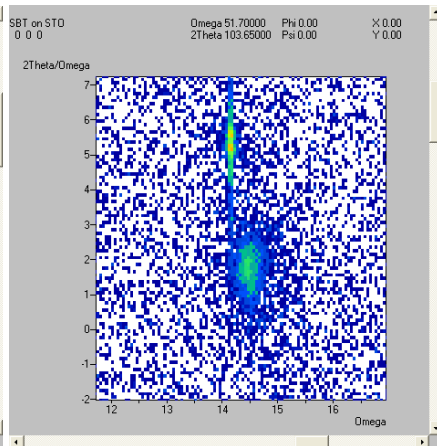


Figure 3-10: Area B

That is the end of this exercise, close all files and close Epitaxy.



Chapter 4. Creating a Wafer Map from a Set of Rocking Curves

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Chapter 4. Creating a Wafer Map from a Set of Rocking Curves

4.1 Introduction

A wafer map shows the variation in a sample parameter (for example: substrate peak width or layer mismatch) as a function of position on the wafer). A series of rocking curves recorded from an array of points on the sample is required as input.

Two sets of example data are provided. The first is an array of rocking curves recorded from a gallium arsenide wafer with a amorphous layer of silicon nitride. The change in position of the substrate peak is used to demonstrate the distortion of the wafer due to the presence of the amorphous layer. The second set is from a strained (i.e. relaxation = 0%) gallium indium arsenide phosphide layer on an indium phosphide substrate with an indium phosphide cap. Here the variation in layer mismatch is calculated from the variation in the separation of the substrate and quaternary layer peaks.

The first example is described in Section 4.2. This analysis does not require a sample file. This type of wafer map can be applied to any substrate material.

The second example is described in Section 4.3. Here a sample is required. This type of wafer map can only be applied to samples with diamond or zinc blende crystal structure.

4.2 Creating a Wafer Map to Demonstrate Substrate Distortion

The sample was a 2 inch gallium arsenide (001) wafer with a deposited layer of amorphous silicon nitride. A regular array of rocking curves was collected using a Wafer Map program using X'Pert Data Collector.

The two files supplied for this example (folder “C:\Program Files\PANalytical\X'Pert Epitaxy\Examples”) are:

GaAs_SiN WM.xrdml - the scan data

2flat30.sol - a file showing the outline of the wafer.

The procedure for creating the wafer maps is described in three parts:

1. Setting the defaults.
2. Opening the data and creating the wafer map.
3. Printing out the results.

To set up the defaults:

- Start X'Pert Epitaxy.
- Select *Customize - Defaults*.
- Click on the “Automatic Peak Search and Label Parameters” tab.

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- Use the options shown in Figure 4-1:

On the left hand side select “Automatic search window size”, “set peak to Gaussian”.

On the right hand side “1-S” should be highlighted for the “Peaks to label” and “S peak has higher intensity” should be highlighted for the “Substrate/layer labeling criteria”.

All the option boxes at the bottom should be unchecked.

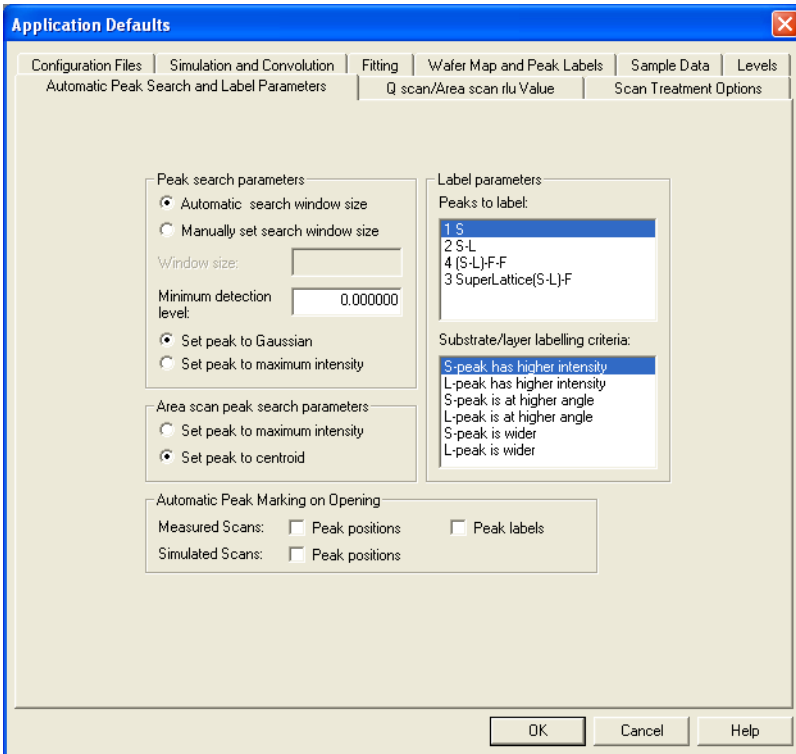


Figure 4-1: The Automatic Peak Search and Label Defaults Setup for Finding One Peak

Chapter 4. Creating a Wafer Map from a Set of Rocking Curves

Now set the wafer mapping defaults:

- Click on the “Wafer Map and Peak Labels” tab.
- Use the options shown in Figure 4-2:

Use the first drop-down list box to set “For wafer map peak table files display” to “Substrate Position (°)”.

Use the second drop-down list box to set “For wafer map results files display” to “Strained Mismatch (ppm)” - this is for the second example.

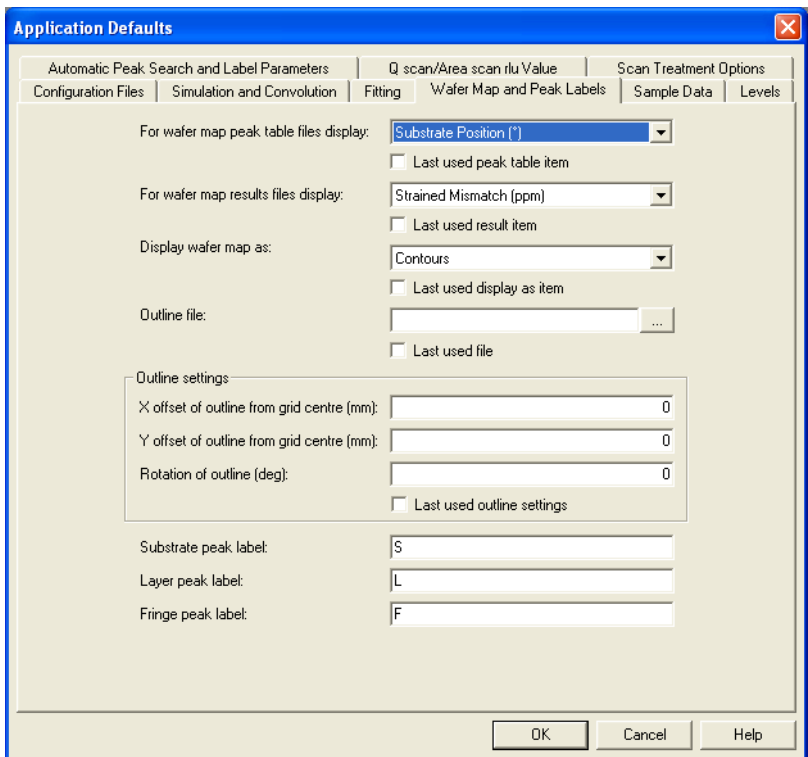


Figure 4-2: The Wafer Map and Peak Label Defaults

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To continue:

- Click to close “Application Defaults” window.
- Select *Wafer Map - Wafer Map from Raw Data*.
- Enter the “Peak table file name” as “GaAs_SiN”.
- Click on .
- Open the file “GaAs_SiN WM.xrxml” (folder “C:\Program Files\PANalytical\X'Pert Epitaxy\Examples”).
- Click to open the file and close the “File Open” window.
- Click on to see the position of the measured rocking curves.
- You will see a 5x5 grid of measured points as shown in Figure 4-3. The points are in the centre of the wafer. The positions are shown in terms of the X and Y co-ordinates of the MRD cradle. The centre of the wafer was at X=2 mm, Y=26 mm.

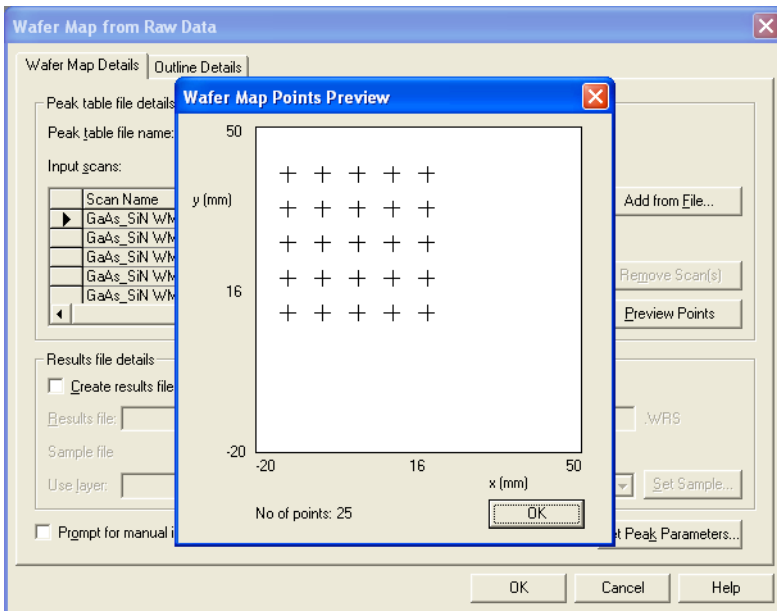


Figure 4-3: The Wafer Map from Raw Data Window with the Preview Display

Chapter 4. Creating a Wafer Map from a Set of Rocking Curves

To add the information about the wafer shape:

- Click to close “Wafer Map Points Preview” window.
- Click on the “Outline Details” tab.
- Enter 2 and 26 for the X and Y offsets (the X and Y positions of the centre of the wafer).
- Click on .
- Select the file “2flat30.sol” - this is a 2 inch wafer with a major flat subtending an angle of 30 at the centre and press .

The outline will be displayed on the tab as shown in Figure 4-4.

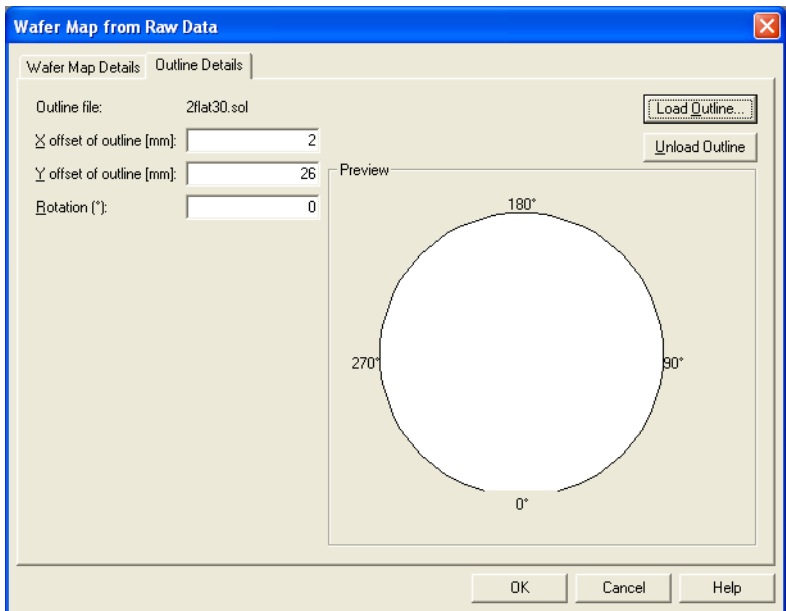


Figure 4-4: The “Outline Details” Tab

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To display and print the map:

- Click to close the wafer map window.

The map should appear as in Figure 4-5. You may need to select View-Linear to observe the contours.

- Select *File - Print*.
- If required click **Options** in the printer window to change the paper orientation and the print quality.

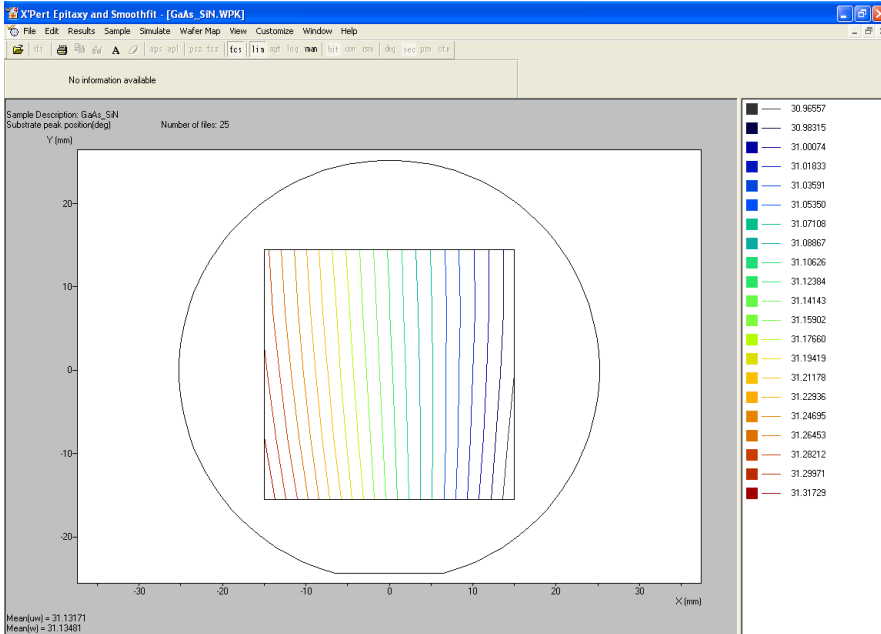


Figure 4-5: The Wafer Map showing the Substrate Peak Position

This wafer map is saved as “GaAs_SiN.wpk”. All the information about the outline file position is saved with it. The wafer map can be opened using *File - Open*.

4.3 Wafer Map to Demo Mismatch Variation in Quaternary Layer

The sample was half a 2 inch indium phosphide (001) wafer with a heteroepitaxial quaternary (gallium indium arsenide phosphide) layer plus an indium phosphide cap. Thirty six individual 004 rocking curves scans are supplied. These were recorded for a 9x4 rectangular array of points. The mismatch will be determined from the substrate-layer peak separation using information about the substrate and layer materials from the sample file.

The sample was mounted on the MRD cradle with the co-ordinates of $X = -1$, $Y = -2$ for the centre point of the full 2 inch wafer.

The files supplied for this example (in folder “C:\Program Files\PANalytical\X’Pert Epitaxy\Examples”) are:

- InP_Q.d00 to InP_Q.d35 - 36 rocking curves in a 4x9 grid
- InP_Q.s00 - the sample file
- Half 2in.sol - the outline file.

We will assume the defaults are as set in Section 4.2.

To load the scans:

- Select *Wafer Map - Wafer Map from Raw Data*.
- Click on .
- Highlight all the file names “InP_Q.d00” to “InP_Q.d35”.
- Click to close the “Add from File” window.
- Click on to see the position of the measured rocking curves.

You should see a complete 4x9 grid of points. If the grid is not complete check the list of scan names in the Wafer Map window to see which files have not been loaded.

You can add these by clicking again and highlighting the missing files.

- Click to close the “Preview” window and then click to close the “Wafer Map from Raw Data” window.

For this example we want to search for the two largest peaks per scan and we wish to make calculations from the peak positions. We need to change the peak search parameters from those used in Section 4.2:

- Click on .

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- In the “Label Parameters” frame change the “Peaks to label” to “2 S-L” - see Figure 4-6.
- Click .

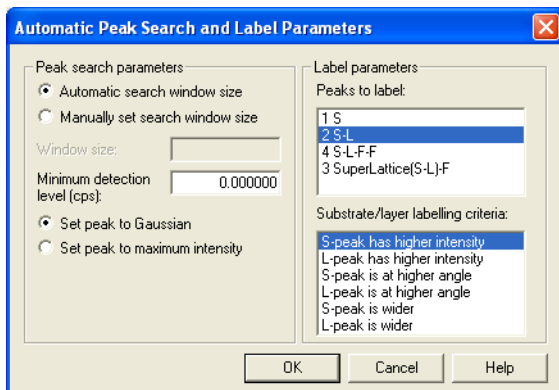


Figure 4-6: The Peak Parameters for the InP_Q Sample

For this example we need to produce a peak table (with information about the peak parameters) and a results file (with the values calculated from the peak positions). We also need to load the sample file:

- Enter “InP_Q” for the “Peak table file name”.
- Tick the “Create results file” option box.
- Enter “InP_Q” for the “Results file” name.
- Click .
- Select the file “InP_Q.s00”.
- Click to load the sample file.
- The “Use layer” drop-down list box should show Layer 1 of the sample (the Q layer).

The “Wafer Map Details” tab should now be as in Figure 4-7.

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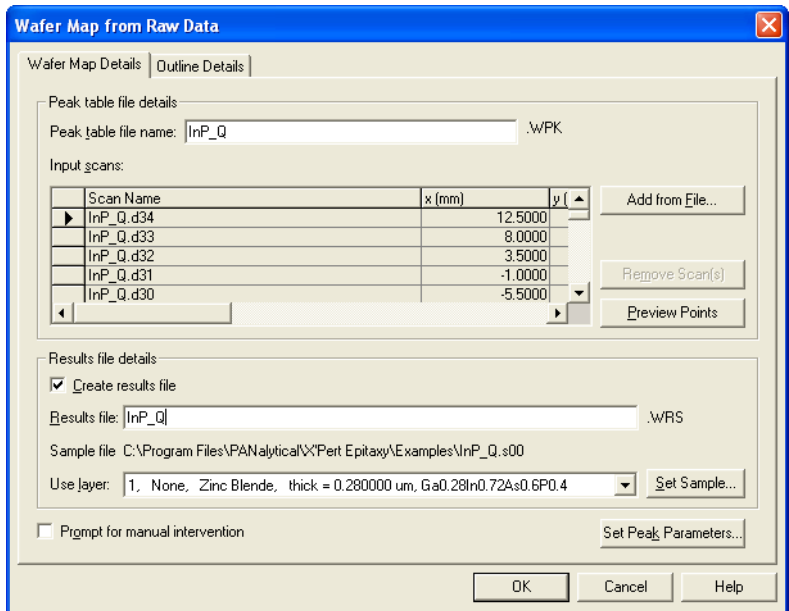


Figure 4-7: The “Wafer Map Details” tab

To add the information about the wafer shape:

- Click on the “Outline Details” tab.
- Enter “-1” and “-2” for the X and Y offsets.
- Click on .
- Select the file “Half 2in.sol” - this is a semicircle with a diameter of 2 inches.
- Click to load the outline file.

The “Outline details” tab should now be as in Figure 4-8.

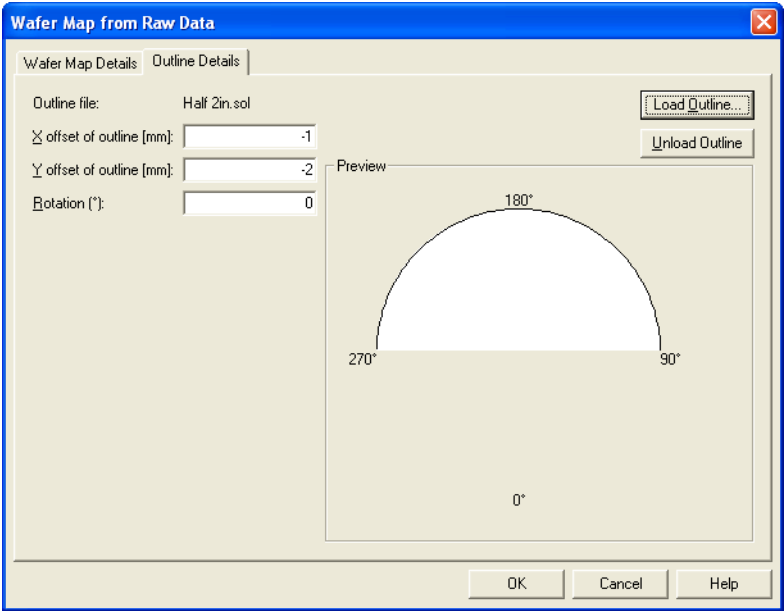


Figure 4-8: The Wafer Outline tab

To display and print the map:

- Click to close the wafer map window.
- Select *File - Print*.
- If required click **Options** in the printer window to change the paper orientation and the print quality.

The map should appear as in Figure 4-9. The layer mismatch is displayed because this is the results file default selected in Figure 4-2.

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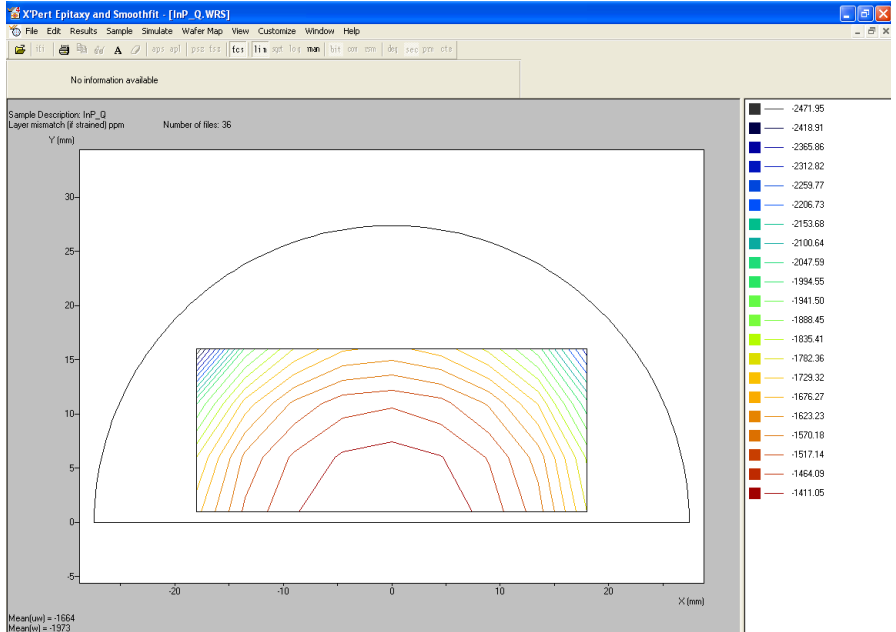


Figure 4-9: The map of Variation in Layer Mismatch

For this example both the peak table file (with extension .wpk) and the results file (with extension .wrs) were created and saved. The default results table item is displayed. If you want to look at a wafer map of any of the peak parameters:

- Select *File - Open*.
- Highlight InP_Q.wpk.
- Click to open the file.

You will see a map of the substrate peak position (default set in Figure 4-2). If you wish to view another parameter from the peak table:

- Move the mouse pointer into the graphics area and click the right mouse button to display the pop-up menu.
- Select *Peak Table Items*.
- Choose the item you require from the submenu. In this example we chose “Width (°)” and the result is as shown in Figure 4-10.

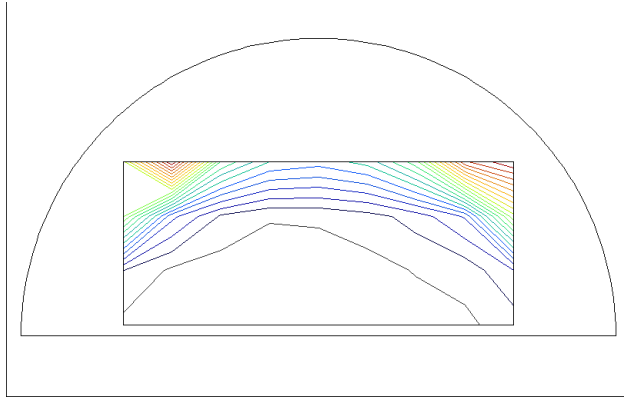


Figure 4-10: The Peak Table having Chosen Width (°)

4.4 Using Your Own Data

This section provides additional information you may need when using your own data. This includes:

- How to create outline files (4.4.1).

- How to create results files from an existing peak file. (4.4.2).

- How to include thickness measurements (4.4.3).

- Changing the viewing options (4.4.4).

- What to do if all peaks are not marked automatically (4.4.5).

- Limitations on structure types (4.4.6).

- Folders used for Wafer map data (4.4.7).

Further information is provided in the X'Pert Epitaxy Help File.

Chapter 4. Creating a Wafer Map from a Set of Rocking Curves

4.4.1 How to Create Outline Files

You can use *Wafer Map - Create Wafer Outline* to produce a circular wafer outline of any diameter with a horizontal flat at the bottom. All you need to specify is the radius in millimeters and the angle where the flat starts (0° is at the bottom of the wafer).

To create an outline for a 4 inch wafer with a flat subtending 50° at the centre of the wafer:

- Select *Wafer Map - Create Wafer Outline*.
- Enter “50.8” as the “Radius”.
- Enter “25” as the “Start” - the window should be as in Figure 4-11.
- Enter “4flat25” as the “File name”.
- Click to save.

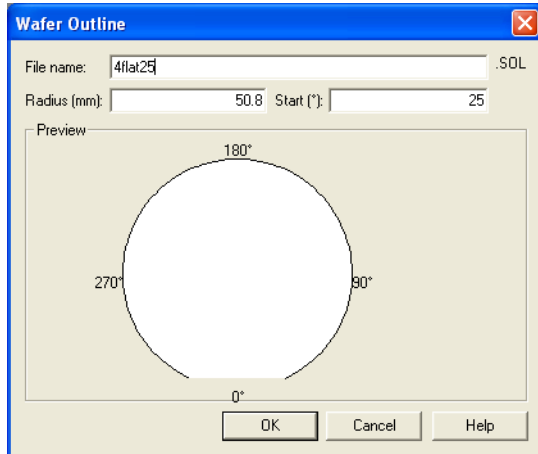


Figure 4-11: The Wafer Outline Window

If the sample is mounted with the flat at an angle to the horizontal use the “Rotation” field of the “Outline Details” tab shown in Figure 4-4 when creating your wafer map.

4.4.2 How to Create Results Files from an Existing Peak File

To create a results file (.wrs) from an existing peak table file (.wpk):

- Select *Wafer Map - Wafer Map from Peak Table*.
- Enter a name in the “Results file” name field.
- Click on **Load Table...**.
- Load the peak file that you want to use.
- Click on **Set Sample...**.
- Load the sample you wish to use.
- If the peak table does not include the outline you want to use, you can edit the “Outline Details” tab.
- Click **OK** to create the results file.

4.4.3 How to Include Thickness Measurements

If your measured files include thickness fringes you can mark these automatically and the layer thickness will be calculated in the results file. To do this proceed as in section 4.3 except that the Automatic Peak Search and Label Parameters should be set as shown in Figure 4-12 instead of as in Figure 4-6 - you may need to change the “Substrate/layer labelling criteria” to apply to your sample.

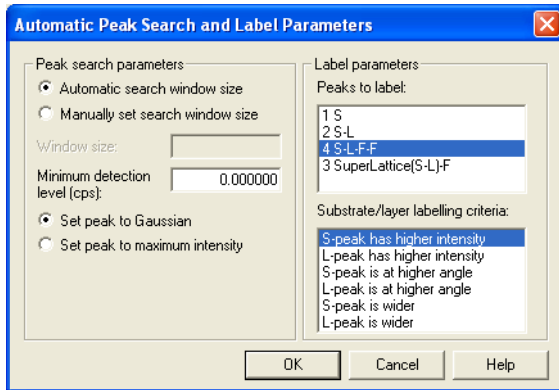


Figure 4-12: Automatic Peak Marking for Thickness Results

If you have problems with peak marking see Section 4.4.5.

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4.4.4 Changing the Viewing Options

In sections 4.2 and 4.3 wafer maps were shown in contours. It is also possible to show the maps as values or as both (i.e. with contours and values). These options are selected using the *View* menu shown in Figure 4-13. Viewing as *Values* is the only available option if the wafer map is for an irregular array of points.

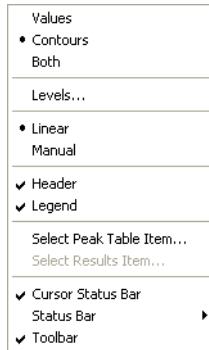


Figure 4-13: The View Menu from a Wafer Map Window

It is also possible to use the *View* menu to change between *Manual* and *Linear* scaling. Select *Levels* to set the *Manual* levels.

Use the *Edit* menu to add Text labels to a wafer map.

4.4.5 What to Do if All Peaks are not Marked Automatically

Often peaks are not marked consistently in all the scans of a wafer map. There are two options for adjusting the peak information:

Use manual intervention

Edit the .wpk with a text processor

To use manual intervention:

- When you are editing the “Wafer Map Details” tab (Figure 4-7) tick the “Prompt for manual intervention” option box.

When you click to start the Wafer Map, each scan will be shown with the peaks marked. If the peak marking is correct, select *Wafer Map - Process Next Scan*. If the peak marking is incorrect, edit it manually before selecting *Wafer Map - Process Next Scan*. When you know that all the inconsistent marking has been removed you can select *Wafer Map - Continue to End*.

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When there are only a small number of problem files in a large data set it may be quicker to edit the .wpk file directly. One mode of working:

- Use *Wafer Map - Wafer Map from Raw Data* to create a peak file (.wpk).
- Use a text processor to look at the .wpk file and note the problem scans which have been inconsistently marked.
- Load each of the problem files as a single scan.
Mark the peaks you wish to use.
Note the peak parameters displayed in the Peak Grid.
- Go back to the text processor and edit the peak information.

4.4.6 Limitations on Structure Types

The calculations used in the results file are the same as those used in *Results - Results Summary* for single scans as shown in Chapter 2. The mismatch and composition values are intended for diamond and zinc blende materials. If you use a sample file which has neither a diamond or a zinc blende substrate all the mismatch and composition values will be set to zero. Only the thickness will be calculated.

For more information about the Results Summary calculations see the X'Pert Epitaxy help file.

4.4.7 Folders Used for Wafer Map Data

When loading data to create a wafer map, the folder which X'Pert Epitaxy uses as the "last used folder" will always be the folder from which you most recently have loaded scan data. The wafer map files you create - the .wpk and .wrs files - will be saved in this folder.

The sample file can be loaded from any folder. This will not influence which folder the wafer map tables are saved in.

The outline files are always stored with Epitaxy.exe.



Chapter 5. Creating Sample Files

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5.1 Introduction

In this chapter you will be shown how to use X'Pert Epitaxy to create sample files which are used to store information about semiconductor epitaxial layer structures. Sample files are required by the results and simulate menus. The chapter is divided into three independent parts one for each of the main materials combinations supported by X'Pert Epitaxy.

The three demonstration samples are:

- Sample A: A silicon substrate with a SiGe graded layer plus a Si capping layer.
- Sample B: A quaternary multiquantum well device structure on an InP substrate
- Sample C: A GaN/GaInN superlattice on a sapphire substrate

For each sample the procedure is described in two parts:

1. Setting the default substrate and layer.
2. Creating the sample file.

In addition, layer linking procedures are described for samples B and C.

Sample A and Sample C are similar to the samples used in Chapter 6 to demonstrate automatic fitting.

Sample B is similar to the sample used in Chapter 6 to demonstrate creating a Batch of Simulations.

5.2 The Procedure for Sample A (Si Substrate)

Figure 5-1 shows the structure of the sample for which we are going to create a sample file.

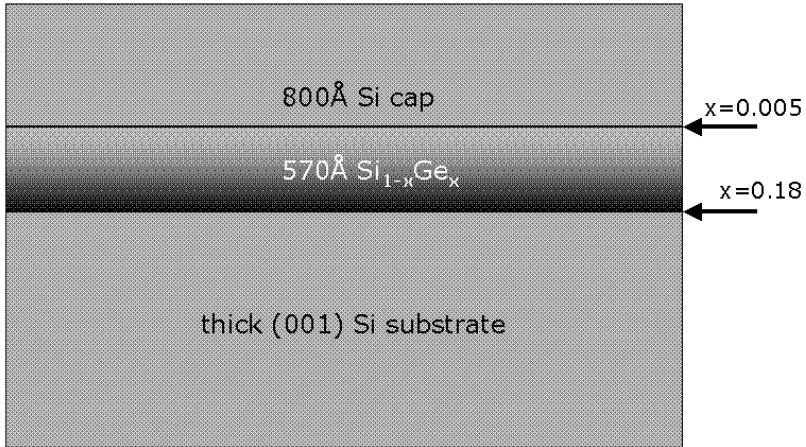


Figure 5-1: Sample Structure

- Start X'Pert Epitaxy.

To set the default substrate and layer:

- Select *Customize - Defaults*.
- Click on the “Sample Data” tab.
- Use the drop-down list box at the top of the tab to set the “Default substrate structure” to Diamond.

Now we want to set the default diamond substrate to (001) Si:

- Click on “Diamond” in the Substrate branch of the tree structure on the left-hand side of the window.
- In the “Site A” frame:
 - set the “No. of elements” to 1.
 - Use the drop-down list box to set the “Element 1” to Si.
- Enter 0 0 4 (0 <space> 0 <space> 4) for the “Simulation HKL”.

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- Enter 0 0 1 (0 <space> 0 <space> 1) for the Primary HKL
- Enter 600 for the “Thickness in microns”.
- Enter 0.0 for the “Offcut angle”.
- Use the drop-down list box to set the “Layer structure” to Diamond.

Now we want to set the default diamond layer to SiGe:

- Click on “Diamond” in the Layer branch of the tree structure.
- In the “Site A” frame:
 - set the “No. of elements” to 2.
 - Use the drop-down list box to set the “Element 1” to Si and “Element 2” to Ge.
 - Enter 0.5 for the Si “Fraction”.
- Enter 0 0 4 as the “Simulation hkl”.
- Enter 0.01 as the “Thickness (mu)”.

Figure 5-2 shows the Sample Data tab after editing the default layer.

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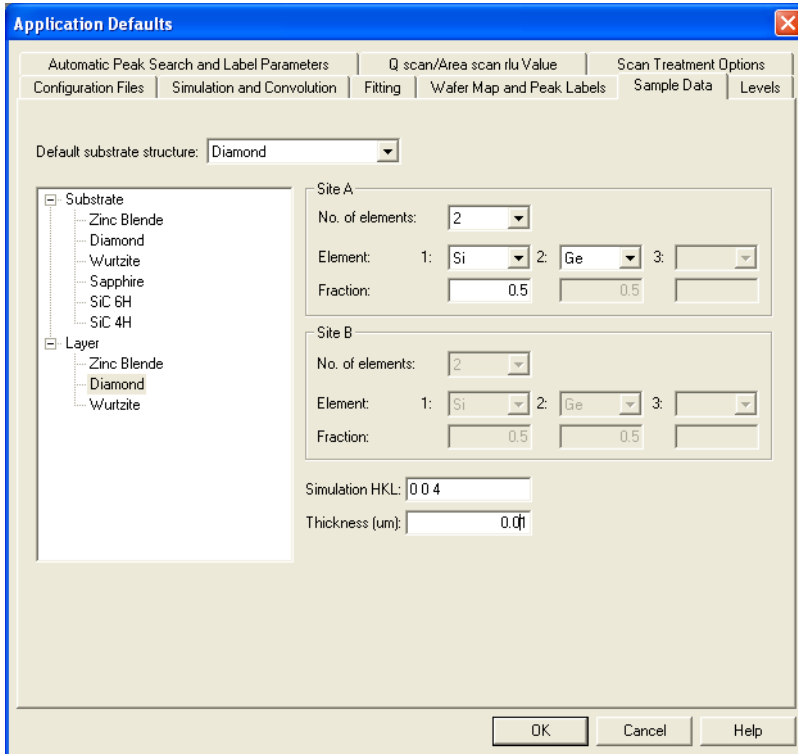


Figure 5-2: Default Sample Tab after Editing the Default Diamond Layer

Click to save the changes you have made to the default sample.

Create the sample file for the structure shown in Figure 5.1:

- Select *Sample - New Sample*.

The “New Sample” window will appear with a silicon substrate as we have just set in the defaults.

Create the full sample file:

- Click on in the “Add as next layer” frame (top left-hand corner of window).

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- Use the “Grading type” drop-down list box to set the grading to Linear.
- Enter 5 for the “No. of steps”.
- In the “Site A” frame:
 - Enter 0.995 for the “Top fraction” of Element Si.
 - Enter 0.82 for the “Bottom Fraction”.
- Enter 0.0057 micron as the “Thickness (um)”.
- Click on Set Layer to transfer this data to the sample tree display.

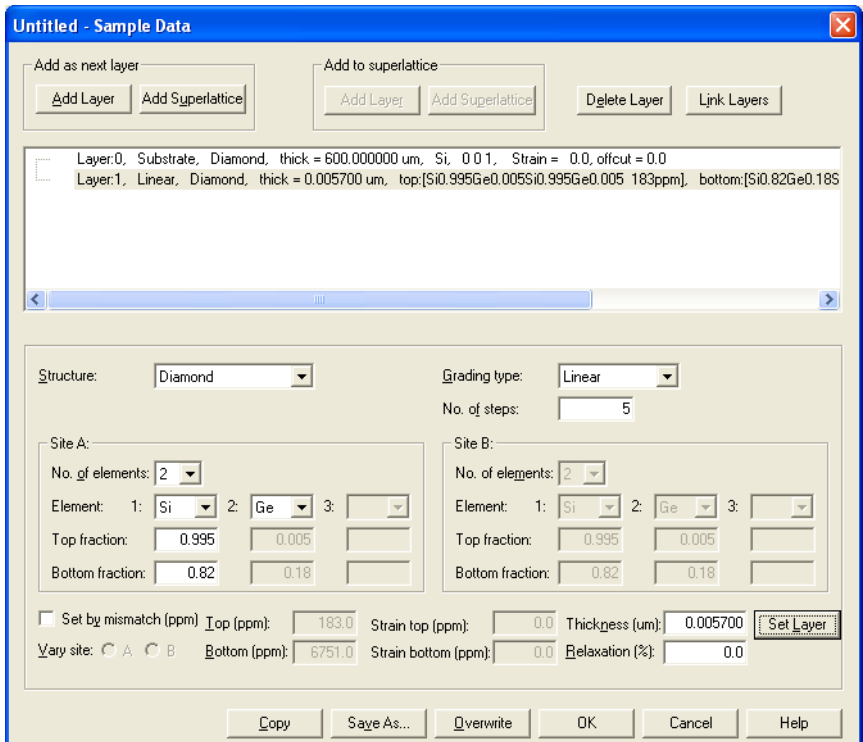


Figure 5-3: Sample Window after Editing the Graded Layer for Sample A

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We are now ready to add the second layer (the Si capping layer):

- Click on in the “Add as next layer” frame.
- Set the “No. of elements” to 1 for the A site - this gives us a Si layer.
- Enter 0.008 micron as the “Thickness (um)”.
- Click on to transfer this data to the sample tree display.

To save the sample data as a sample file:

- Click on at the bottom of the “Sample Edit” window.

The sample file save window will appear as in Fig 5.4

- Enter “Sample A” as the “File name”.
- Click on .

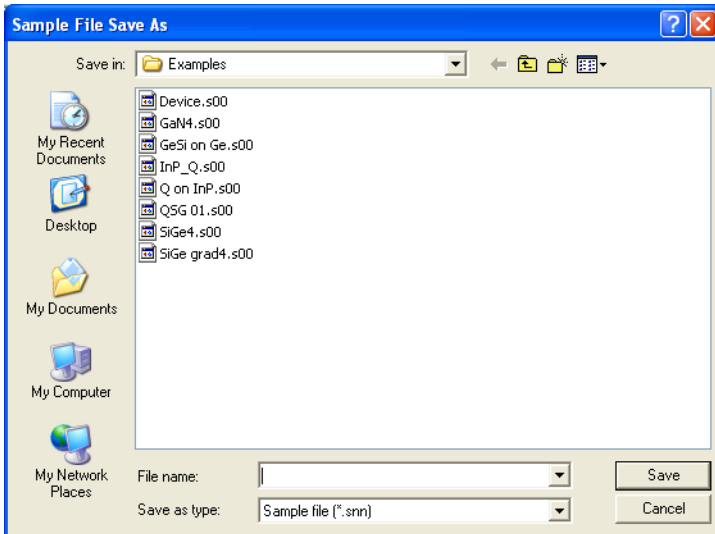


Figure 5-4: Sample Edit Window

Sample A will be saved in the current sample folder.

5.3 The Procedure for Sample B (InP substrate)

Figure 5.5 shows the structure of the sample for which we are going to create a sample file:

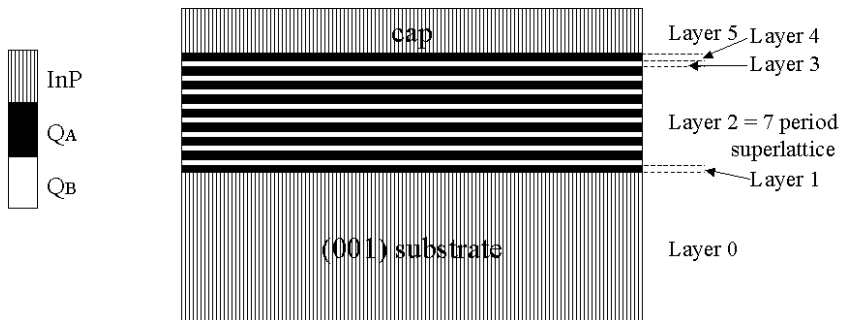


Figure 5-5: Device Structure with Seven Quantum Wells on InP

The sample has an (001) indium phosphide substrate and capping layer, with alternating layers of two different compositions of indium gallium phosphide arsenide ($\text{In}_x\text{Ga}_{(1-x)}\text{P}_y\text{As}_{(1-y)}$). The x and y values for the two quaternaries are: Q_A $x=0.6764$, $y=0.5000$; Q_B $x=0.8040$, $y=0.2000$. To create the sample file we will divide the sample into layers as indicated on the right-hand side of the figure. The layer thicknesses in microns are:

layer	Material	Thickness
0	InP	250
1	Q_A	0.01
2	7 periods	0.1470×7
2.0	Q_B	0.0070
2.1	Q_A	0.0140
3	Q_B	0.0070
4	Q_A	0.01
5	InP	0.10

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Set the default substrate and layer:

- Start X'Pert Epitaxy.
- Select *Customize - Defaults*.
- Click on the “Sample Data” tab.
- Use the drop-down list box at the top of the tab to set the “Default substrate structure” to Zinc Blende.

Now we want to set the default Zinc Blende substrate to InP:

- In the left-hand tree structure of Sample tab click on “Zinc Blende” in the “Substrate” branch.
- In the “Site A” frame:
 - Set the number “Elements” to 1.
 - Use the drop-down list box to set the “Element” to In.
- In the “Site B” frame:
 - Set the number of “Elements” to 1.
 - Use the drop-down list box to set the Element to P.
- Enter 0 0 4 (0 <space> 0 <space> 4) for the “Simulation hkl”.
- Enter 0 0 1 (0 <space> 0 <space> 1) for the “Primary hkl”.
- Enter 250 for the “Thickness (um)” (as for layer 0 in Figure 5-5).
- Enter 0.0 for the “Offcut Angle”.
- Use the drop-down list box to set the “Layer structure” to Zinc Blende.

Now we want to set the default Zinc Blende layer to Q_A - the composition of layers 1, 2.1 and 4 in Figure 5-5.

- Click on “Zinc Blende” in the “Layer” branch of the left-hand tree.
- In the “Site A” frame:
 - Set the “No of Elements” to 2.
 - Use the drop-down list boxes to set Element 1 to In and Element 2 to Ga.
 - Enter 0.6764 for the fraction of In.
- Set the “No of Elements” on Site B to 2.

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- Use the drop-down list boxes to set Element 1 to P and Element 2 to As.
- Enter 0.5 for the fraction of P.
- Enter the “Simulation hkl” as 0 0 4 (0 <space> 0 <space> 4).
- Enter the “Thickness” as 0.01 (as required for layers 1 and 4).
- Click to save the default sample information.

To create the sample file for the structure shown in Figure 5-5.

- Select *Sample - New Sample*.
- If required, click to clear the existing sample.

The New Sample window will appear with an InP substrate as we have just set in the defaults.

To enter the Layer 1:

- Click on in the “Add as next layer” frame (top left-hand corner of window).
- Click on Set Layer.

To enter Layer 2:

- Click on in the “Add as next layer” frame at the top of the window
- Enter 7 for the “No. of repeats” in the bottom half of the window.
- Click in the bottom right-hand corner.

A Default Zinc Blende layer has been entered as the first layer of the superlattice (Layer 2.0). We need to add a second layer (layer 2.1) to the superlattice:

- Click on in the “Add to superlattice” frame in the middle of the window at the top.

We need to edit both the composition and thickness of layer 2.0 and the thickness of layer 2.1:

- Highlight Layer 2.0 by clicking on it.
- Enter 0.007 for the “Thickness”.
- Enter 0.804 for the “Top Fraction” of In.

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- Enter 0.2 for the “Top Fraction” of P.
- Click on .
- Highlight Layer 2.1.
- Enter 0.014 for the “Thickness”.
- Click on .

We can use copy and paste to add layer 3 and layer 4 as they are the same as layer 2.0 and layer 1.

- Highlight Layer 2.0 by clicking on it.
- Click the right mouse button to display the pop-up menu (the mouse pointer should be in the sample tree view).
- Select *Copy*.
- Highlight Layer 2 (the first line of the superlattice entry) by clicking on it.
- Select *Paste* from the pop-up menu to add the copied layer as layer 3.
- Highlight layer 1 by clicking on it.
- Click the right mouse button to display the pop-up menu.
- Select *Copy*.
- Highlight Layer 3 by clicking on it.
- Select *Paste* from the pop-up menu to add the copied layer as layer 4.

Now add the InP cap (Layer 5)

- Click on in the “Add as next layer” frame.
- Change the number of “Elements” on site A to 1.
- Change the number of “Elements” on site B to 1.
- Enter 0.1 for the thickness.
- Click on .

The sample edit window should now appear as shown in Figure 5-6.

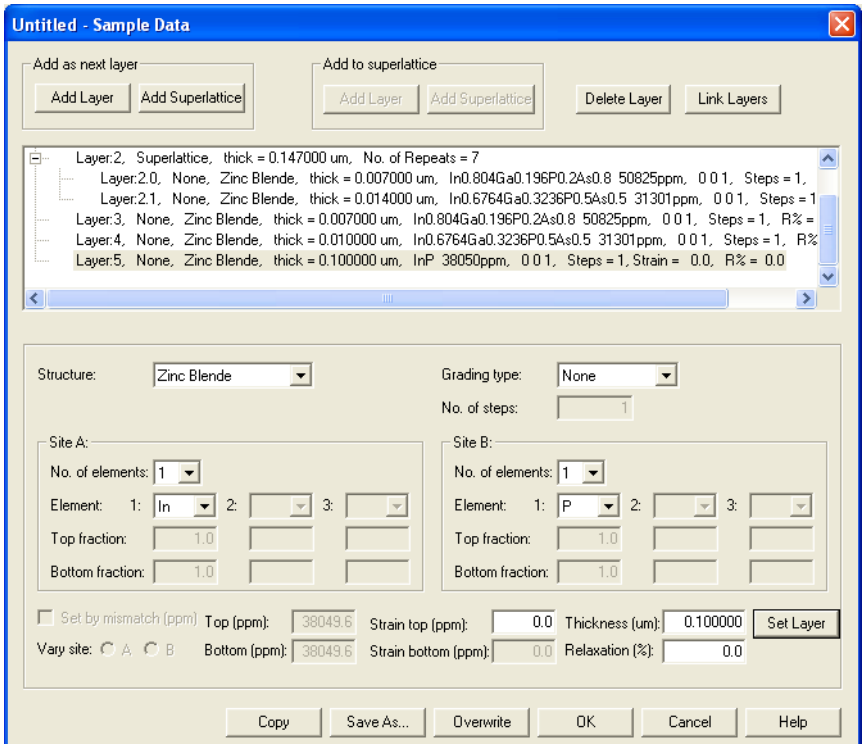


Figure 5-6: The Sample Edit Window after Entering the Layers for Sample B

Now save the sample:

- Click on to exit from the edit window.
- On the “Sample Save” window enter the sample name “Sample B”.
- Click to save the sample information.

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For this sample we can set up links. We will set up standard links between the site A compositions of all the layers of composition Q_A . We will do the same for all the layers of composition Q_B . We will set up a total link for the layer thickness of Layers 2.0 and 2.1. Once these links have been set up, the A site occupancy of all the Q_A layers and all the Q_B layers will all change together whenever any one of the layers is edited. The combined thickness of Layers 2.0 and 2.1 will remain constant whenever the thickness of either layer is edited. These links are saved in the sample file and will be active during manual editing and when using automatic fitting.

- Select *Sample - Edit Sample*.
- Click **Link Layers** (button at top right-hand side of the window).
- Hold down the **Ctrl** key and highlight lines 1, 7 and 13 by clicking on them.
- Click **Standard Link** (button at bottom left-hand side of the window).

The link window should now appear as in Figure 5-7. A link has been created between all the site A compositions of the Q_A layers.

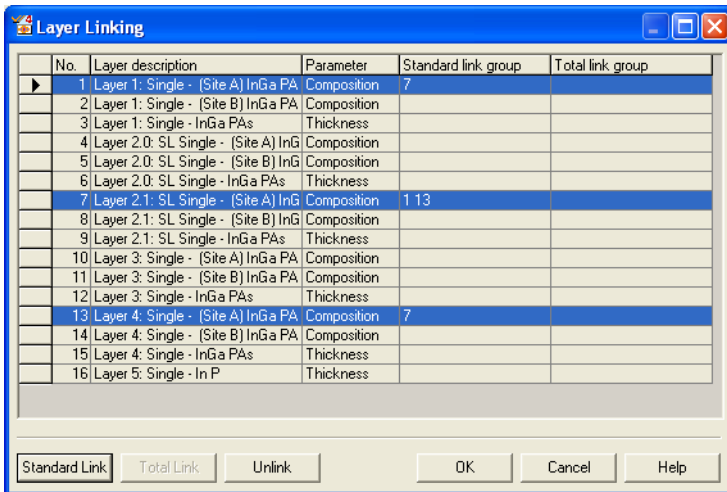


Figure 5-7: The linking Window After Linking the A Site Composition of all the Q_A Layers

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We will now create the remaining links:

- Click on line 4 to highlight it.
- Hold down the **Ctrl** key and click on line 10.
- Click .
- Click on line 6 to highlight it.
- Hold down the **Ctrl** key and click on line 9.

To save the sample with links:

- Click .
- Click (bottom of the window).

Figure 5.8 shows the linking window with all three links made.

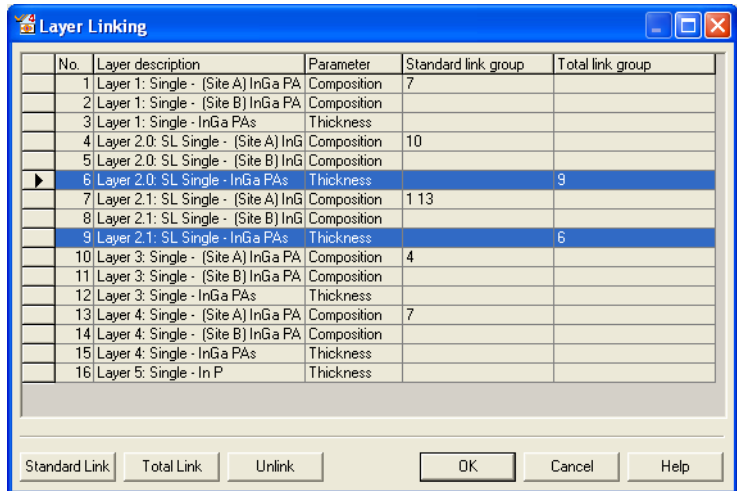


Figure 5-8: The Linking Editor After All Three Linked Groups Have Been Made

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Click **Overwrite** in “Sample edit” window.

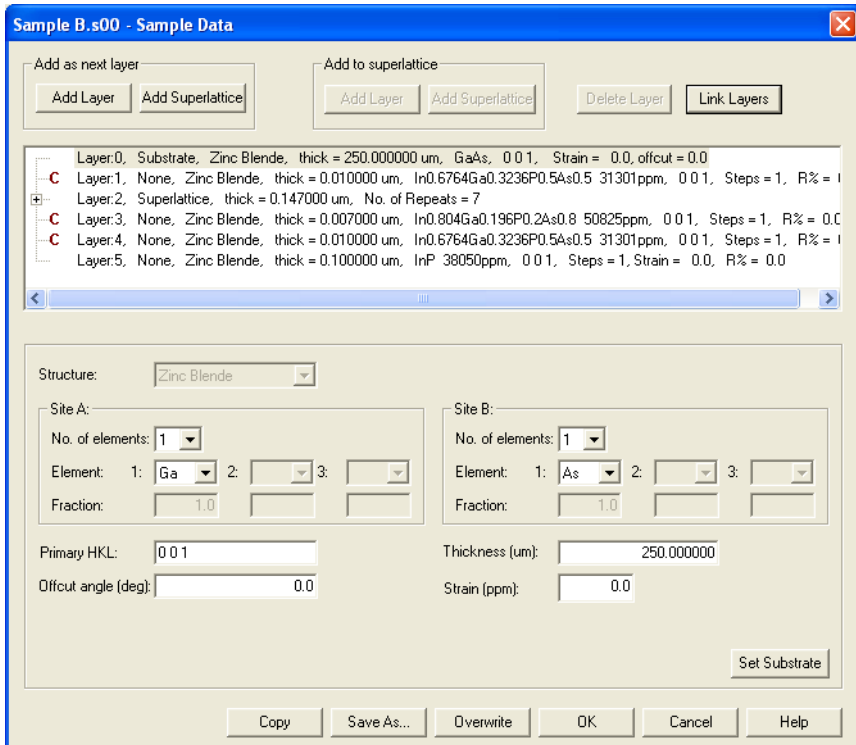


Figure 5-9: The Linking Editor After “Overwrite” has been Pressed

5.4 The Procedure for Sample C (Sapphire Substrate)

Figure 5-10 shows the structure for which we are going to create a sample. For this sample the interface between the sapphire and the GaN buffer layer is assumed to be totally relaxed.

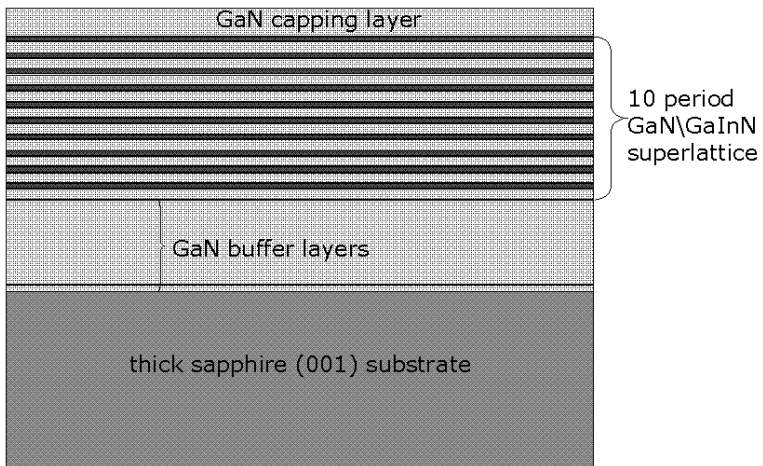


Figure 5-10: Sample with Sapphire Substrate

- Start X'Pert Epitaxy.

Set the default substrate and layer:

- Select *Customize - Defaults*.
- Click on the “Sample Data” tab.
- Use the drop-down list box at the top of the tab to set the “Default substrate structure” to Sapphire.
- Click on Sapphire substrate in the left-hand tree structure of “Sample” tab.
- Check that the substrate details are as shown in Figure 5-11.
- Click on the “Wurtzite” in the left-hand “Layer” tree.

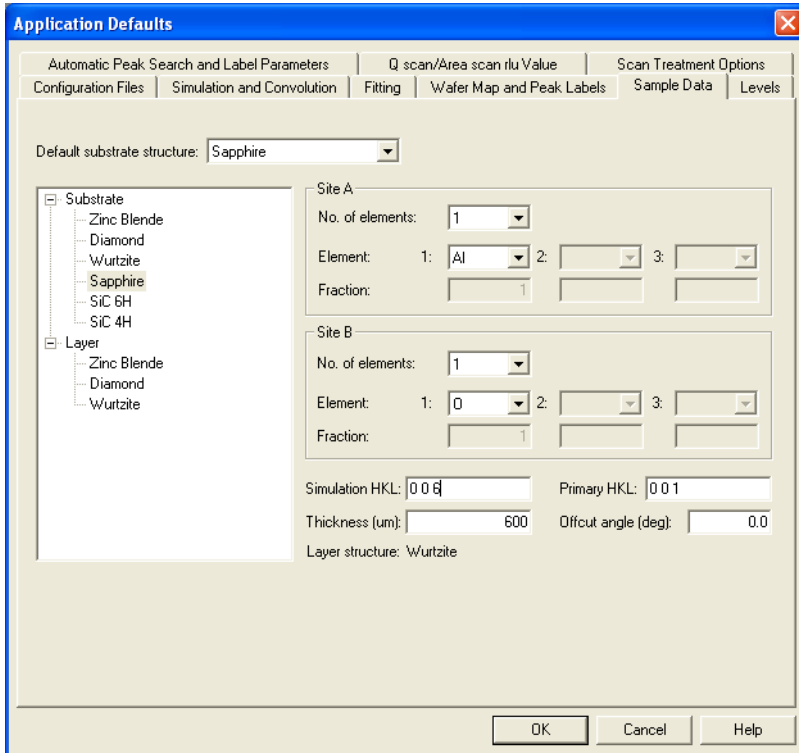


Figure 5-11: The Default Sample Data Tab Edited for a Sapphire Substrate

- Set the “No of Elements” on Site A to 2.
- Use the drop-down list boxes to set “Element” 1 to Ga and “Element” 2 to In.
- Enter the “Simulation hkl” as 0 0 2 (0 <space> 0 <space> 2).
- Enter the “Thickness” as 0.1.
- Enter the “In plane rotation” as 30, the tab should be as shown in Figure 5-12.
- Click to save the default sample information.

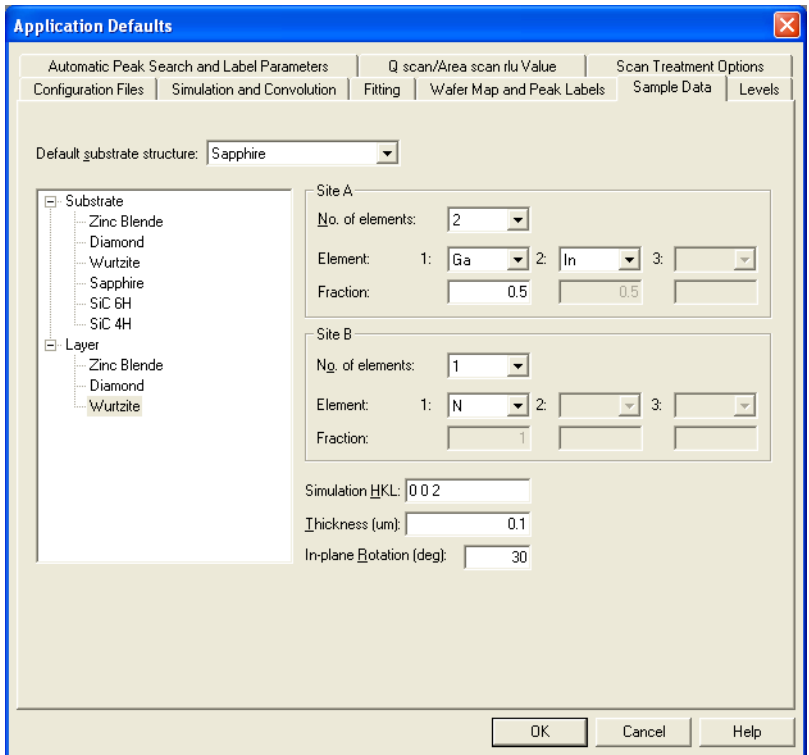


Figure 5-12: The Default Sample Data Tab Edited for a Wurtzite Layer

Create the sample file for the structure shown in Figure 5-10.

- Select *Sample - New Sample*.

The New Sample window will appear with a sapphire substrate as we have just set in the defaults.

Enter the relaxed GaN buffer layer which is 1.525 microns thick:

- Click on **Add Layer** in the “Add as next layer” frame (top left-hand corner of the window).
A 0.1 micron $\text{Ga}_{0.5}\text{In}_{0.5}\text{N}$ layer has appeared as we set in the defaults. We need to edit this:

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
Set the “Number of elements” on site A to 1.

Enter 1.525 for the “Thickness”.


Enter 100.0 the “Relaxation %”.

Click on .

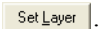

To enter the superlattice which consists of 10 repeats of (25Å of Ga_{0.87}In_{0.13}N plus 70Å of GaN):

- Click on  in the “Add as next layer” frame at the top of the window.
- Enter 10 for the “No. of repeats” in the bottom half of the window.
- Click  in the bottom right-hand corner.

A Default Wurtzite layer has been entered as the first layer of the superlattice (Layer 2.0). We need to add a second layer to the superlattice:

- Click on  in the “Add to superlattice” frame in the middle of the window at the top.

A second layer (layer 2.1) appears. To edit the two layers:

- Highlight Layer 2.0 by clicking on it.
- Enter 0.87 for the “Top fraction” of Element 1.
- Enter 0.0025 for the “Thickness”.
- Enter 0 for the “Relaxation %”.
- Click on .
- Highlight Layer 2.1.
- Set the “No. of elements” on Site A to 1.
- Enter 0.07 for the “Thickness”.
- Enter 0 for the “Relaxation %”.
- Click on .

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We now need to add the 500Å GaN capping layer:

- Highlight “Layer 2” in the tree structure display of the sample (i.e. the main superlattice description).
- Click on in the “Add as next layer” frame.
- Set the “Number of elements” on site A to 1.
- Enter 0.05 for the “Thickness”.
- Enter 0 for the “Relaxation %”.
- Click on .

Figure 5-13 shows the sample edit window with all the layers entered.

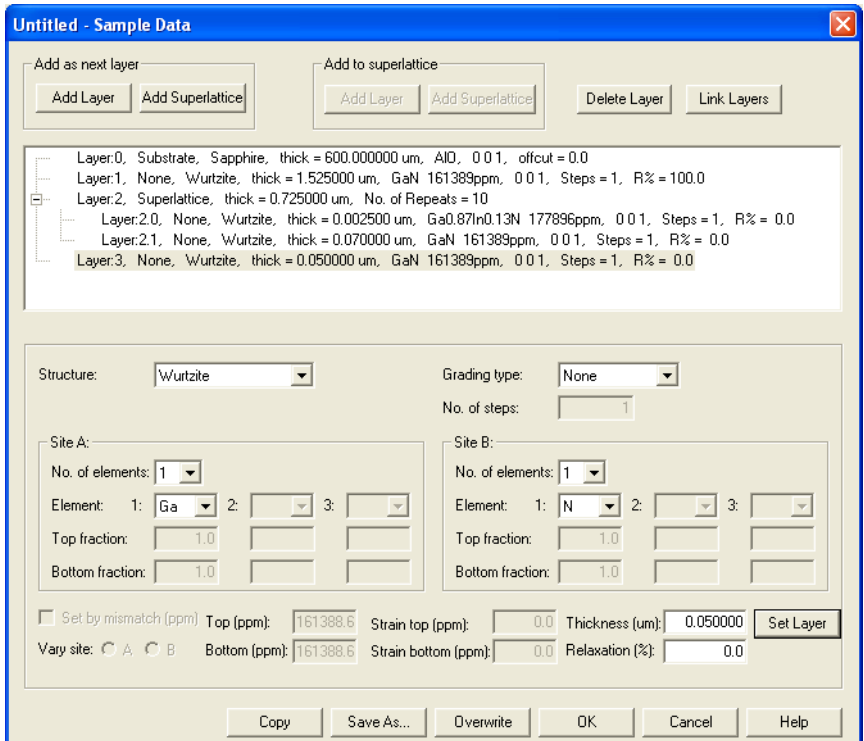


Figure 5-13: The Sample Edit Window after Entering all Layers

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To save the structure:

- Click on to exit from the edit window.
- On the “Sample save” window enter the sample name “SAMPLE C”.
- Click to save.

For this sample we can add one total link to fix the superlattice period. This link will be saved in the sample file and will be active during manual editing and when using automatic fitting (see Chapter 6).

- Select *Sample - Edit Sample*.
- Click (button at top right-hand side of the window).
- Hold down the **Ctrl** key and highlight lines 3 and 4 by clicking on them.
- Click (button at bottom left-hand side of the window).

The link window should now appear as in Figure 5-14.

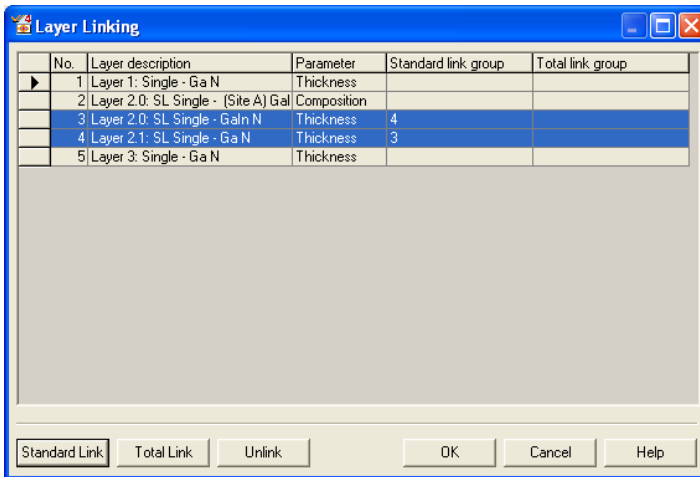


Figure 5-14: Linking Window after Creating Total Link for Sample C

To save the sample with links:

- Click (bottom of window).
- Click in “Sample edit” window to save the sample file with links.

Chapter 6. Making Simulations and Using Automatic Fitting

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6.1 Introduction

This chapter demonstrates the simulation and fitting functionality.

The demonstration is in three parts:

- Using Batch Simulation

- Using the Simulation and Fit pane to make simulations

- Using the Simulation and Fit pane for automatic fitting.

There is a final section indicating the best procedures for using your own scan data.

NOTE: To follow all the instructions in this chapter you will need an X'Pert Epitaxy License and a Smoothfit License. If you do not have X'Pert Smoothfit License you will not be able to do automatic fitting.

6.2 Simulating a Batch of Rocking Curves

We will learn how to set up the defaults for simulations and convolutions and create simulations from existing sample files. A sample file “Q on InP.s00” is provided in folder: “C:\Program Files\PANalytical\X'Pert Epitaxy\Examples”. This is similar to the sample file “Sample B.s00” we created in Chapter 5.

- Start X'Pert Epitaxy.
- Select *Customize - Defaults*.
- Click on the “Simulation and Convolution” tab.

The window will appear as in Figure 6-1. The values will normally be set for your diffractometer. We will set the values shown in the figure.

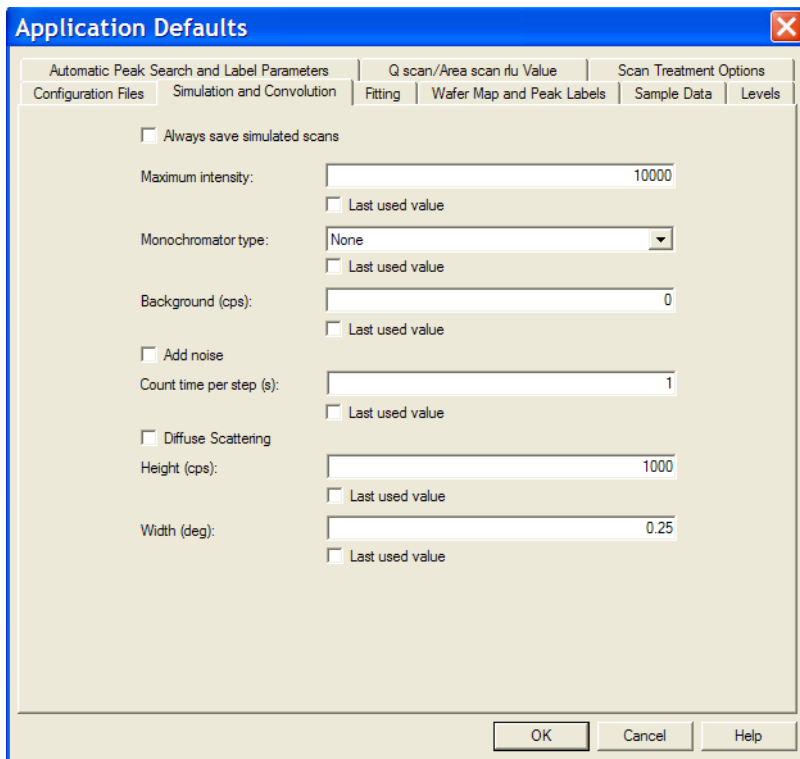


Figure 6-1: The Window for Setting the Default Convolution Conditions

- Check the “Always save simulated scans” box in the top corner of the window. The simulated files will be saved in the folder names on the “Folders” tab.
- Enter 50000000 in the “Maximum Intensity field”.
- Use the drop-down list box to set the “Monochromator type” to Ge(220) 4-Crystal.
- Enter 11 in the “Background (cps)” field.
- Make sure the “Add Noise” and “Diffuse Scattering” option boxes are NOT checked.

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- Click .

We will now make a batch of simulations using file “Q on InP.s00” which is similar to “sample B.s00” created in Section 5.3 of this Quick Start Guide:

- Select *Simulate - Batch Simulation*.
- Click on the button on the bottom left of the window.
- Select “Q on InP.s00”.

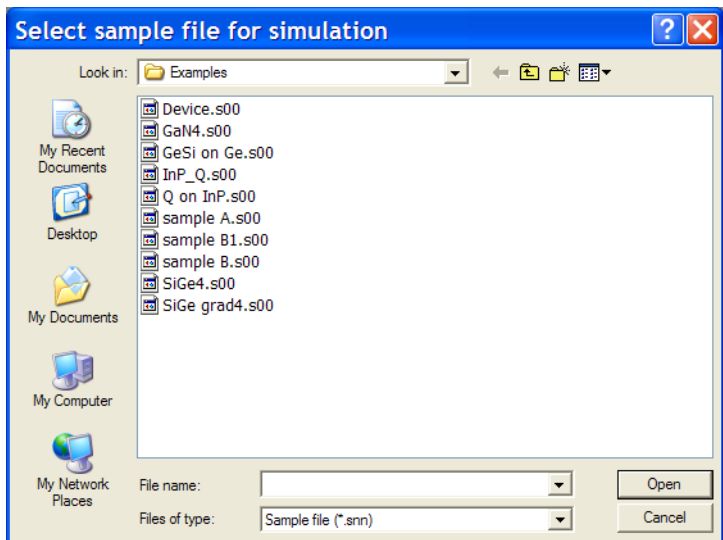


Figure 6-2: The Select Sample File Window

Figure 6-3 shows the Batch Simulation window after “Q on InP.s00” has been inserted. You may need to drag on the dividers between the columns to see all the information available. The Sample file name is in the second column. The first column is the file name which will be used for the simulated data - this ends in .z00. The convolution conditions are shown in code in column 3 - in this case the default convolution conditions. The remainder of the columns show the reflection used, the substrate Bragg angle and the range and step size. The layer and substrate hkl values in columns 5 and 6 are taken from the default sample tab. The range has been calculated to show all the Bragg peaks from the layers plus a few thickness fringes beyond the outermost peaks. The step size is based on the expected thickness fringe spacings.

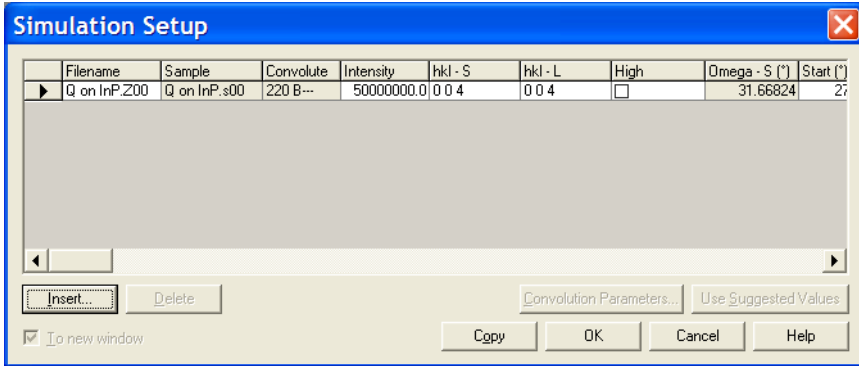


Figure 6-3: The Batch Simulation Window after Inserting One Sample

In this batch we will show how to add further simulations using different convolution conditions and different reflections.

- Highlight the existing entry for the batch by clicking on the left-hand end of the line.
- Click the right mouse button to display the pop-up menu.
- Select *Copy*.
- Click the right mouse button to display the pop-up menu again.
- Select *Paste* - this will add a second simulation with simulation file name extension .z01.
- Repeat the last two actions - this will add a third simulation with simulation file name extension of .z02.

We will edit the line with simulation file ending in .z01 to have different convolution conditions to the first file and then we will edit the line with simulation file ending in .z02 to use a different reflection.

- Highlight the line with simulation file name ending in .z01 by clicking on the left-hand end.
- Click on the **Convolution Parameters...** button.
- Enter 1 in the “Background (cps)” field, so we can see the effect of having a smaller background.
- Click **OK**.

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The convolution parameters window is shown in Figure 6-4.

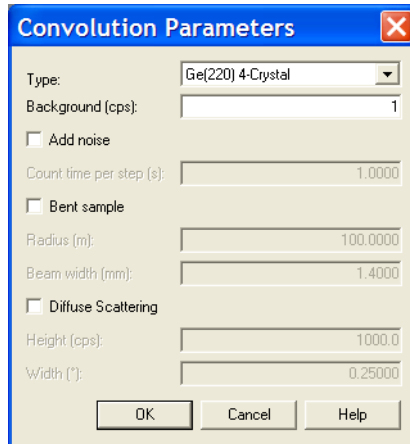


Figure 6-4: The Window for Editing the Convolution Parameters

- Highlight the line with simulation file name ending in .z02 by clicking on the left-hand end.
- Enter 0 0 2 (0<space>0<space>2) in columns 5 and 6 for this line, so we can simulate a different reflection.

The “Simulation Setup” window should be as in Figure 6-5.

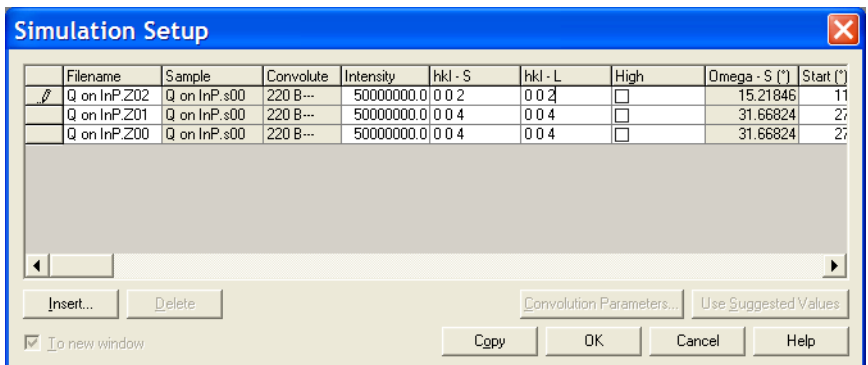


Figure 6-5: The Simulation Setup Window with Three Simulations

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To perform the simulations:

- Click .

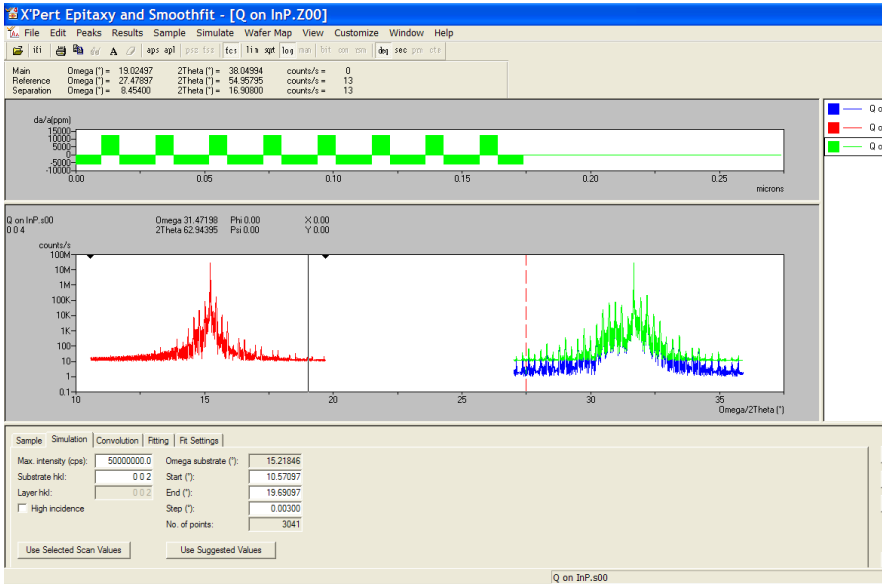


Figure 6-6: The Graphics Display of the Three Simulations

Figure 6-6 shows the graphics display you will see. The following *View* menu options were used:

- Mismatch plot selected
- Logarithmic intensity scaling
- Plot in degrees

These three simulations demonstrate the loss of detail with increasing background noise (compare “Q on InP.z00” and “Q on InP.z01”) and difference in satellite intensities in the 004 and 002 reflections (compare “Q on InP.z00” and “Q on InP.z02”).

6.3 Simulating Using the Simulate and Fit Pane

This section gives you step-by-step instructions for simulating a rocking curve using the “Simulation and Fit” pane. It is possible to edit parameters on the different tabs of the “Simulation and Fit” pane to rapidly improve the fit between a simulated curve and a measured curve.

The sample structure used is shown in Figure 6-7 - a SiGe heterojunction bipolar transistor (HBT) with two discrete SiGe layers and a Si cap. Two files are provided, the measure scan, SiGe.d00 and a sample file, SiGe4.s00. The files are inserted in the folder “C:\Program Files\PANalytical\X’Pert Epitaxy\Examples” when X’Pert Epitaxy is installed.

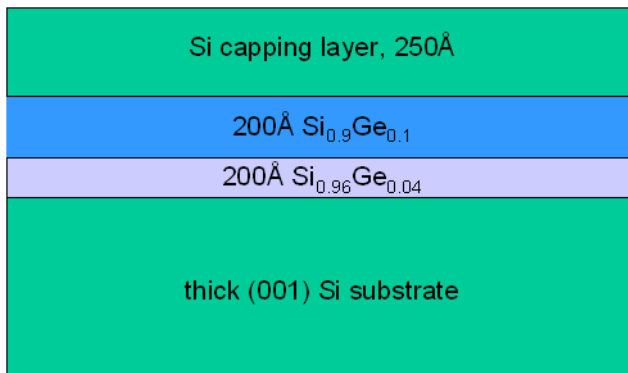


Figure 6-7: The SiGe HBT Structure with Two SiGe Layers

To begin:

- Start X’Pert Epitaxy.

First we will set some defaults:

- Select *Customize - Defaults*.
- Click on the “Simulation and Convolution” tab.
- Set all values as shown in Figure 6-8.
- Select the “Automatic Peak Search and Label Parameters” tab.
- Set all values as shown in Figure 6-9.
- Click to close the “Applications Defaults” window.

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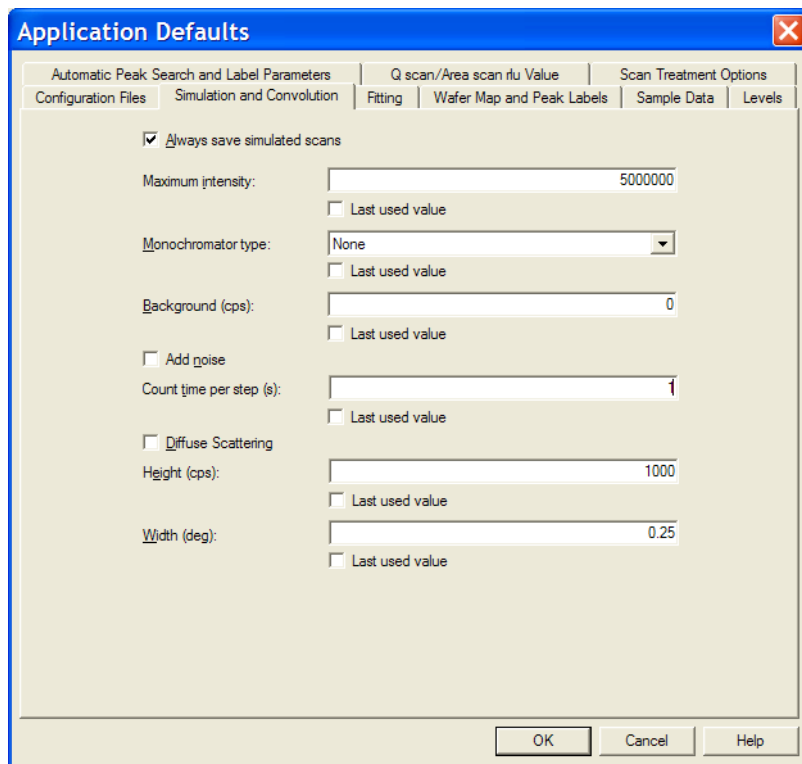


Figure 6-8: The Simulation and Convolution Defaults Tab

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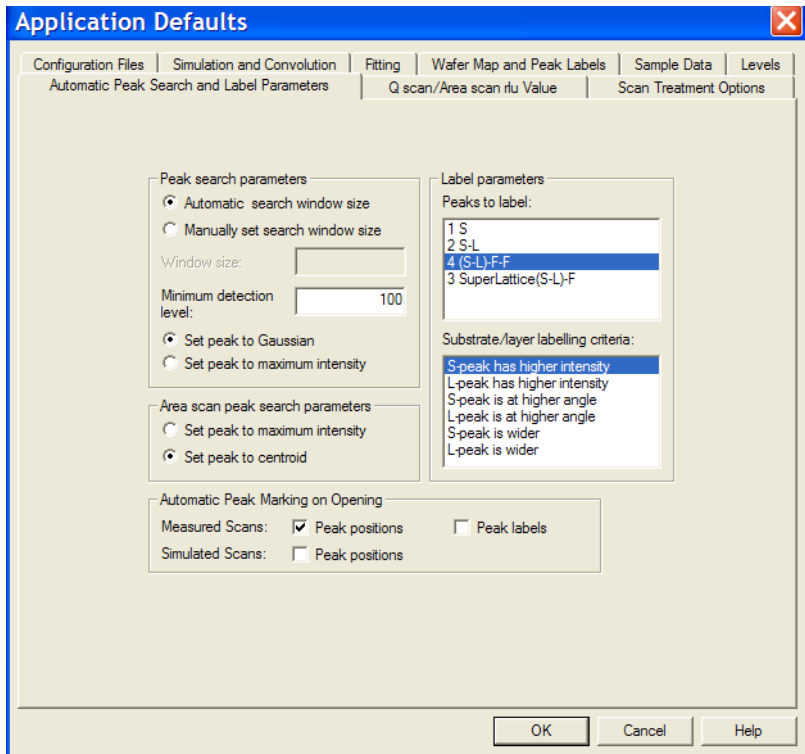


Figure 6-9: The Automatic Peak Search and Label Defaults Tab

Now we will load the experimental scan and the sample file:

- Select *File - Open*.
- Open SiGe.d00.
- Select *Sample - Open Sample*.
- Select the file SiGe4.s00.
- Click to open the file, and then .
- Select *Simulate - Simulate and Fit*.

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The display should be as in Figure 6-10. You may need to select *View - Results* to see the results pane and you may need to adjust the splitter bars to get a better view of the results pane. You may also need to select *View - Plot in Relative Seconds* and *View - Logarithmic*.

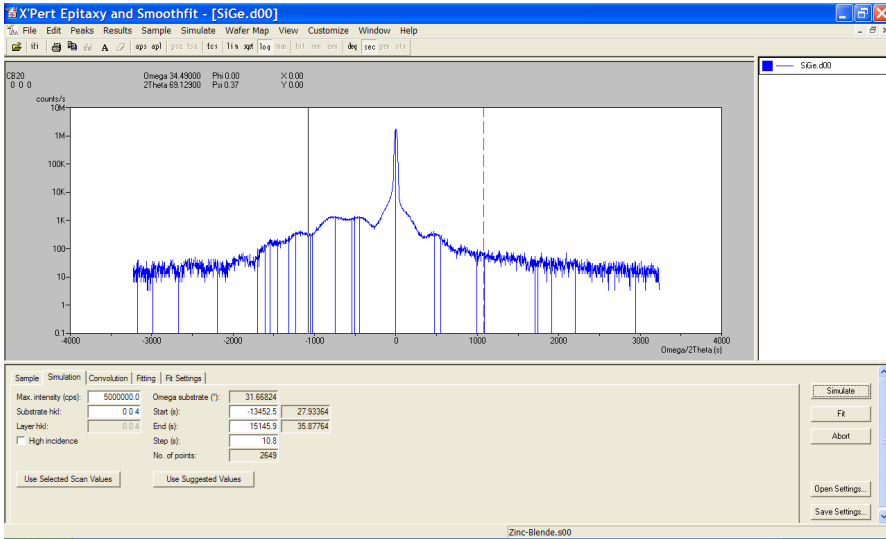


Figure 6-10: The Measured Data with the Simulation and Fit Pane

To make the first simulation:

- Click on the **Use Selected Scan Values** button.
- Click on the **Simulate** button.

The simulated curve is shown as a temporary file (file name ends in #) as shown in Figure 6-11. The simulated curve has not been convoluted with a monochromator and the background count was set at zero (see defaults set in Figure 6-8).

If you checked “View-mismatch plot” for the previous example you may need to uncheck it for this example.

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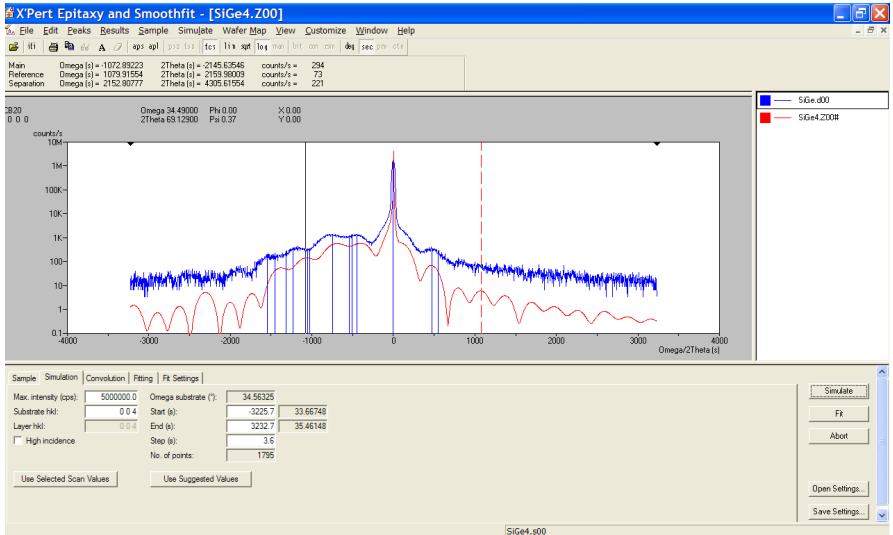




Figure 6-11: First Simulation Displayed with Measured Curve

To add instrumental effects:

- Select the “Convolution” tab of the “Simulation and Fit” pane.
- Use the drop-down list box to set the monochromator as “Ge(220) asym 4-Crystal”.
- Enter 12 in the “Background (cps)” field.
- Enter 2 in the “Intensity Multiplier” field.
- Click the  button.

The simulated curve now matches the measured curve better but the peaks due to the SiGe layers are not well matched.

To edit the sample:

- Select the “Sample” tab of the “Simulation and Fit” pane.
- Use the drop-down list box to select “Layer 2 Single Diamond SiGe”.
- Enter 0.98 for the Si concentration for the A site.
- Click the  button.

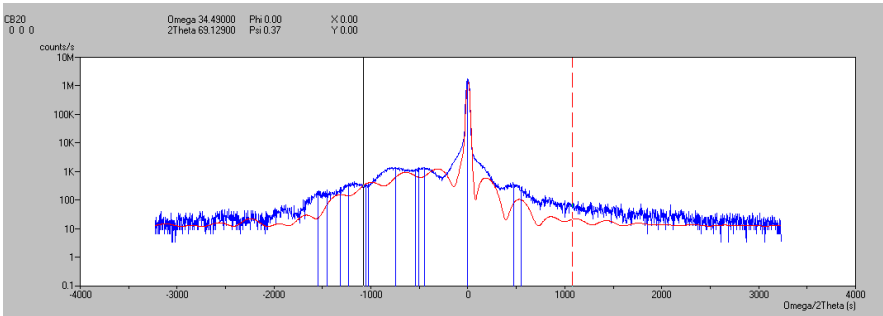


Figure 6-12: A Small Improvement in Fit after Changing Layer 2

Figure 6-12 shows that there is a small improvement in the fit. This change in the sample can be saved:

- Select *Sample - Edit Sample*.
- Click on .
- In the Sample File “Save As..” window enter “My SiGe”.
- Click to save.
- Click to close the “Sample Edit” window.
- Select File - Close and then click on to close without saving.

6.4 Fitting Using the Simulate and Fit Pane

Further improvements could be made by editing the sample tab. However at this point we will demonstrate how automatic fitting can be used to achieve a match between the measured and simulated curve. Data is provided for three samples:

A SiGe HBT structure with two discrete SiGe layers (as used in Section 6.3)

A SiGe HBT structure with a graded SiGe layer

A GaN/GaNN superlattice on a sapphire substrate.

Chapter 6. Making Simulations and Using Automatic Fitting

6.4.1 A SiGe HBT Structure With Two Discrete SiGe Layers

The procedure is described in four parts:

1. Opening the measured scan, sample file and settings file.
2. Understanding the tabs used during fitting.
3. Saving the sample file.
4. Printing out the results.

To open all the files:

- Select *File - Open*.
- Select the file SiGe.d00.
- Select *Sample - Open Sample*.
- Select the file SiGe4.s00.
- Click to open the file.
- Click on the button on the “Simulate and Fit” pane.
- Select the file SiGe4.fit.
- Click to open the file.

SiGe4.s00 and SiGe4.fit contain all the information required for successful automatic fitting. Before starting to fit we will look at the information provided.

To see the information from SiGe4.s00:

- Select the “Fitting” tab of the “Simulate and Fit” pane.

Sample Simulation Convolution Fitting Fit Settings										
No.	Adjust	Parameter	Type	Initial value	Current value	Start increment	Final increment	Lower limit	Upper limit	
1	<input checked="" type="checkbox"/>	Layer 1: Single - SiGe	Composition	0.90000		0.04500	0.00090	0.01000	0.99000	
2	<input checked="" type="checkbox"/>	Layer 1: Single - SiGe	Thickness	0.02000		0.00200	0.00002	0.01500	0.02500	
3	<input checked="" type="checkbox"/>	Layer 2: Single - SiGe	Composition	0.96000		0.04800	0.00096	0.06400	1.00000	
4	<input checked="" type="checkbox"/>	Layer 2: Single - SiGe	Thickness	0.02000		0.00200	0.00002	0.01500	0.02500	
5	<input checked="" type="checkbox"/>	Layer 3: Single - Si	Strain	0.0		0.00	0.00	0.0	0.0	
6	<input checked="" type="checkbox"/>	Layer 3: Single - Si	Thickness	0.02500		0.00250	0.00003	0.01875	0.03125	
7	<input checked="" type="checkbox"/>	Background (cps)	Convolution	10.0		0.100	0.0100	8.0	12.0	
8	<input checked="" type="checkbox"/>	Intensity multiples	Convolution	1.00		0.1000	0.01000	0.80	1.20	
9	<input checked="" type="checkbox"/>	Diffuse scattering width	Convolution	800.0		32.000	4.0000	640.0	960.0	
10	<input checked="" type="checkbox"/>	Diffuse scattering height	Convolution	800.0		32.000	4.0000	640.0	960.0	

Figure 6-13: The Fitting Tab

Figure 6-13 shows the tab. This displays all the sample and convolution parameters that can be adjusted during fitting. All the tick boxes in the “Adjust” column should be checked. The “Initial value” of each parameter is from the original sample information (Figure 6-7). The start and final increments were saved in the sample file (SiGe4.s00) with the layer information. If this had not been done the increments would have been taken from the “Fitting” tab of *Customize - Defaults*. The initial values should be large enough to change the rocking curve significantly, while the final values should be just below the smallest observable change for the measured scan step size. More information is given in the X'Pert Epitaxy Help file. Whenever you edit the “Fitting” tab you can save the changes in the sample file by selecting *Sample - Edit Sample*, followed by **Overwrite** or **Save as....** The convolution parameters are saved in the xxx.fit file. This can be updated at any time by clicking on .

- Then select the “Fit Settings” tab of the “Simulate and Fit” pane

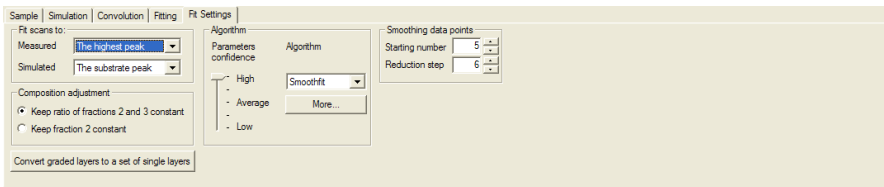


Figure 6-14: The Fit Settings Tab

Figure 6-14 shows the tab. This displays all the parameters used for fitting. More information is given in the X'Pert Epitaxy Help file. Whenever you edit the “Fit Settings” tab you can save the changes in the fit file by clicking on .

To select the fitting algorithm:

- In the “Algorithm” frame use the drop-down menu to select “Smoothfit”.
- Click on the button and ensure that the “Target Function: value is $1e^{-004}$ and then press .
- In the “Smoothing datapoints” frame change the starting number to 25 and the reduction step to 20.

To perform the fit:

- Select *Peaks - Automated Peak Search* and press .
- Click on the button.
- If a message saying “!Lower limit should be smaller than upper limit” appears, press .

Chapter 6. Making Simulations and Using Automatic Fitting

- Click on the “Fitting” tab, the limit(s) in question will be highlighted:

No.	Adjust	Parameter	Type	Initial value	Current value	Start increment	Final increment	Lower limit	Upper limit
1	<input checked="" type="checkbox"/>	Layer 1: Single - SiG	Composition	0.90000		0.04500	0.00050	0.81000	0.99000
2	<input checked="" type="checkbox"/>	Layer 1: Single - SiG	Thickness	0.02000		0.00200	0.00002	0.01500	0.02500
3	<input checked="" type="checkbox"/>	Layer 2: Single - SiG	Composition	0.96000		0.04800	0.00096	0.86400	1.00000
4	<input checked="" type="checkbox"/>	Layer 2: Single - SiG	Thickness	0.02000		0.00200	0.00002	0.01500	0.02500
5	<input checked="" type="checkbox"/>	Layer 3: Single - Si	Strain	0.0		0.00	0.00		0.0
6	<input checked="" type="checkbox"/>	Layer 3: Single - Si	Thickness	0.02500		0.00250	0.00003	0.01975	0.03125
7	<input checked="" type="checkbox"/>	Background (cpt)	Convolution	10.0		0.100	0.0100	8.0	12.0
8	<input checked="" type="checkbox"/>	Intensity multiplier	Convolution	1.00		0.1000	0.01000	0.80	1.20
9	<input checked="" type="checkbox"/>	Diffuse scattering wvd	Convolution	800.0		32.000	4.0000	640.0	960.0
10	<input checked="" type="checkbox"/>	Diffuse scattering hvd	Convolution	800.0		32.000	4.0000	640.0	960.0

- Change the values for row 5 so that they are non-zero, for example: “Initial value” = 10, “Start increment” = 50, “Final increment” = 1, “Lower limit” = -500, “Upper limit” = 500.
- Click again.

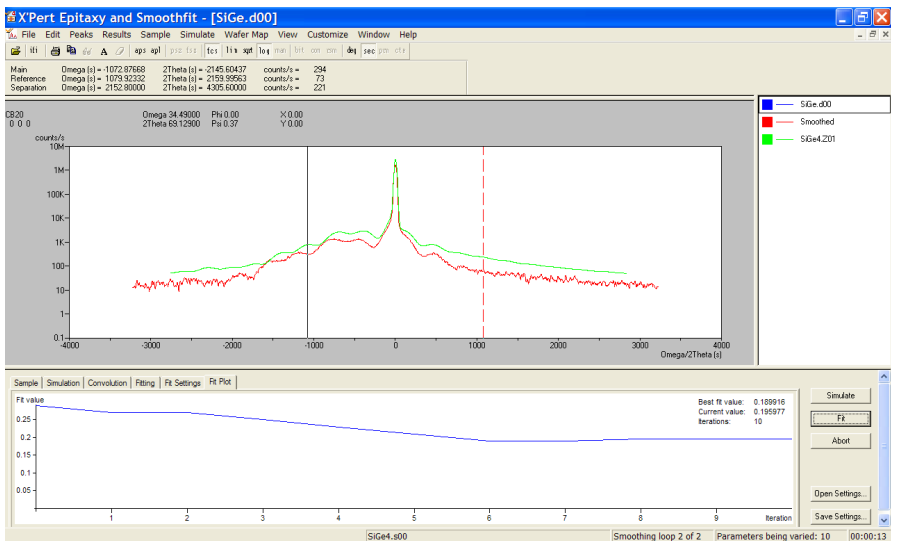


Figure 6-15: The Fit Plot Tab Viewed Whilst Fitting

During fitting, only two curves are displayed in the graphics area. These are the smoothed measured curve and the current simulated curve. The progress of the fitting is indicated at the right hand end of the status line.

At the end of the fitting the final simulated curve is displayed together with the measured scan. Any scans which were previously loaded in the same window will

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also be shown. A message saying “Fitting has finished. Save or update fitting results via “Fitting tab of “Simulate and Fit” tab” should appear.

- Press .
- Look in the “Fitting” tab to see if any cells are highlighted.

No.	Adjust	Parameter	Type	Initial value	Current value	Start increment	Final increment	Lower limit	Upper limit
1	<input checked="" type="checkbox"/>	Layer 1: Single - SiGe	Composition	0.90000		0.04500	0.00090	0.01000	0.99000
2	<input checked="" type="checkbox"/>	Layer 1: Single - SiGe	Thickness	0.02000		0.00200	0.00002	0.01500	0.02500
3	<input checked="" type="checkbox"/>	Layer 2: Single - SiGe	Composition	0.96000		0.04800	0.00096	0.06400	1.00000
4	<input checked="" type="checkbox"/>	Layer 2: Single - SiGe	Thickness	0.02000		0.00200	0.00002	0.01500	0.02500
5	<input checked="" type="checkbox"/>	Layer 3: Single - Si	Strain	0.0		0.00	0.00	0.0	0.0
6	<input checked="" type="checkbox"/>	Layer 3: Single - Si	Thickness	0.02500		0.00250	0.00003	0.01695	0.03125
7	<input checked="" type="checkbox"/>	Background (cps)	Convolution	10.0		0.100	0.0100	8.0	12.0
8	<input checked="" type="checkbox"/>	Intensity multiplier	Convolution	1.00		0.1000	0.01000	0.80	1.20
9	<input checked="" type="checkbox"/>	Diffuse scattering w/c	Convolution	800.0		32.000	4.0000	640.0	960.0
10	<input checked="" type="checkbox"/>	Diffuse scattering h/c	Convolution	800.0		32.000	4.0000	640.0	960.0

- Change the “Lower limits” for rows 9 and 10 to 300.
- Click again.

NOTE: If you get the message “required peak is not available” make sure that the measured scan is selected by clicking on the measured data file name in the upper right corner of the graphics pane. If there is no peak marked on the data file, run through section from the beginning to enable “Automatic peak label”. Or else you can manually label the substrate peak (see the Help text for more details).

- At the end of the fitting look once again at the “Fitting” tab to make sure that none of the limits have been reached.

If any have been reached, change the limits, click again.

NOTE: Some of the values are highlighted when they are close to but not equal to the limit, in this case they do not need to be changed.

- At the end of the fitting when no limits have been reached, right-click in the “Fitting” pane, select “Update sample” and answer the resulting question by pressing . Right-click in the “Fitting pane and select “Update convolution parameters”.
- Press and save these settings as “My SiGe4”.
- As long as “Always save simulated scans” was selected at *Customize - Defaults - Simulation and Convolution* the sample file will be saved.

6.4.2 A SiGe HBT Structure with a Graded SiGe Layer

This example uses the sample structure shown in Figure 5-1 for which a sample file was created in Section 5.2. To demonstrate automatic fitting for this sample three files are supplied:

SiGe grad.x00 which is a measured 004 rocking curve

SiGe grad4.s00 which is a sample file describing the intended layer structure

SiGe grad4.fit which contains all the information about simulation and fitting parameters

The procedure for fitting is described in four parts:

1. Opening the input files.
2. Fitting as a graded layer.
3. Treating the graded layer as a series of separate layers.
4. Printing out the results and saving files for fitting similar samples.

To open the three files required for this example:

- Select *File - Open*.
- Select the file SiGe grad.x00.
- Click **Open**.
- Select *Sample - Open Sample*.
- Select the file “SiGe grad4.s00”.
- Click and then .
- Select *Simulate - Simulate and Fit* (you may need to drag the splitter bar up in order to see all the buttons).
- Click the button.
- Select “SiGe grad4.fit”.
- Click .

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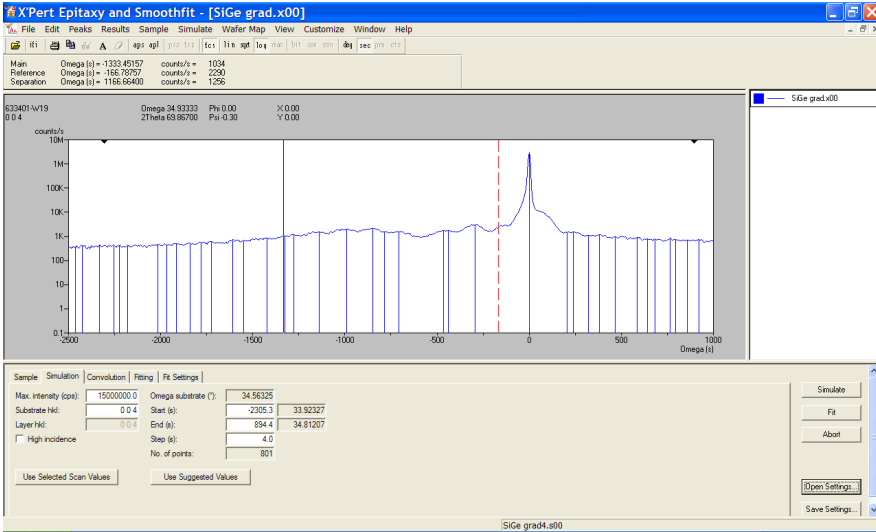


Figure 6-16 : The Display after Loading the Three Files

The display should appear as in Figure 6-16 - if necessary use the *View* menu to set logarithmic scaling.

- The peaks are automatically marked if “Automatic peak marking upon opening measured scan” has been checked in *Customize - Defaults - Automatic peak search and label parameters*.
- The sample and settings files you have loaded contain all the information to fit the sample as a linearly graded layer.
- Click on the “Fitting” tab and uncheck “Adjust” for item 4 which is the layer 2, Single Si, Strain.

No.	Adjust	Parameter	Type	Initial value	Current value	Start increment	Final increment	Lower limit	Upper limit
1	<input checked="" type="checkbox"/>	Layer 1: Graded - Ti	Composition	0.00500		0.00050	0.00001	0.00450	0.00950
2	<input checked="" type="checkbox"/>	Layer 1: Graded - Bi	Composition	0.19000		0.01800	0.00019	0.16200	0.19800
3	<input checked="" type="checkbox"/>	Layer 1: Graded - Ge	Thickness	0.05700		0.00570	0.00006	0.04275	0.07125
4	<input type="checkbox"/>	Layer 2: Single - Si	Strain	0.0		0.00	0.00	0.0	0.0
5	<input checked="" type="checkbox"/>	Layer 2: Single - Si	Thickness	0.08000		0.00800	0.00008	0.06000	0.10000
6	<input checked="" type="checkbox"/>	Background (cps)	Convolution	75.5		0.755	0.0755	60.4	90.6
7	<input checked="" type="checkbox"/>	Intensity multiplier	Convolution	1.00		0.0100	0.00100	0.90	1.20
8	<input checked="" type="checkbox"/>	Diffuse scattering wd	Convolution	585.6		5.856	0.5856	468.5	702.7
9	<input checked="" type="checkbox"/>	Diffuse scattering hc	Convolution	1341.2		13.412	1.3412	1073.0	1609.4

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- In the “Fit Settings” tab, make sure that the “Smoothfit algorithm has been selected.

To start the fit:

- Click on the button.
- At the end of fitting zoom in on the measured curve to examine the fit.

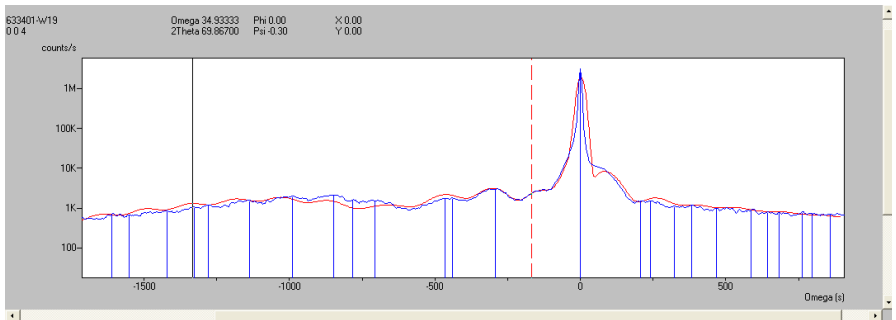


Figure 6-17: Zoomed View of the Measured Scan after Fitting to a Graded Layer

Figure 6-17 shows the fit achieved. It is not particularly good. This may be because the variation of Ge concentration with depth in the layer is not linear as we have assumed in our sample file. We will now see if we can achieve an improved fit allowing the Ge gradient to change. In the sample file the graded is defined as having 5 steps. We will now treat the SiGe layer as five discrete layers starting with a linear composition gradient.

To fit the SiGe layer as five discrete layers:

- Click on the “Fit Settings” tab.
- Click on the button.
- Click to confirm you want the conversion.
- Click on the “Fittings” tab to view the five separate layers.
- Remove the checks from the check boxes on lines 4, 6 and 8 as shown in Figure 6-18. Note that the layer strain that was formerly item 4 has become item 11 and should remain unchecked.
- Click the button.

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- If you get a message saying “!Lower limit should be smaller than initial value”, press . Then adjust the highlighted values accordingly and press the button again.
- If necessary, continue making changes and pressing the button until the fitting starts.

No.	Adjust	Parameter	Type	Initial value	Current value	Start increment	Final increment	Lower limit	Upper limit
1	<input checked="" type="checkbox"/>	Layer 1: Single - GeS	Composition	0.18000	0.00500	0.01800	0.00018	0.16200	0.19800
2	<input checked="" type="checkbox"/>	Layer 1: Single - GeS	Thickness	0.01140	0.17775	0.00570	0.00006	0.04275	0.07125
3	<input checked="" type="checkbox"/>	Layer 2: Single - GeS	Composition	0.13625	0.04887	0.01800	0.00018	0.16200	0.19800
4	<input type="checkbox"/>	Layer 2: Single - GeS	Thickness	0.01140	0.0	0.00570	0.00006	0.04275	0.07125
5	<input checked="" type="checkbox"/>	Layer 3: Single - GeS	Composition	0.09250	0.08400	0.01800	0.00018	0.16200	0.19800
6	<input type="checkbox"/>	Layer 3: Single - GeS	Thickness	0.01140	75.5	0.00570	0.00006	0.04275	0.07125
7	<input checked="" type="checkbox"/>	Layer 4: Single - GeS	Composition	0.04875	0.93	0.01800	0.00018	0.16200	0.19800
8	<input type="checkbox"/>	Layer 4: Single - GeS	Thickness	0.01140	702.7	0.00570	0.00006	0.04275	0.07125
9	<input checked="" type="checkbox"/>	Layer 5: Single - GeS	Composition	0.00500	1341.2	0.01800	0.00018	0.16200	0.19800
10	<input checked="" type="checkbox"/>	Layer 5: Single - GeS	Thickness	0.01140	0.00570	0.00570	0.00006	0.04275	0.07125
11	<input type="checkbox"/>	Layer 6: Single - Si	Strain	0.0	0.0	0.00	0.00	0.0	0.0
12	<input checked="" type="checkbox"/>	Layer 6: Single - Si	Thickness	0.08000	0.00080	0.00080	0.00008	0.06000	0.10000
13	<input checked="" type="checkbox"/>	Background (cps)	Convolution	75.5	-0.755	0.0755	0.0755	60.4	90.6
14	<input checked="" type="checkbox"/>	Intensity multiplier	Convolution	1.00	0.0100	0.00100	0.00100	0.90	1.20
15	<input checked="" type="checkbox"/>	Diffuse scattering w	Convolution	585.6	5.856	5.856	5.856	488.5	702.7
16	<input checked="" type="checkbox"/>	Diffuse scattering he	Convolution	1341.2	13.412	13.412	1.3412	1073.0	1609.4

Figure 6-18: The Fitting Tab after Converting the Graded Layer to Five Layers

Originally there were 12 adjustable parameters for the SiGe layers. We have now reduced this to 8 to decrease the fitting time. These 8 parameters allow sufficient flexibility to model the lattice parameter variation. Figure 6-19 shows a zoomed view of the final fit which is a significant improvement on the fit shown in Figure 6-17.

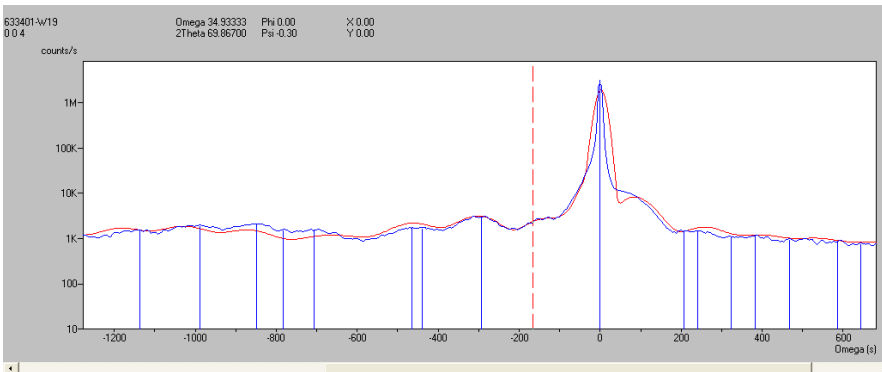


Figure 6-19: Zoomed View of the Measured Scan after Converting the Graded Layer to Five Layers

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If you had several similar samples to fit you can save the sample and settings file now so that they can immediately be analyzed as using seven parameters to fit the five discrete SiGe layers.

To print out the results shown in Figure 6-17 and save the sample and settings files:

- Select *File - Print*.
- Click .
- Select the “Fitting” tab.
- When the mouse pointer is on the “Fitting” tab, click the right mouse button to display the pop-up menu.
- Select *Update Sample*.
- Confirm you wish to save the sample by clicking - it will be saved as “SiGe grad4.s01”.
- Click on the button (you may need to drag the splitter bar up in order to see all the buttons).
- Enter “SiGe gradx54” as the file name.
- Click .

6.4.3 A GaN/GaN Superlattice on a Sapphire Substrate

This example uses the sample structure shown in Figure 5-10 for which a sample file was created in 5.4. To demonstrate automatic fitting with for this sample three files are supplied:

GaN.d00 which is a measured rocking curve

GaN4.s00 which is a sample file describing the intended layer structure

GaN4.fit which contains all the information about simulation and fitting parameters.

The procedure for fitting is described in three parts:

1. Opening the input files.
2. Fitting.
3. Printing out the results and saving files for fitting similar samples.

To open the three files required for this example:

- Select *File - Open*.

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- Select the file GaN.d00.
- Click .
- Select *Sample - Open Sample*.
- Select the file GaN.s00.
- Click .
- Select *Simulate - Simulate and Fit*.
- Click the Button.
- Select GaN4.fit.
- Click .
- Click on the “Fit Settings” tab.

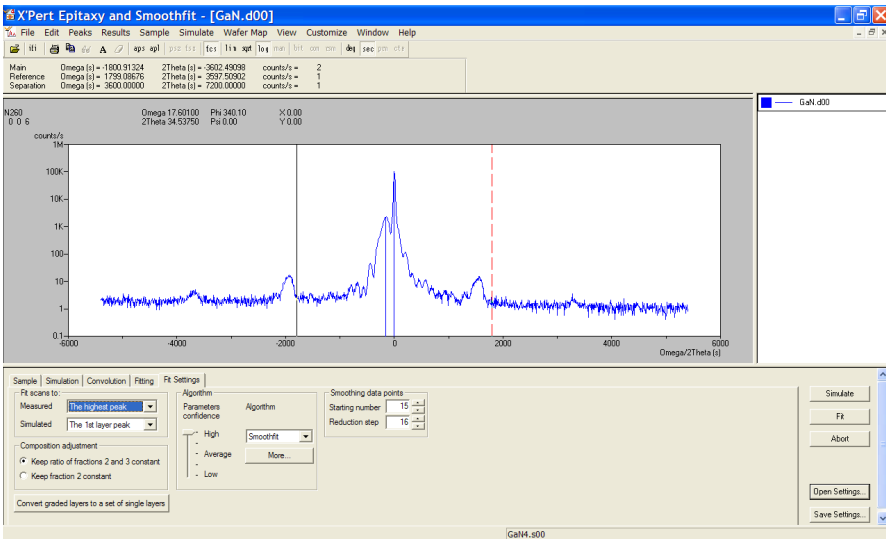


Figure 6-20: The Display with Fit Settings Tab after Having Loaded the Three Files

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The display will be as in Figure 6-20. In this case the first layer peak of the simulated scan is being matched to the highest peak of the measured scan. This is because the sapphire peak is beyond the range of the measured scan. For this example we are using a sample file with a total link. To view information about the link:

- Click on the “Sample” tab.
- Click on the button.

You will see the Layer Linking window shown in Figure 6-21. There is a total link between the two layers of the superlattice. This has been done because it was possible to get a good estimate of the period (the combined thickness of the two layers) from the satellite peak positions. In the sample file GaN4.s00 the period was made equal to the estimated period and we do not wish this to change during fitting.

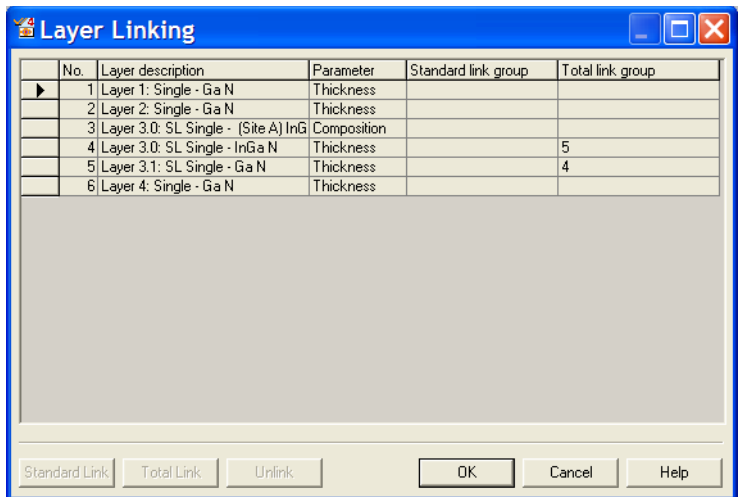


Figure 6-21: The Layer Linking Window for Sample GaN4.s00

To start fitting:

- Close the “Layer Linking” window by clicking on the button.
- Click on the button.
- When fitting is finished click on the “Fitting” tab.
- Look for the highlighted cells.

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- Change the limits on the highlighted cell so that they are no longer equal to the current value. For example:

No.	Adjust	Parameter	Type	Initial value	Current value	Start increment	Final increment	Lower limit	Upper limit
1	<input checked="" type="checkbox"/>	Layer 1: Single - Ga	Thickness	0.02500	0.02500	0.00025	0.00003	0.01875	0.03125
2	<input checked="" type="checkbox"/>	Layer 2: Single - Ga	Thickness	1.50000	1.50000	0.01500	0.00150	1.12500	1.87500
3	<input checked="" type="checkbox"/>	Layer 3:0: SL Single	Composition	0.13000	0.11700	0.00130	0.00013	0.05000	0.14300
4	<input checked="" type="checkbox"/>	Layer 3:0: SL Single	Thickness	0.00250	0.00188	0.00003	0.00000	0.00050	0.00313
5	<input checked="" type="checkbox"/>	Layer 3:1: SL Single	Thickness	0.00700					
6	<input checked="" type="checkbox"/>	Layer 4: Single - Ga	Thickness	0.05000	0.05000	0.00050	0.00005	0.03750	0.06250
7	<input type="checkbox"/>	Background (cps)	Convolution	1.5	1.5	0.075	0.0015	1.2	1.8
8	<input type="checkbox"/>	Intensity multiplier	Convolution	1.00	1.00	0.0500	0.00100	0.80	1.20
9	<input type="checkbox"/>	Diffuse scattering w/	Convolution	100.0	100.0	5.000	0.1000	80.0	120.0
10	<input type="checkbox"/>	Diffuse scattering he	Convolution	10.0	10.0	0.500	0.0100	8.0	12.0

- Click on the **Fit** button.
- repeat the previous steps until no limits are reached.

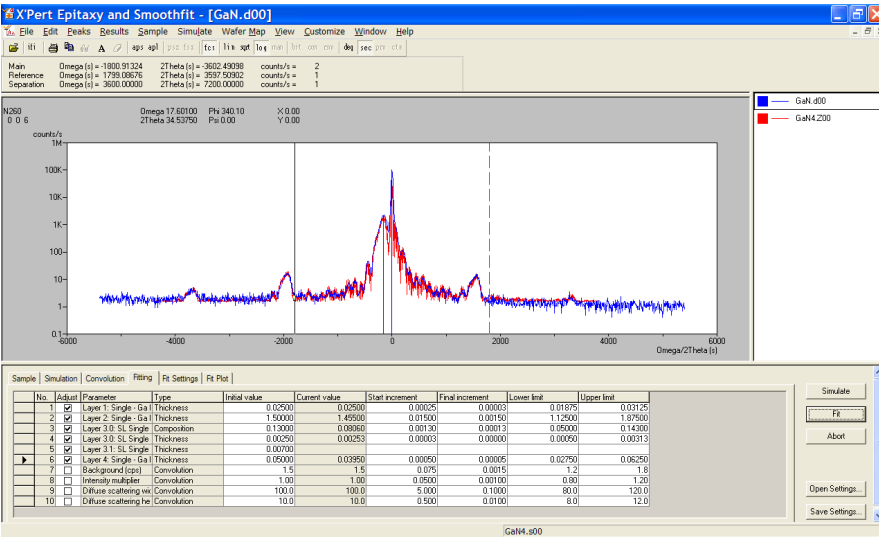


Figure 6-22: Final Fit for GaN Sample Displayed with the Best Sample Data Tab

To print out the results shown in Figure 6-22 and save the sample file:

- Select **File - Print**.
- Click **OK**.

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- Move the mouse pointer into the “Fitting” tab.
- Click the right mouse button to display the pop-up menu.
- Select *Update Sample*.
- Confirm you wish to save the sample by clicking - it will be saved as GaN4.s01.

6.5 Using Simulating and Fitting with your Own Data

If you plan to use the simulation and fit pane to simulate or fit your own data you may find it useful to make use of the grippers to set the simulation and fit range. The behavior of these grippers depends upon the entries in the “Fit scans to:” frame of the “Fit Settings” tab, the substrate offset and whether the graphics are displayed as relative seconds or degrees. More information is given in the help file.

If you wish to use the grippers you are advised to use relative seconds scaling and check that the “X centre point:” is set at “Fit Position”. This is set by selecting *View - Axes* as shown in Figure 6-23.

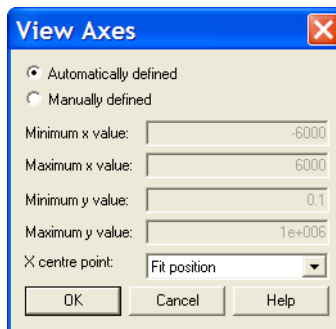

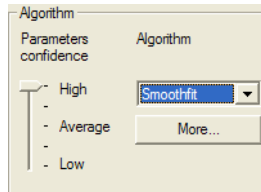



Figure 6-23: Setting the X Centre Point when using Relative Seconds

If you prefer to work in degrees you should be aware that the measured and simulated scans will never overlap in the graph unless the substrate offset angle set in the sample file is equal to the value for the measured scan. The Fit Parameter will be calculated for the situation where the two peaks indicated in the “Fit scans to:” frame of the “Fit Settings” tab are superimposed, regardless of how they are plotted in the graph.

6.6 Fitting Using Other Algorithms

- If you wish to try fitting using the other algorithms the procedure is similar to that given in section 6.4. However, prior to clicking on the  button, select the algorithm that you wish to use; either by using the slider or the drop-down menu in the “Algorithm” frame of the “Fit Settings” tab.



Input optimization parameters for the selected algorithm can be edited by clicking on the  button.

For information about the algorithms and their optimization parameters refer to the help file and the references therein.



Chapter 7.

Determining Composition & Relaxation from Rocking Curves

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Chapter 7. Determining Composition & Relaxation from Rocking Curves

7.1 Introduction

This chapter demonstrates how to determine the composition and percentage relaxation of a layer from four rocking curves. Four curves are supplied from a gallium indium arsenide ($\text{Ga}_{1-x}\text{In}_x\text{As}$) layer on a (001) GaAs substrate:

GaInAs004a.d00	GaInAs004b.d00
GaInAs224a.d00	GaInAs224b.d00

These files can all be found in the folder: “C:\Program Files\PANalytical\X'Pert Epitaxy\Examples”.

The rocking curves are for 004 and 224 reflections with the [110] direction horizontal with $\Phi = 90$ (for scans with file names ending in A) and $\Phi = -90$ (for scans with file names ending in B). All four rocking curves show two peaks - the weaker peak is from the layer in all curves.

The four scans provided are the optimum set required to calculate relaxation from rocking curves. They are two symmetrical reflections, measured before and after a 180 rotation in Φ . There are two rocking curves using the same asymmetrical reflection, one with low angle of incidence and one with high angle of incidence and Φ rotated by 180. Information about the approximations involved in using fewer rocking curves is given in the Help Topic “Using Results - Mismatch and Relaxation.”

The procedure described in this chapter is available for diamond, zinc blende and wurtzite structures. It cannot be used for wurtzite layers on sapphire or silicon carbide substrates.

Section 7.2 describes the procedure in three parts:

1. Setting the default sample, plot and peak search criteria.
2. Opening the data files.
3. Displaying and printing.

Section 7.3 provides some information on additional steps which may be necessary when you analyze your own data:

1. What to do if the hkl values are not included in the scan data.
2. How to use an existing sample file.
3. Calculating the composition for quaternary layers.
4. Using the results to update the sample file.

7.2 The Procedure

To begin:

- Start X'Pert Epitaxy.

7.2.1 Setting the Defaults

Now we will set all the defaults we require:

- Select *Customize - Defaults*.

First we will set the default sample:

- Click on the “Sample Data” Tab.
- Use the drop-down list box to set the “Default substrate structure” to Zinc Blende.
- In the “Substrate” branch of the tree view on the left of the tab, highlight the Zinc Blende.
- For “Site A” set the number of elements as 1.
- Set Element 1 as Ga.
- For “Site B” set the number of elements as 1.
- Set Element 1 as As.
- In the lower part of the tab enter 0 0 4 (0=zero<space>0<space>4) for the “Simulation HKL”; 0 0 1 for the “Primary HKL”; 600 microns for the “Thickness” and 0.0 for the “Off cut angle”.
- Use the drop-down list box to set the “Layer Structure” to Zinc Blende.
- In the “Layer” branch of the tree view highlight the Zinc Blende.
- For “Site A” set the number of elements as 2.
- Set Element 1 as Ga; Element 2 as In.
- For “Site B” set the number of elements as 1.
- Set Element 1 as As.
- Enter 0 0 4 for the “Simulation HKL”.
- Enter 0.1 micron for the “Thickness” of the layer.

Chapter 7. Determining Composition & Relaxation from Rocking Curves

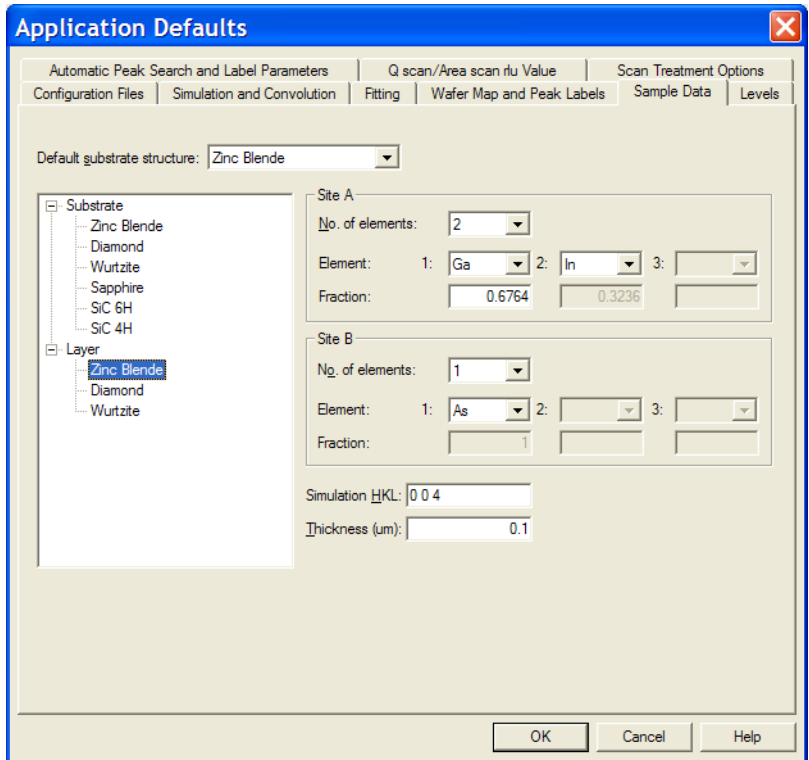


Figure 7-1: Default Sample Data tab after editing the Layer

The Sample Data tab after editing the default layer is shown in Figure 7-1.

Then we set the default peak search parameters:

- Click on the “Automatic Peak Search and Label Parameters” Tab.
- In the “Peak search parameters” frame:
 - Select the radio button for “Automatic search window size”.
 - Enter 500 for the “Minimum detection level.” - this is set just above the background level.
 - Select the radio button for “Set peak to Gaussian”.
- In the “Label parameters” frame:

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Select “2S-L” for “Peaks to Label” and “S peak has higher intensity” in the “Label Parameters” frame.

- In the “Automatic Peak Marking on Opening” frame:

Select (check the boxes) for “Measured scans:” “Peak positions”, and “Peak labels”.

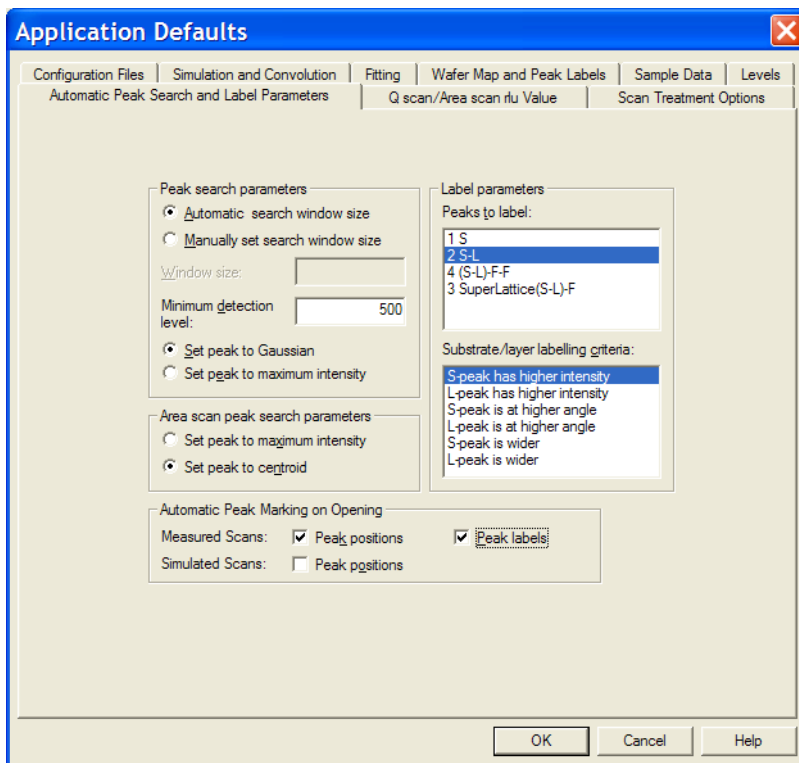


Figure 7-2: The Peak Labeling Parameters After Setting

Chapter 7. Determining Composition & Relaxation from Rocking Curves

The Automatic Peak Search and Label Parameters tab is shown in Figure 7-2 with these peak labeling parameters set. Peaks will be found and labelled in each measured scan as it is loaded.

- Click to save the default values.

Now set the plot options:

- Select *Customize - Single Scan Options*.
- Select the radio button for “Relative Second plot” as the Default X-scaling type.
- Select the radio button for “Logarithmic” as the Default Y-scaling type.
- Select the radio button for “Automatically defined” as the Axis Labels.
- Select the radio button for “Highest Peak” for defining how to Set seconds plotted relative to.

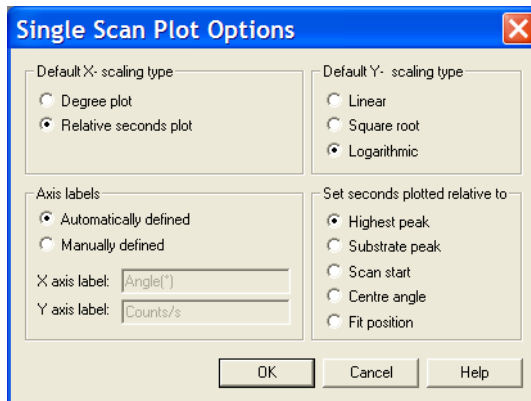



Figure 7-3: Single Scan Plot Options Window for this Example

The Single Scan Plot Options Window is shown in Figure 7-3.

- Press .

7.2.2 Opening the Data Files

To open the measured scan files:

- Select *File - Open*.
- Use the drop-down list in the “Look in:” box at the top of the “File Open” window to select the folder “C:\Program Files\PANalytical\X'Pert Epitaxy\Examples”.
- Select the four files GaInAs004a.d00, GaInAs004b.d00, GaInAs224a.d00 and GaInAs224b.d00 - hold down the **Ctrl** key and click on each file.
- Click .

7.2.3 Displaying and Printing Results

- Select *Results - Mismatch and Relaxation* - you may need to pull up the splitter bar at the bottom of the graphics area to display the full results pane.

The four measured rocking curves plus the calculated relaxation and composition of the layer are now displayed as in Figure 7-4. Relaxation and composition can be calculated from three curves (omitting any one of the four) or two curves (which must include one asymmetrical scan). You can alter the check marks beside the scan names to see the effect of using different combinations of scans.

Chapter 7. Determining Composition & Relaxation from Rocking Curves

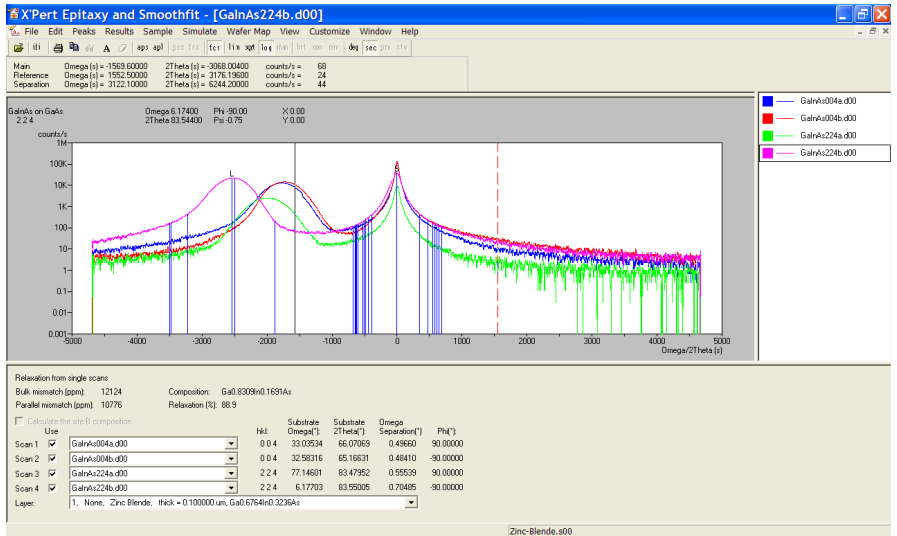


Figure 7-4: The Four Measured Scans Displayed with the Relaxation and Composition on the Results Pane

To print out the graphics plus the results pane:

- Select *File -Print*.
- Select the Printer you wish to use.
- If necessary use “Properties” to change the paper orientation or print quality.
- Click

7.3 Analyzing Your Own Data

Section 7.2 demonstrated how the composition and relaxation could be calculated from four rocking curves using the default sample structure. This section describes some additional actions which may be required when analyzing your own data. Section 7.3.1 describes how to edit the HKL parameters not correctly entered during data collection. Section 7.3.2 describes how to use an existing sample file instead of the default sample. Section 7.3.3 describes your options when you have a sample with more elements. Section 7.3.4 describes how to use the results to update a sample file.

7.3.1 Editing HKL Values

The mismatch, composition and relaxation calculations require the HKL values for each of the curves used in the analysis. If your scan data does not include the correct HKL information, you can use the edit menu to provide the required information:

- Open all the files you wish to use with *File - Open*.
- For each scan which does not contain the correct HKL information.
 - Select the scan by clicking on its name in the legend area - the scan name will be surrounded by a box.
 - Select *Edit - Scan Information*.
 - Enter the required HKL in the Substrate hkl field as:
<H><space><K><space><L> in the window (see Figure 7-5).
 - Click .

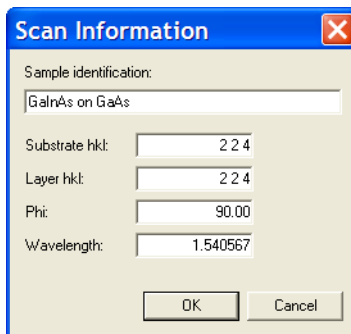


Figure 7-5: Window for Editing the Reflection Used

Chapter 7. Determining Composition & Relaxation from Rocking Curves

When calculating relaxation and composition from rocking curves it is only necessary to edit the Substrate HKL. The Layer HKL is assumed to be the same. You can also use *Edit - Scan Information* to change the Phi value for the scan and to change the wavelength value used in the calculation. The wavelength value is normally saved from the X'Pert Data Collector.

7.3.2 How to Use an Existing Sample File

If you have already created a sample file to use with your data you should open the sample file using *Sample - Open Sample* after you have loaded all the scan data in a window using *File - Open*.

Use the drop-down list box at the bottom of the result pane to choose the correct layer to use for the relaxation calculation.

7.3.3 Calculating the Composition for Quaternary Layers

If your sample has more than one element on both the A site and the B site you have the choice of adjusting the A site or the B site. To adjust the B site click on the tick box "Calculate the site B composition". The ratio of the second and third elements will be held constant if there are three elements on the site you have chosen to adjust.

7.3.4 Using the Results to Update the Sample File

You can transfer the values calculated in *Results - Mismatch and Relaxation* to the sample file when the results are displayed in the results pane. To do this:

- Drag the splitter bar upwards so that you can see all of the results pane.
- Move the mouse pointer into the results pane.
- Click the right mouse button to display the pop-up menu.
- Select *Update Sample*.
- Select *Sample - Edit Layer*. At this time you may be asked to select various options; answer the questions as required.
- Select *Sample - Edit Sample*. If you press it will overwrite the original sample, if you click on you can save the sample with a different name.



Chapter 8. Determining Composition and Relaxation from Maps

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Chapter 8. Determining Composition and Relaxation from Maps

8.1 Introduction

This chapter demonstrates how to determine the composition and percentage relaxation of a layer from four diffraction space maps. Four maps are supplied from a gallium indium arsenide ($\text{Ga}_{1-x}\text{In}_x\text{As}$) layer on a (001) GaAs substrate:

Map004a.a00	Map004b.a00
Map444a.a00	Map444b.a00

These files can all be found in the folder: “C:\Program Files\PANalytical\X'Pert Epitaxy\Examples”.

All four maps show two peaks - the weaker peak is from the layer in every map. The set of maps consists of a symmetrical 004 and an asymmetrical 444 reflection recorded in two orthogonal reciprocal lattice planes which are normal to the substrate surface. The pair of maps with $\Phi = 0$ have file names ending in a, the pair of maps with $\Phi = 90$ have file names ending in b.

The four maps provided can be used to calculate the three layer unit cell parameters. One pair of maps allows the calculation of the unit cell in one reciprocal lattice plane. The relaxation is assumed to be the same in the orthogonal plane if composition is calculated from a single pair of maps. Composition and relaxation can be calculated from a single asymmetrical map. In this case substrate surface planes are assumed to be parallel to the same planes in the layer in addition to assuming the relaxation is the same in the orthogonal direction.

The procedure described in this chapter is available for diamond, zinc blende and wurtzite structures. It cannot be used for wurtzite layers on sapphire or silicon carbide substrates.

Section 8.2 describes the procedure in three parts:

1. Setting the default sample, peak search criteria and plot options
2. Opening the data files and marking peaks
3. Displaying and printing

Section 8.3 provides additional information for analyzing your own data.

8.2 The Procedure

To begin:

- Start X'Pert Epitaxy.

8.2.1 Setting the Defaults

Now we will set all the defaults we require:

- Select *Customize - Defaults*.

First we will set the default sample:

- Click on the “Sample Data” tab.
- Use the drop-down list box to set the “Default substrate structure” to Zinc Blende.
- In the “Substrate” branch of the tree view on the left of the tab, highlight “Zinc Blende”.
- For “Site A” set the number of elements as 1.
- Set Element 1 as Ga.
- For “Site B” set the number of elements as 1.
- Set Element 1 as As.
- In the lower part of the tab enter 0 0 4 (0=zero<space>0<space>4) for the “Simulation HKL”; 0 0 1 for the “Primary HKL”; 600 microns for the “Thickness” and 0.0 for the “Off cut angle”.
- Use the drop-down list box to set the “Layer Structure” to “Zinc Blende”.
- In the “Layer” branch of the tree view highlight “Zinc Blende”.
- For “Site A” set the number of elements as 2.
- Set Element 1 as Ga; Element 2 as In.
- For “Site B” set the number of elements as 1.
- Set Element 1 as As.
- Enter 0 0 4 for the “Simulation HKL”.
- Enter 0.1 micron for the “Thickness” of the layer.

Chapter 8. Determining Composition and Relaxation from Maps

The Sample Data tab after editing the default layer is shown in Figure 8-1.

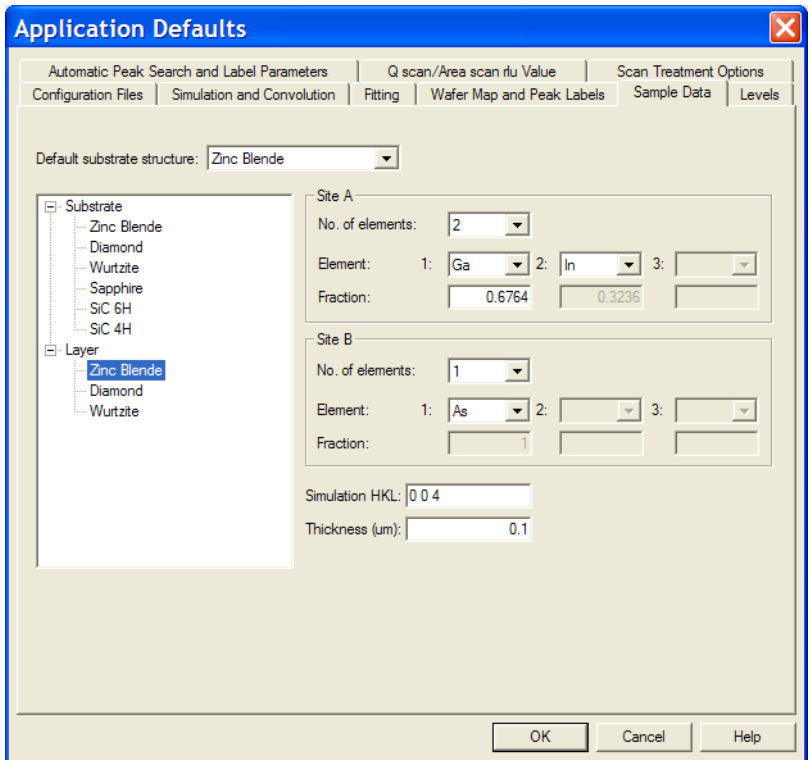


Figure 8-1: Default Sample Data tab after Editing the Layer

Then we set the default peak search parameters:

- Click on the “Automatic Peak Search and Label Parameters” Tab.
- Select the “Set peak to Centroid” radio button in the “Area scan peak search parameters” frame.
- Select “2S-L” for “Peaks to Label” and “S peak has higher intensity” in the “Label Parameters” frame.
- Set “Minimum detection level” to “0.0”.
- Make sure that the “Peak position” box is not checked.

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- Make sure that the “Peak labels” box is not checked.

The Automatic Peak Search and Label Parameters tab is shown in Figure 8-2 with these options set.

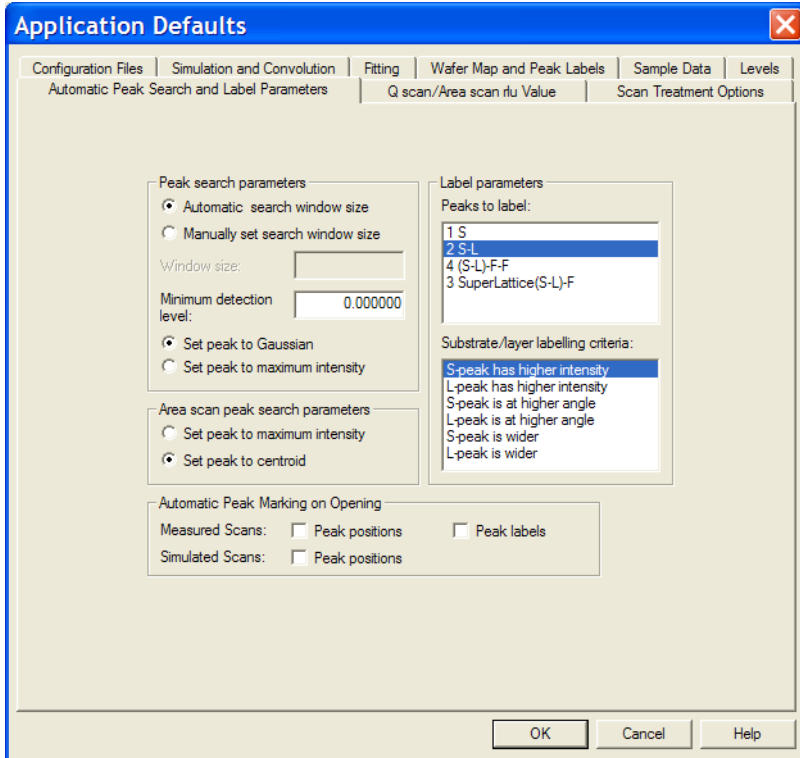


Figure 8-2: After Setting The Peak Labeling Parameters

- Click to save the default values.

Now set the plot options:

- Select *Customize - Area Scan Options*.
- Select the “Bitmap (degrees)” radio button as the Plot type.
- Select the “Automatically defined” radio button for Axis labels.

Chapter 8. Determining Composition and Relaxation from Maps

- Select the “Logarithmic” radio button as the Intensity scaling.
- Check on the “Use Whole Plot Area” option box.

The Area Scan Plot Options Window should be as in Figure 8-3.

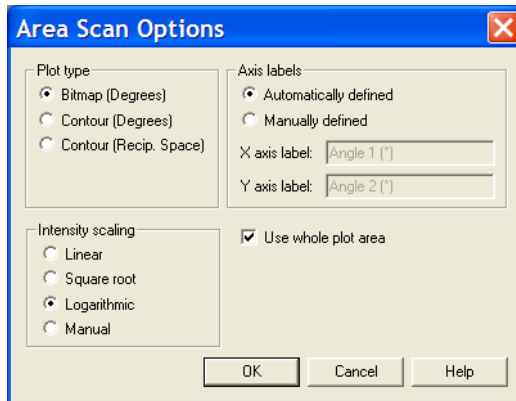


Figure 8-3: Area Scan Plot Options Window for this Example

- Click to close the window.

8.2.2 Opening the Data Files

To open the measured scan files:

- Select *File - Open*.
- Use the drop-down list in the “Look in:” box at the top of the “File Open” window to select the folder “C:\Program Files\PANalytical\X’Pert Epitaxy\Examples”.
- Use the drop-down list in the “Files of type” box to choose “Area scan (*.ann, *.ynn, *.xrdml)”.
- Select the four files Map004a.a00, Map004b.a00, Map444a.a00 and Map444b.a00 - hold down the **Ctrl** key and click on each file.
- Click .

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Now we need to find and label the substrate and layer peaks for each scan:

- Select *Peaks - Semi-Automatic Peak Search*.

Mark and label the substrate and layer peaks for all four scans:

- Double-click on the scan name in the legend area (MAP004A.A00).
- Define a rectangle by clicking and dragging around the substrate (right-hand) peak.
- Release the mouse button and a cross should appear at the peak position.
- Define a rectangle by clicking and dragging around the layer (left-hand) peak.
- Release the mouse button and a cross should appear at the peak position.
- Select *Peaks - Automatic Peak Label* to label the peaks.
- Repeat these actions for the remaining three scans (MAP444A.A00, MAP004B.A00, MAP444B.A00).

8.2.3 Displaying and Printing Results

- Select *Results - Layer Relaxation* - you may need to pull up the splitter bar at the bottom of the graphics area to display the full results pane.

The results pane after marking & labeling the peaks in all four of the scans is shown in Figure 8-4. The results value which are displayed depend on whether the “Use substrate Omega and 2Theta angles calculated from materials data” is checked. When the box is not checked the Bragg angles are calculated from the 2Theta positions of the peaks. Otherwise the expected position of the substrate peak is calculated from the layer lattice parameter stored in the data base and the wavelength. The layer angles are calculated from substrate peak position and the measured peak separations.

You can use the radio buttons above the scan names in the results pane to change the number of scans used in the calculation.

Chapter 8. Determining Composition and Relaxation from Maps

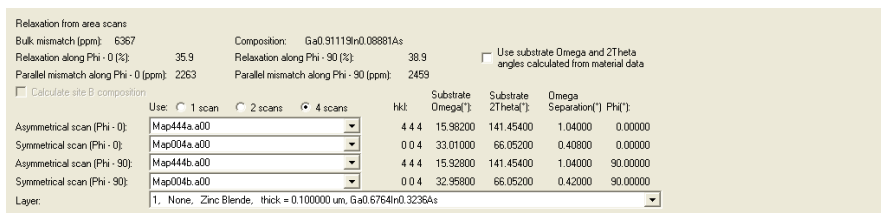


Figure 8-4: The Results Pane after Marking All of the Peaks

To print out the graphics plus the results pane:

- Select *File -Print*.
- Select the Printer you wish to use.
- If necessary use “Properties” to change the paper orientation or print quality.
- Click .

8.3 Analyzing Your Own Data

Section 8.2 demonstrated how the composition and relaxation is calculated from maps using the default sample structure. Additional steps may be necessary when you analyze your own data. All the possibilities described for analyzing rocking curves in Chapter 7 also apply to analyzing maps. Section 7.3.1 describes what you need to do if the hkl values for the reflection were not stored correctly when the data was collected. Section 7.3.2 describes how to use an existing sample file. Section 7.3.3 describes the options available for a layer with more than one element on both the A site and the B site. Section 7.3.4 describes how to update the sample file.

You may wish to select peak positions using the cursors rather than by using *Semi-Automatic Peak Search*. To do this for the selected scan:

- Select *View - Reposition Cursors*.
- Drag the main cursor to the peak position.
- Either press **Ctrl + F9** to define the cursor position as the Substrate Peak, or press **Ctrl + F10** to define the cursor position as the Layer Peak.

Chapter 9. Automating Your Diffraction Measurements/Analyses

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9.1 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 2.0, or by using X'Pert Epitaxy 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.

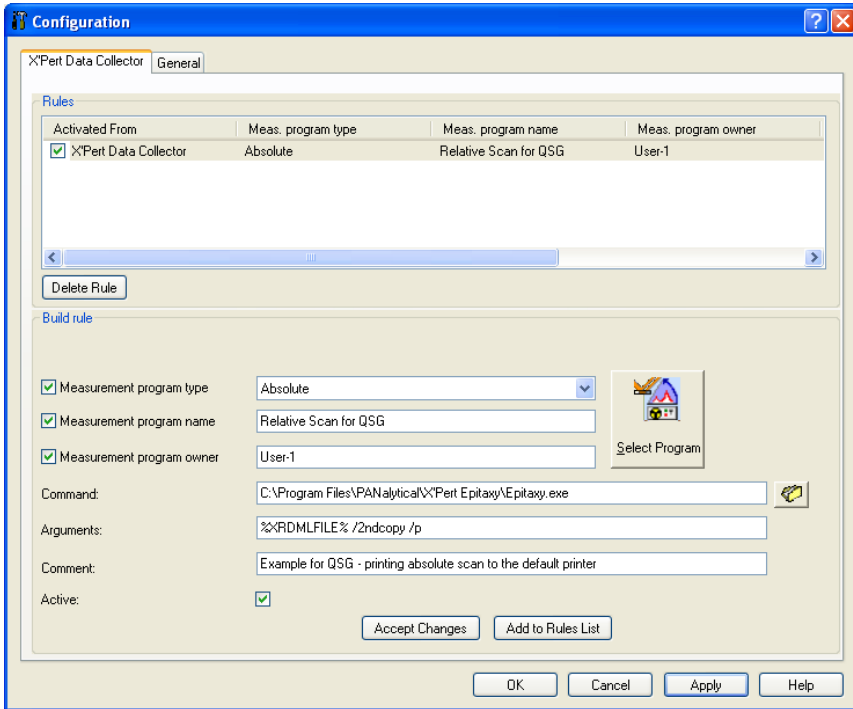
The first example shows how to automatically print out your scan data immediately after it has been measured using the X'Pert Data Collector. The second example shows how to automatically perform the analysis described in Chapter 2.

9.2 Automatic Printing of Scan Data using the APP

Assume that you are working with the X'Pert Data Collector and you have created a relative scan program called Program 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 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 Epitaxy: “C:\Program Files\PANalytical\X'Pert Epitaxy\Epitaxy.exe”.
- In the “Arguments” field enter %XRDMLFILE% /2ndcopy /p
where: %XRDMLFILE% is used to indicate the measured file
/2ndcopy indicates that a second copy of Epitaxy be opened
/P indicates that the scan must be printed.
- Activate the rule you have just saved by ticking the “Active:” tick box.
- Click .
- Click on the button.

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

9.3 Automating the Analysis Described in Chapter 2

If you want to regularly analyze similar samples you can create an Epitaxy icon which can be used to do the analysis automatically. This can be done for any analysis which does not need manual intervention. The example in Chapter 2 fulfills this criterion because all the peak marking can be done automatically.

Create another Epitaxy shortcut:

- If necessary exit from X'Pert Epitaxy.
- Use the right mouse button to click on the X'Pert Epitaxy icon on the desktop.

A menu similar to the one shown in Figure 9-1 will be displayed.

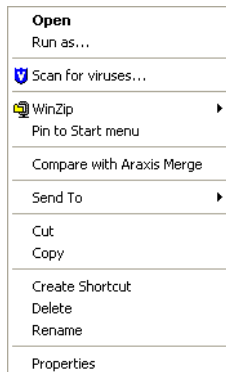



Figure 9-1: The Pop-up Menu Available from the Icon

- Select *Create Shortcut* - another X'Pert Epitaxy icon will appear on the desktop.
- Use the right mouse button to click on the new icon to display the pop-up menu.
- Select *Rename*.
- You can now type another name below the icon - type “Results Summary”.

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- Press *Enter*.
- Use the right mouse button to re-display the pop-up menu and select *Properties*.
- Edit the entry in the “Target” field to:
“C:\Program Files\PANalytical\X'Pert Epitaxy\Epitaxy.exe” “C:\Program Files\PANalytical\X'Pert Epitaxy\ResSum.ini” “C:\Program Files\PANalytical\X'Pert Epitaxy\Examples\004 GeSi on Ge.xrdbl” /
2ndcopy /p.
The “ResSum.ini” file is the file that you created at the end of Chapter 2.
- Click  to close the window.

The formatting of this line must be correct, refer to the Help file for more information about this. A space must be present immediately before each slash (/). File names which include spaces must be put in quotation marks.

The key /2ndcopy is added to start a new instance of X'Pert Epitaxy. This avoids the possibility of disturbing a copy of X'Pert Epitaxy which is running on the same computer. The automatically started instance of X'Pert Epitaxy will be closed after the print command (/p) has been executed.

To run the analysis automatically:

- Check your printer is switched on.
- Start X'Pert Epitaxy using the “Results Summary” icon.

The X'Pert Epitaxy Help File gives more information about using a wider range of input files and options.

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