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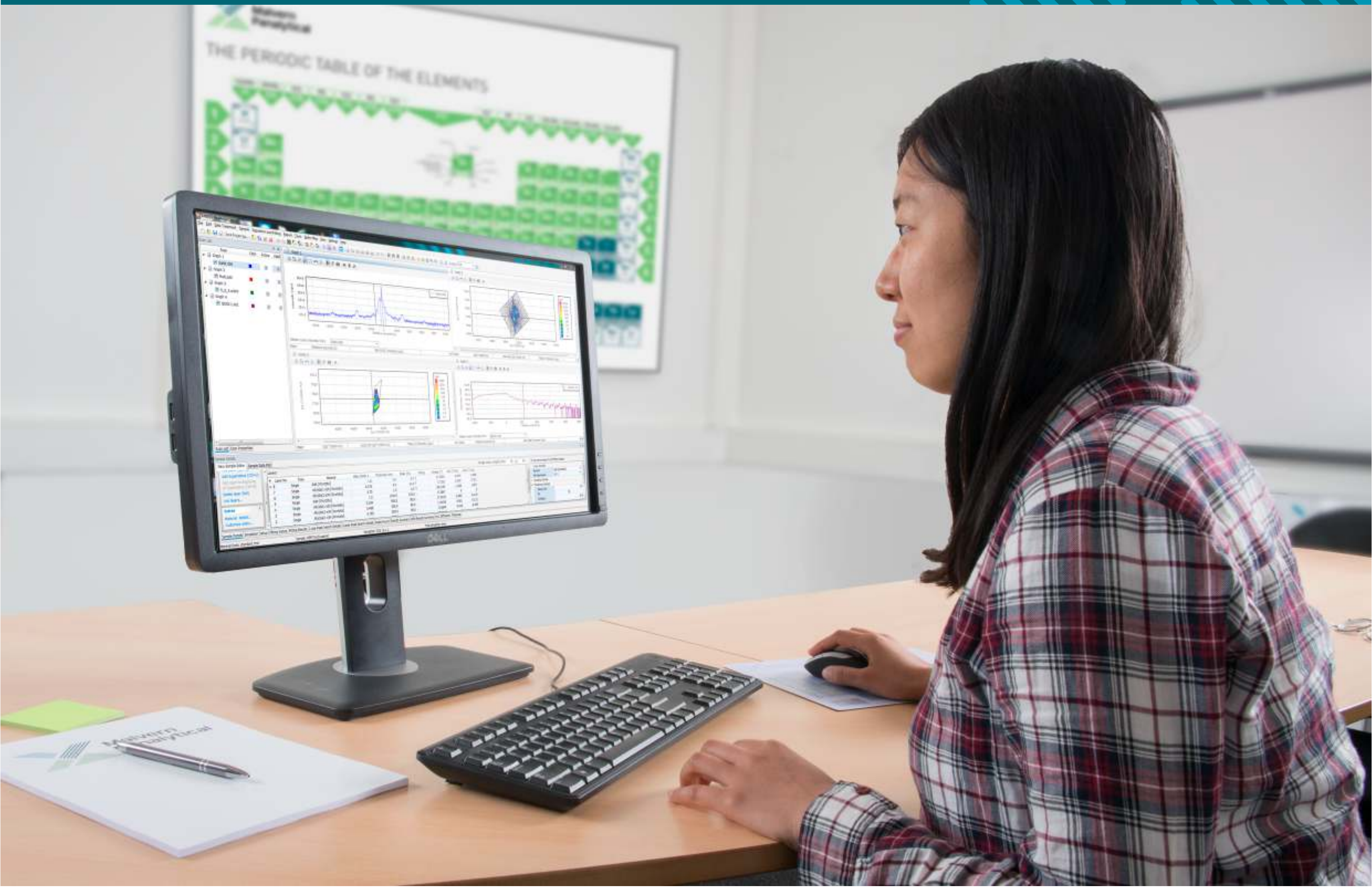
AMASS
APPLICATION GUIDE



AMASS

APPLICATION GUIDE

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This is the original publication of Edition 2 of this document, to be used with AMASS version 1.0 or higher.

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CHAPTER 1 INTRODUCTION

1.1 Introduction

This Application Guide helps you to get started with AMASS quickly.

The examples in this Application Guide show you how to use the software to do simple tasks.

For all the tasks in the examples, there can be other possible ways to complete them, but then you must experiment with AMASS and learn the other possibilities yourself.

There can be differences between the example screens in this Application Guide and what you see on your screen. If that occurs, follow the instructions on your screen.

1.2 Contents of the Application Guide

These are the worked examples used in this Application Guide:

Chapter 2: Measure composition and thickness from a rocking curve

This chapter gives information about how to plot a rocking curve and find the layer thicknesses and compositions from marked peak positions in rocking curves from cubic semiconductor samples.

Chapter 3: Find the thickness of a layer from a specular reflectivity curve

This chapter gives information about how to open a measured data file and use 2 different methods to evaluate the thickness of a layer.

Chapter 4: Make and edit sample information

This chapter gives information about how to make sample files for samples with more than one layer and how to link layers. The sample files are necessary when you use the automatic fit functionality. The chapter is divided into 4 independent sections; one for each of the major sample types supported: SiGe alloy structures, III-V alloy structures and 2 hexagonal nitride materials.

Chapter 5: Use graphics with area scans

This chapter gives information about how to load and show area data and mark peaks for area scans. Information is also given about how to merge area scans, and how to extract single scans from an area scan and project an area scan as a single scan.

Chapter 6: Find composition and relaxation from rocking curves

This chapter gives information about how to find layer composition and relaxation for semiconductor samples from a set of rocking curves.

Chapter 7: Find composition and relaxation from maps

This chapter gives information about how to find layer composition and relaxation for semiconductor samples from a set of reciprocal space maps.

Chapter 8: Make simulations and use automatic fitting of rocking curves

This chapter gives information about how to simulate a rocking curve and use automatic fitting.

Chapter 9: Make simulations and use automatic fitting of specular reflectivity curves

This chapter gives information about how to simulate a specular reflectivity curve and use automatic fitting.

Chapter 10: Make a wafer map from a set of diffraction data

This chapter gives information about how to use the AMASS Wafer Map function to make maps that show the variation in a sample parameter (for example, substrate peaks width or layer mismatch) as a function of position on the wafer from a set of diffraction data.

Chapter 11: Diffuse scatter

This chapter gives information about how to open an omega scan and find out what Hurst parameter and lateral correlation lengths are used best for the sample.

Chapter 12: Automate your diffraction measurements and analyses

This chapter gives information about how to automate your analyses with AMASS directly from the command line or use the AMASS Controller application.

1.3 Start AMASS

To start AMASS, use one of these procedures:

- On the desktop, double-click the icon AMASS.
- Click the Windows Start button and then on the list of apps or programs, go to **PANalytical AMASS > AMASS**.

1.4 Customize AMASS

1.4.1 Customize the default parameters

A wide range of default parameters can be set in the **Settings** menu:

- Options for calculations and to show wafer maps
- Default peak search and labeling when scans are opened or on scan simulations
- Default substrate and layer materials for sample files
- Default convolution parameters for simulated scans
- Default fitting parameters for automatic fitting
- Default plot settings for single and area scans
- Options for the direct analysis of opened single and area scans
- Defaults for the used length units and the number of decimal places of parameters

1.4.2 Customize the toolbar

1. Right-click on the menu bar or toolbar and select **Customize**. The **Customize** window has 3 tabs where you can customize the toolbar.

   NOTE: The default menu bar and toolbar cannot be renamed or deleted.

2. If you want to add a command to the toolbar, do as follows:
   a. Go to the **Commands** tab.
   b. Drag and drop the command that you want to add to the toolbar.
3. If you want to remove a command from the toolbar, do as follows:
   a. Make sure that the **Customize** window is open.
   b. Drag and drop the command that you want to remove away from the toolbar.
4. If you want to reset the toolbar to its original settings, do as follows:
   a. Go to the **Toolbars** tab.
   b. Select the **ToolBar** check box.
   c. Click **Reset**.
   d. Click **OK**.
5. If you want to make your own toolbar, do as follows:
   a. Go to the **Toolbars** tab.
   b. Click **New**.
   c. In the **Toolbar Name** field, enter a name. For example, "My Toolbar".
   d. Click **OK**. My Toolbar is added to the list and there is a small box under the default toolbar which is the new toolbar.
   e. If you want to move the new toolbar, drag and drop it to the new position.
   f. Go to the **Commands** tab.
   g. Drag and drop the commands that you want to use in the toolbar.

Figure 1.1 My Toolbar

6. If you want to hide or show toolbars, do as follows:
   1. Go to the **Toolbars** tab.
   2. Clear or select the check boxes of the toolbars that you want to hide or show.
7. If you want the toolbar buttons shown as large icons, do as follows:
   1. Go to the **Options** tab.
   2. Select the **Large icons** check box.
8. Click **OK** to close the **Customize** window.
9. If you want to hide or show buttons on the customized toolbar, do as follows:
   1. Click the arrow button ▾ at the end of the toolbar.
   2. Click **Add or Remove Buttons**.
   3. Click the button that you want to hide or show.

1.5 Data files used in this Application Guide

Data files that are used in the exercises of this Application Guide are supplied with the software. The files are installed in your Documents folder: **C:Users\User.Name\Documents\PANalytical\AMASS\Examples**.

Table 1.1 *Data files*

Chapter	Data file
Chapter 2	004 GeSi on Ge.xrdml
Chapter 3	SiGe_Si_XRR.x00
Chapter 5	SBTN fibre.A00, Multi_2.A01, Multi_2.A02
Chapter 6	GaInAs004a.d00, GaInAs004b.d00, GaInAs224a.d00, GaInAs224b.d00
Chapter 7	Map004a.a00, Map004b.a00, Map444a.a00, "Map444b.a00
Chapter 8	SiGe.d00, GaN_MQW.aprjxl, GaN.d00
Chapter 9	XRR-1.x00
Chapter 10	X_Y_1.xrdml, X_Y_4.xrdml, InP_Q.asamxl, InP_Q.d00 to InP_Q.d35
Chapter 11	QSG11.asamxl

CHAPTER 2 MEASURE COMPOSITION AND THICKNESS FROM A ROCKING CURVE

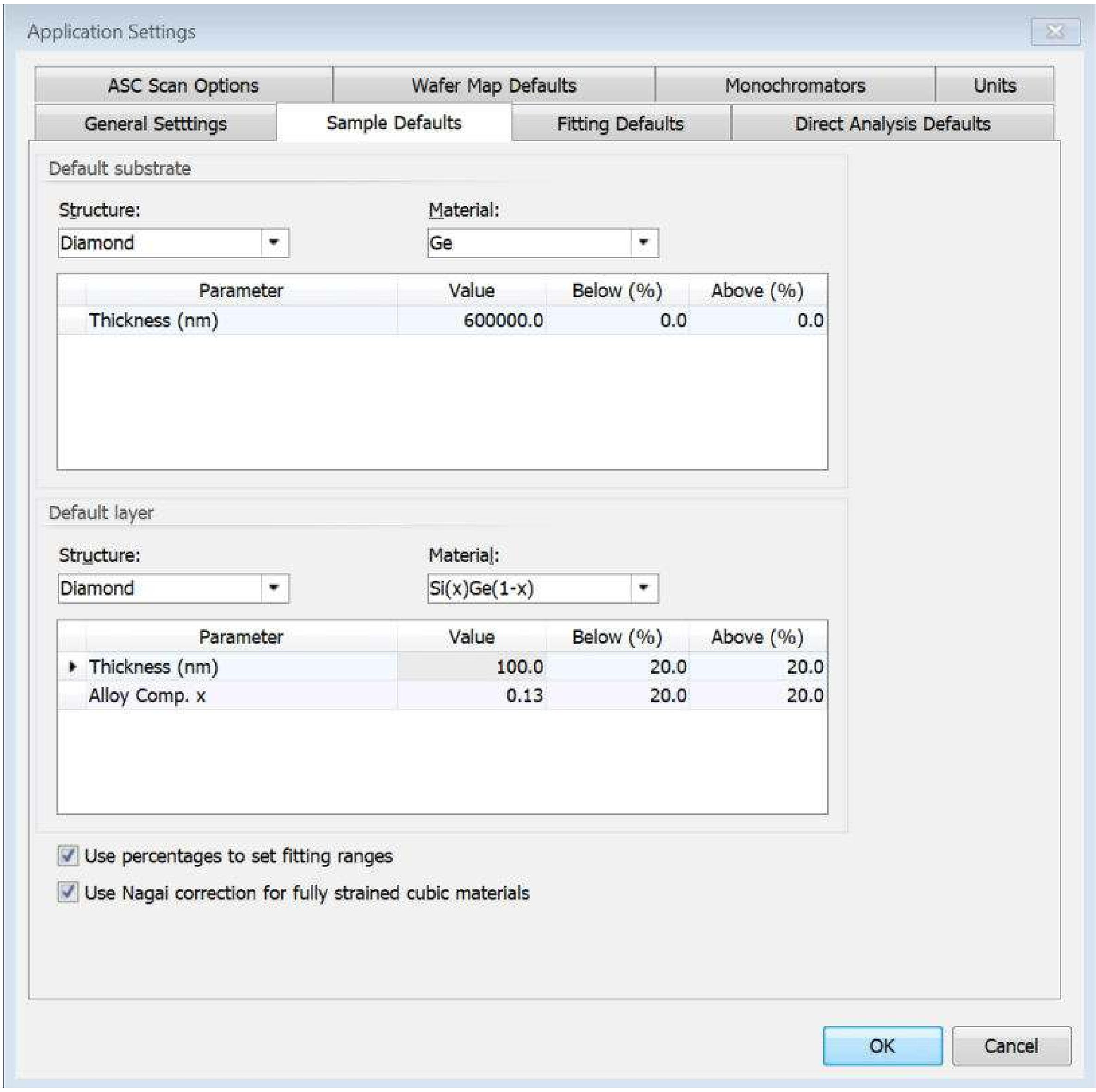
2.1 Introduction

This chapter gives information about how to show a rocking curve from a single crystal substrate with a heteroepitaxial layer and find the composition and thickness of the layer.

This example uses an 004 rocking curve from a (001) germanium substrate with a strained heteroepitaxial layer of germanium silicon recorded with an X'Pert PRO MRD. The scan file "004 GeSi on Ge.xrdml" is an ω/2θ scan which was recorded with a mirror plus a Ge 220 4-crystal monochromator as primary optics modules and with a receiving slit as secondary optics module.

2.2 Set the sample defaults

1. Start AMASS.
2. Go to **View > View as H.R. diffraction**.
3. Set the substrate as follows:
   a. Go to **Settings > Application Settings**.
   b. Go to the **Sample Defaults** tab.
   c. In the **Default substrate** frame, select **Diamond** from the **Structure** drop-down list.
   d. In the **Default substrate** frame, select **Ge** from the **Material** drop-down list. The list only contains materials that are part of the chosen structure type.
4. Set the layer as follows:
   a. In the **Default layer** frame, select **Diamond** from the **Structure** drop-down list.
   b. In the **Default layer** frame, select **Si(x)Ge(1-x)** from the **Material** drop-down list.
   c. If applicable, change the default values for thickness and composition.
   d. If applicable, select the **Use percentages to set fitting ranges** check box. When this check box is selected, you can change the percentage values that will be used to set the fitting ranges.



Default substrate

Structure: Diamond

Material: Ge

Parameter	Value	Below (%)	Above (%)
Thickness (nm)	600000.0	0.0	0.0

Default layer

Structure: Diamond

Material: Si(x)Ge(1-x)

Parameter	Value	Below (%)	Above (%)
Thickness (nm)	100.0	20.0	20.0
Alloy Comp. x	0.13	20.0	20.0

☑ Use percentages to set fitting ranges

☑ Use Nagai correction for fully strained cubic materials

Figure 2.1 Sample Defaults tab for GeSi layer

e. Go to the **Direct Analysis Defaults** tab.

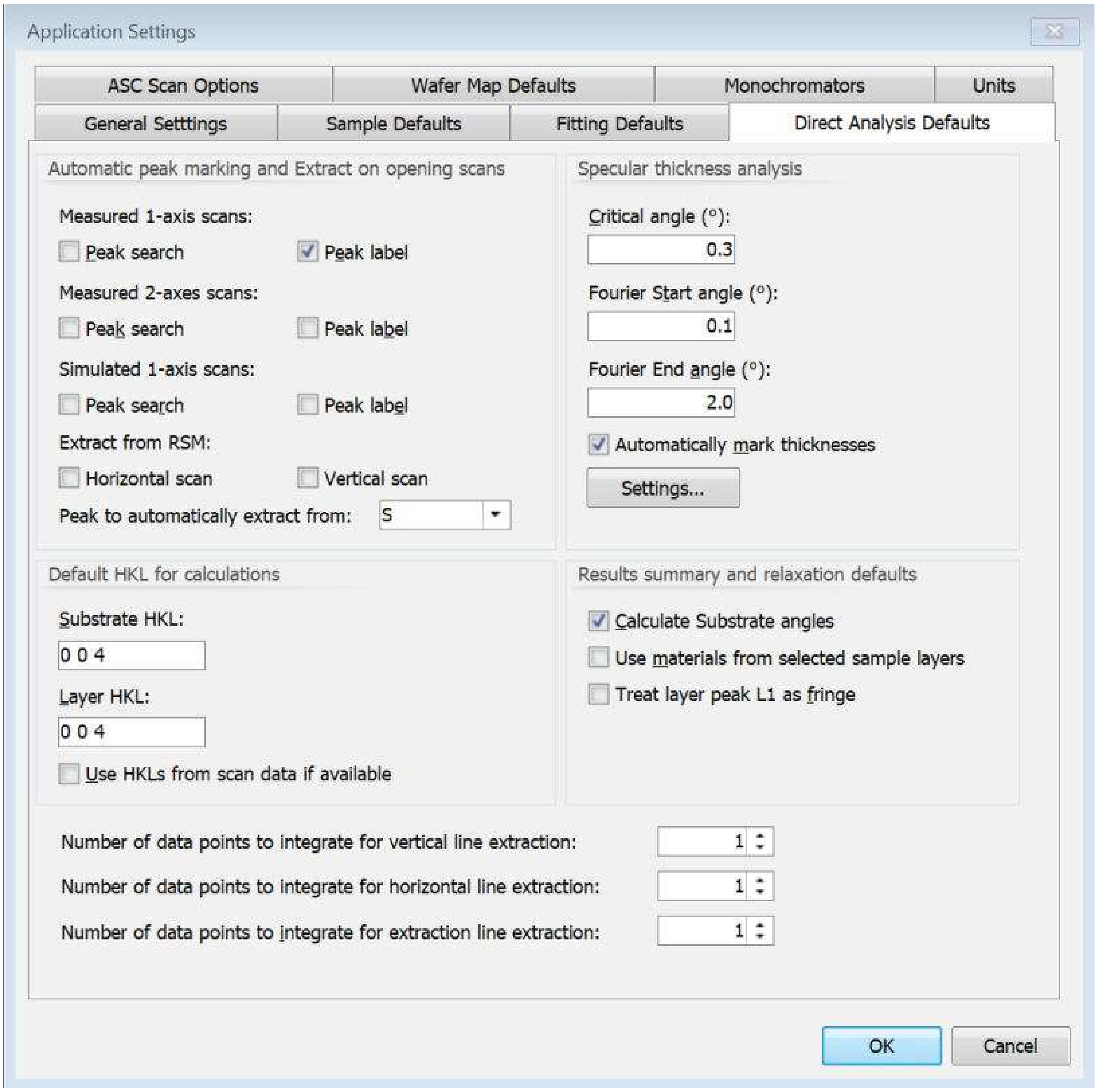
f. In the **Substrate HKL** field, enter "0 0 4".

NOTE: Make sure that you enter the value as 0, space, 0, space, 4.

g. In the **Layer HKL** field, enter "0 0 4"

NOTE: Make sure that you enter the value as 0, space, 0, space, 4.

5. In the **Automatic peak marking on opening scans** frame, select the **Peak label** check box for **Measured 1-axis scans**.



Automatic peak marking and Extract on opening scans

Measured 1-axis scans:
☐ Peak search ☑ Peak label

Measured 2-axes scans:
☐ Peak search ☐ Peak label

Simulated 1-axis scans:
☐ Peak search ☐ Peak label

Extract from RSM:
☐ Horizontal scan ☐ Vertical scan

Peak to automatically extract from: S

Specular thickness analysis

Critical angle (°): 0.3

Fourier Start angle (°): 0.1

Fourier End angle (°): 2.0

☑ Automatically mark thicknesses

Default HKL for calculations

Substrate HKL: 0 0 4

Layer HKL: 0 0 4

☐ Use HKLs from scan data if available

Results summary and relaxation defaults

☑ Calculate Substrate angles
☐ Use materials from selected sample layers
☐ Treat layer peak L1 as fringe

Number of data points to integrate for vertical line extraction: 1
Number of data points to integrate for horizontal line extraction: 1
Number of data points to integrate for extraction line extraction: 1

Figure 2.2 Direct Analysis Defaults tab for GeSi layer

6. Click **OK** to save the settings and close the window.

2.3 Make a new sample

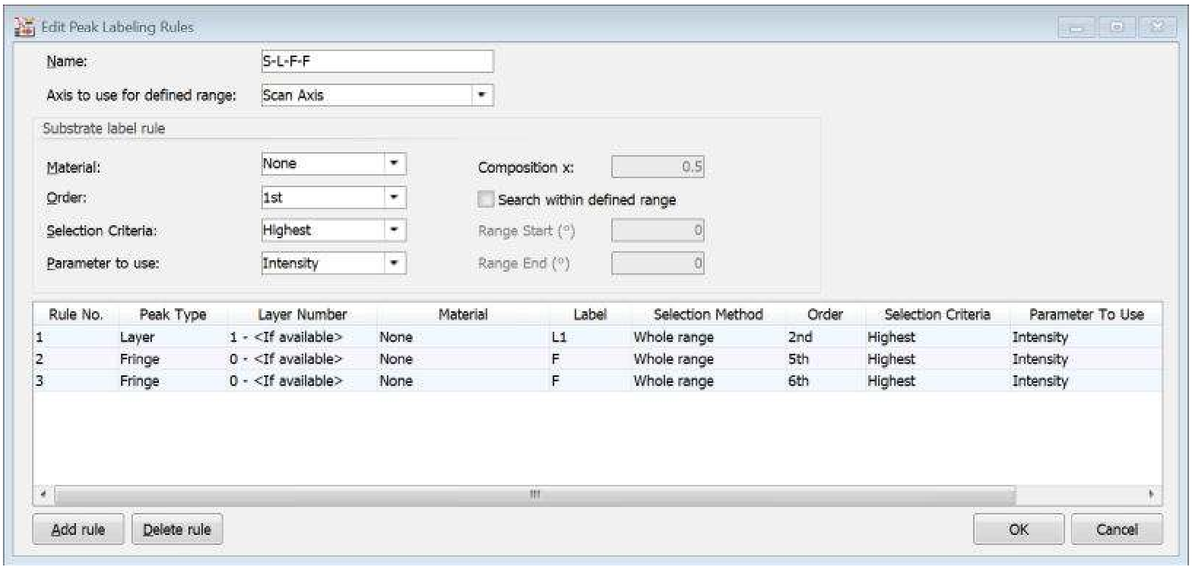
1. Go to **Sample > New Sample**. At the bottom of the screen, the **New Sample Editor** tab opens with the default material of the substrate. If necessary, this can be edited.
2. In the **Layers** pane, click **Add Layer**. The substrate layer moves down 1 row and the new layer is the top row. The default material and parameters are used. Relaxation is set to 0 %.
3. If necessary, edit the material, alloy composition, thickness or relaxation.

2.4 Set default peak labeling

Set peak search and peak labeling rules for the layer, substrate peaks and 2 thickness fringes:

1. Go to the **1-axis Peak Search Details** tab.

2. Click **Add**. A window opens where you can edit the rules for labeling peaks.
3. In the **Name** field, enter "S-L-F-F".
4. Click **Add rule** 3 times to add 3 rules.
5. Use these settings:



Name: S-L-F-F
Axis to use for defined range: Scan Axis
Material: None
Order: 1st
Selection Criteria: Highest
Parameter to use: Intensity
Composition x: 0.5
☐ Search within defined range
Range Start (°): 0
Range End (°): 0

Rule No.	Peak Type	Layer Number	Material	Label	Selection Method	Order	Selection Criteria	Parameter To Use
1	Layer	1 - <If available>	None	L1	Whole range	2nd	Highest	Intensity
2	Fringe	0 - <If available>	None	F	Whole range	5th	Highest	Intensity
3	Fringe	0 - <If available>	None	F	Whole range	6th	Highest	Intensity

Figure 2.3 *Edit Peak Labeling Rules window*

6. Click **OK**. When a measured scan is loaded, peak positions are marked with vertical lines. The substrate and layer peaks are marked "S" and "L" respectively and the 2 thickness fringes are labeled "F".

2.5 Open measured data

1. Set the default single scan options as follows:
   a. Go to **Settings > Default Single Scan Plot Settings**.
   b. In the **Intensity scale** field, select **Logarithmic**.
   c. In the **Intensity units** field, select **cps**.
   d. In the **Show x axis as** field, select the correct setting:
      - Select **Absolute angle (deg)** if you want to plot in degrees.
      - Select **Relative seconds** if you want to plot in seconds.
   e. Click **OK** to close the window.
2. Go to **File > Open Scan(s)**.
3. Go to **C:\Users\User.Name\Documents\PANalytical\AMASS\Examples**.
4. Select "004 GeSi on Ge.xrdml".
5. Click **Open**. The scan data shows in a single scan graphics window.

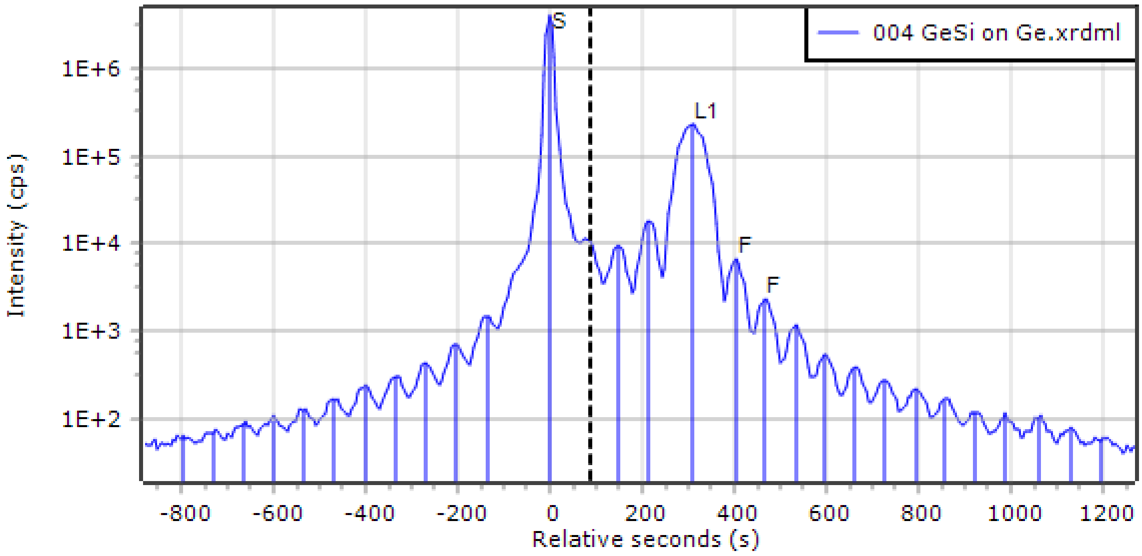


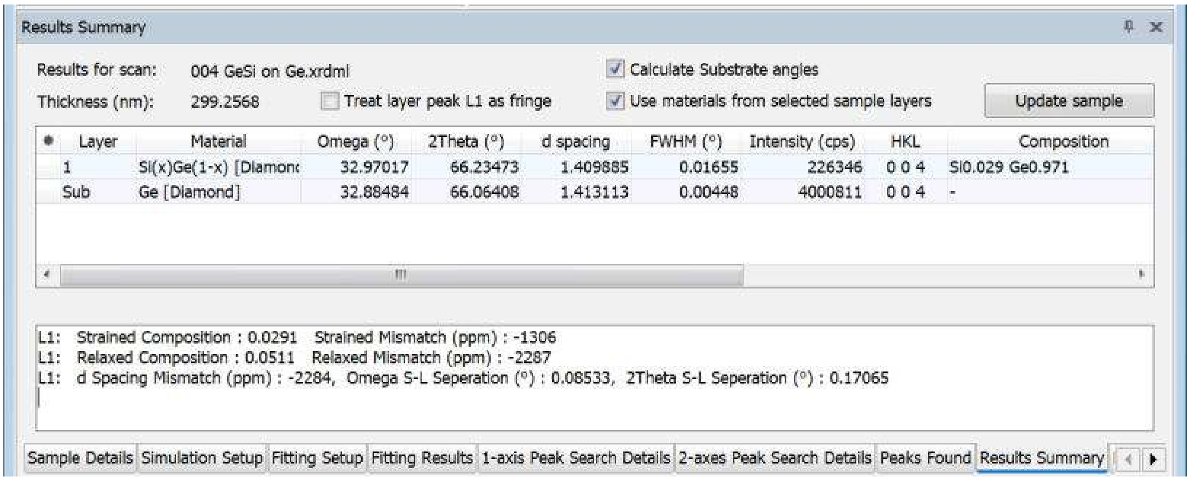
Figure 2.4 Graph area in relative seconds

The file name is shown in the **Scan List** tab on the left of the screen. The scan information can be found in the **Scan Properties** tab. If you cannot see these areas, go to **View** and select them.

6. If you want to adjust the plot, do as follows:
   - To zoom in, click and drag the cursor to zoom in into that area. Horizontal and vertical scroll bars are available to move around the full area of the plotted data. Double-click or click 🔍 to see the full-size plot. To go back to the previous size, click 🔍.
   - To change the intensity scaling settings to linear, square root or logarithmic or to change other relevant single scan settings, click 📈. You can also use the **Intensity scale** in the toolbar Intensity scale: Logarithmic ▾.
   - To change between plot in degrees or plot in relative seconds, click x° (degrees) or xs (relative seconds).
   - To change between plot intensity in counts or counts per second, click CPS.
   - To change the color of the plot, double-click the color symbol in the **Scan List** tab, select the new color and then click **OK**.
   - To change the plot style and line style, click 📈.

2.6 Find the layer composition and thickness

1. Go to the **Results Summary** tab.
2. Select the **Use materials from selected sample layers** check box.



Results for scan: 004 GeSi on Ge.xrdml

Thickness (nm): 299.2568

☐ Treat layer peak L1 as fringe

☑ Calculate Substrate angles

☑ Use materials from selected sample layers

●	Layer	Material	Omega (°)	2Theta (°)	d spacing	FWHM (°)	Intensity (cps)	HKL	Composition
	1	Si(x)Ge(1-x) [Diamonc	32.97017	66.23473	1.409885	0.01655	226346	0 0 4	Si0.029 Ge0.971
	Sub	Ge [Diamond]	32.88484	66.06408	1.413113	0.00448	4000811	0 0 4	-

```
L1:   Strained Composition : 0.0291   Strained Mismatch (ppm) : -1306
L1:   Relaxed Composition : 0.0511   Relaxed Mismatch (ppm) : -2287
L1:   d Spacing Mismatch (ppm) : -2284,  Omega S-L Seperation (°) : 0.08533,  2Theta S-L Seperation (°) : 0.17065
```

Figure 2.5 *Results Summary pane*

The layer and substrate peak positions, intensities and half widths are given together with values of the layer thickness. There are 2 values supplied for the mismatch and composition; 1 value is for a fully relaxed layer and 1 value is for the fully strained layer. As the thickness fringes are very clear, the layer is apparently fully strained, thus the fully strained value is the correct value for this sample.

This procedure is the peak position based method to find the composition and mismatch for a cubic sample. As an alternative, use the fitting procedure. Refer to Chapter 8.

For more information about how to interpret single scans with the used equations, refer to the AMASS Help. You can also mark all the fringes on the right side of the layer peak to find the layer thickness more accurately. This information is also given in the AMASS Help.

2.7 Set up a report

1. Go to **Report > Report Setup**.
2. In the **Available report items** field, select the item that you want to include in the report.
3. Click >.
4. Go back to step 2 until you have added all the items that you want to include in the report.
5. Click **OK**.
6. If you want to print the report, go to **Report > Print Report**.
7. If you want to save the report, go to **Report > Save Report To File As** and select the format that you want to save the report as.

2.8 Prepare for work on equivalent samples

If this sample was the first of many equivalent samples to be measured, you can save the sample file and the INI file to automate the analysis of further samples. Refer to Chapter 12.

1. Go to the **Results Summary** tab.
2. Click **Update sample**.
3. Select **Strained composition values** and the **Update thickness** check box.
4. Click **OK** to change the layer details into the sample definition.

5. Save the sample:
   a. Go to **Sample > Save Sample As**.
   b. In the **File name** field, enter "GeSi on Ge.asamxl".
   c. Click **Save** to save the sample details as a sample file.
6. Save the default settings in an INI file for future use:
   a. Go to **Settings > Save Settings As**.
   b. In the **File name** field, enter "ResSum.ini".
   c. Click **Save** to save the default settings in an INI file.
7. As an alternative, you can also save all settings including all data in a project file. Do as follows:
   a. Go to **File > Save Project As**.
   b. In the **File name** field, enter "ResSum.aprjxl".
   c. Click **Save**.

CHAPTER 3 FIND THE THICKNESS OF A LAYER FROM A SPECULAR REFLECTIVITY CURVE

3.1 Introduction

This chapter gives 2 different methods to examine the thickness of the layer of SiGe on a Si substrate:

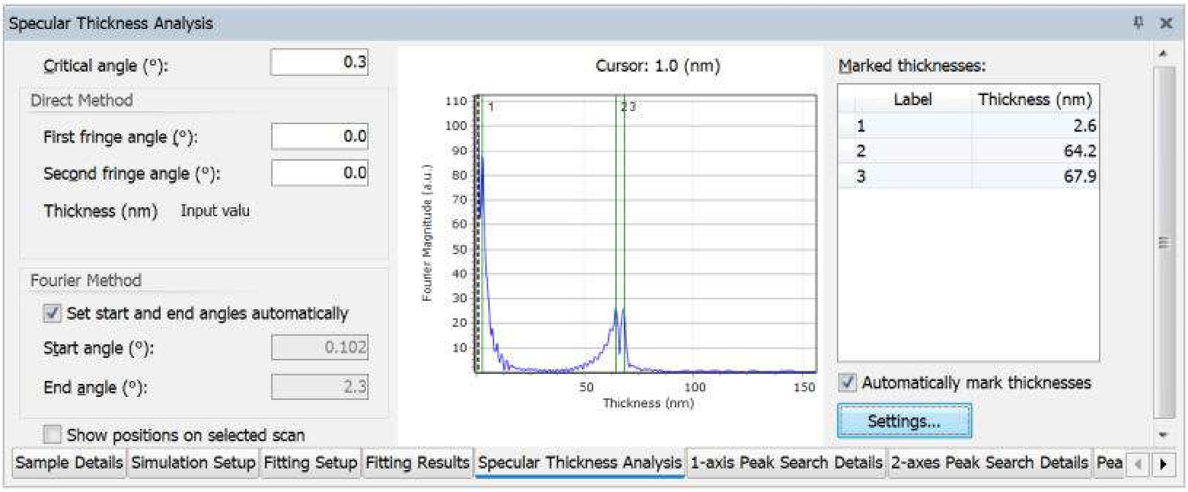
- Fourier method
- Direct method

3.2 Open measured data

1. Start AMASS.
2. Go to **File > Open Scan(s)**.
3. Go to **C:\Users\User.Name\Documents\PANalytical\AMASS\Examples**.
4. Select "SiGe_Si_XRR.x00".
5. Click **Open**.

3.3 Use the Fourier method

1. Go to the **Specular Thickness Analysis** tab. If the tab is not shown in the results and working area, go to **View > Specular Thickness Analysis**.



Critical angle (°): 0.3

First fringe angle (°): 0.0

Second fringe angle (°): 0.0

Thickness (nm) Input valu

☑ Set start and end angles automatically

Start angle (°): 0.102

End angle (°): 2.3

☐ Show positions on selected scan

Label	Thickness (nm)
1	2.6
2	64.2
3	67.9

☑ Automatically mark thicknesses

Figure 3.1 Specular Thickness Analysis tab

There are 2 frames in this tab, **Direct Method** and **Fourier Method**. In this section, the Fourier method is used to find the thickness of the SiGe layer.

2. On the main scan, drag the cursor line to the critical angle. If the cursor line is not visible, click .

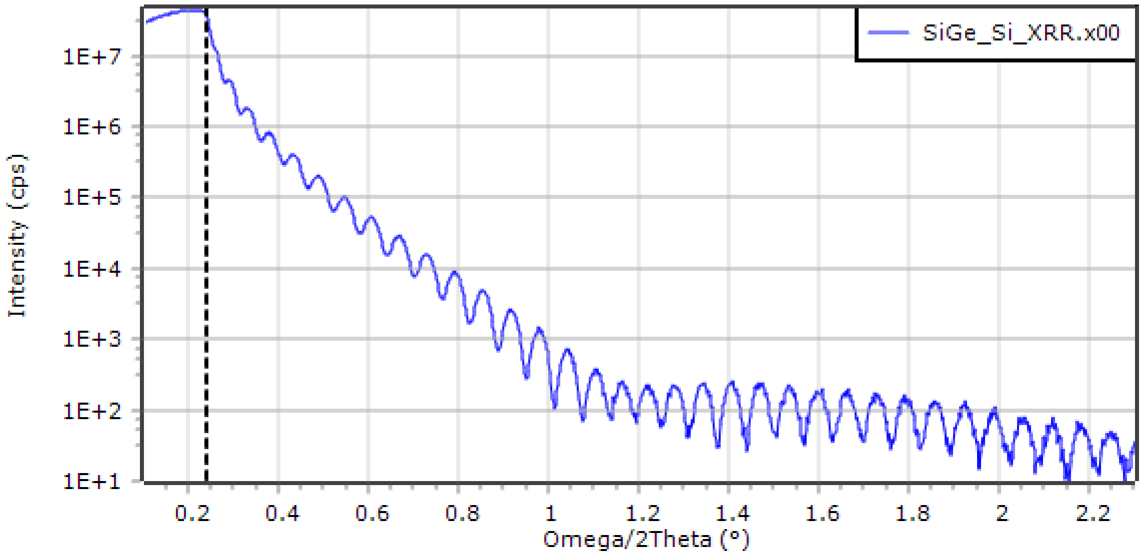
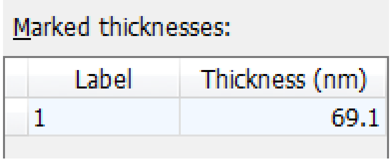


Figure 3.2 Cursor line at the critical angle

3. Right-click at the critical angle and go to **Specular Thickness Analysis > Define Cursor Position as Critical Angle**. The position is shown in the **Critical angle (deg)** field in the **Specular Thickness Analysis** tab. To show the manually set cursor position, select the **Show positions on the selected scan** check box.
4. If applicable, select the **Set start and end angles automatically** check box. The start and end angle values are taken from the open scan. The 2 positions can also be set by the cursor:
   a. To set the start angle, right-click and go to **Specular Thickness Analysis > Define Cursor Position as Fourier Analysis Start Angle**.
   b. To set the end angle, right-click and go to **Specular Thickness Analysis > Define Cursor Position as Fourier Analysis End Angle**.
5. Select the **Automatically mark thicknesses** check box. The related thicknesses are shown in the **Marked thicknesses** table.
6. If you want to change the peak search criteria, do as follows:
   a. Click **Settings**.
   b. Change the peak search criteria.
   c. Click **OK**.
7. In the **Specular Thickness Analysis** tab, click and drag the cursor on the peak to zoom in.
8. Move the cursor line to the top of the peak.
9. Right-click and select **Mark Cursor Position as Thickness**. The result is shown in the **Marked thicknesses** table. In this experiment, the thickness is measured at 69.1 nm.


Marked thicknesses:

Label	Thickness (nm)
1	69.1

Figure 3.3 Marked thicknesses table

3.4 Use the direct method

The direct method measures the distance between 2 fringes to find the thickness of the layer.

1. On the main scan, zoom into an area with clearly defined peaks or valleys.
2. Move the cursor to a peak or valley.

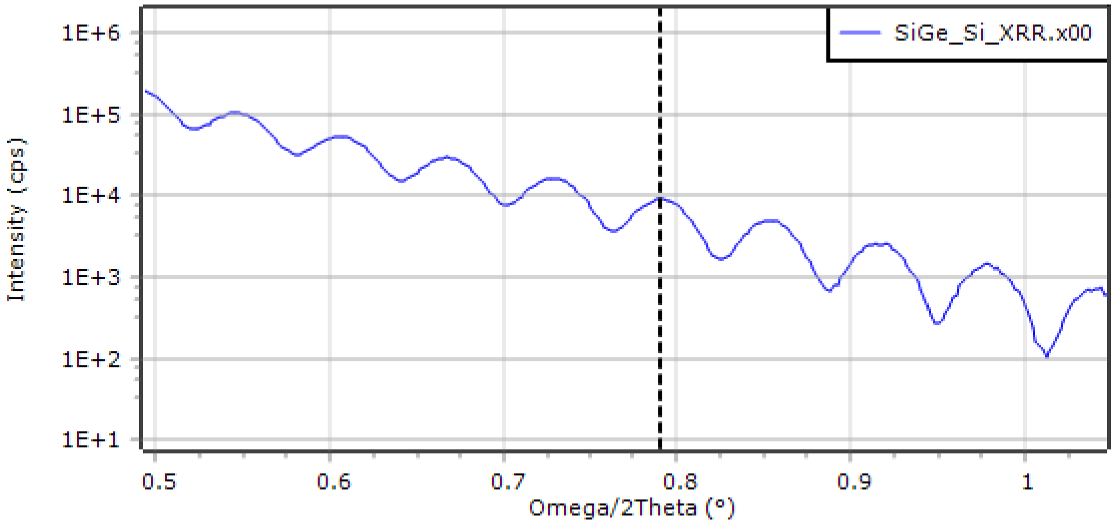
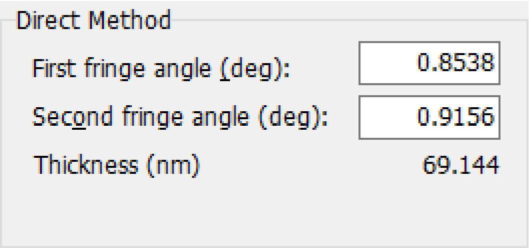


Figure 3.4 Main scan zoomed in

3. Right-click and go to **Specular Thickness Analysis > Define Cursor Position as First Fringe Angle**.
4. Move the cursor to the next peak or valley.
5. Right-click and go to **Specular Thickness Analysis > Define Cursor Position as Second Fringe Angle**. The results are shown in the **Direct Method** frame. In this example, the thickness is 69.144 nm.


Direct Method

First fringe angle (deg): 0.8538
Second fringe angle (deg): 0.9156
Thickness (nm) 69.144

Figure 3.5 Direct Method frame

The results of the Fourier method and the direct method are very close. It shows that the thickness is approximately 69 nm.

NOTE: If you need a more accurate result, you need the average of more adjacent fringes (4, 6, 8, and so on). If more fringes are used, the result must be multiplied by the number of fringes used.

CHAPTER 4 MAKE AND EDIT SAMPLE INFORMATION

4.1 Introduction

This chapter gives information about how to make sample files which are used to keep information about semiconductor epitaxial layer structures. Sample files are necessary for the results and simulate functions. The chapter is divided into 4 independent parts, 1 for each of the main materials combinations supported by AMASS.

These are the demonstrations samples:

- 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.
- Sample D: An InGaN layer on GaN substrate (or buffer layer) with a-plane orientation

For each sample, the default substrate and layer must be set and the sample file must be made.

For samples B and C, layer linking procedures are also given.

4.2 Sample A (Si substrate)

This is the sample structure used for the sample file in this example:

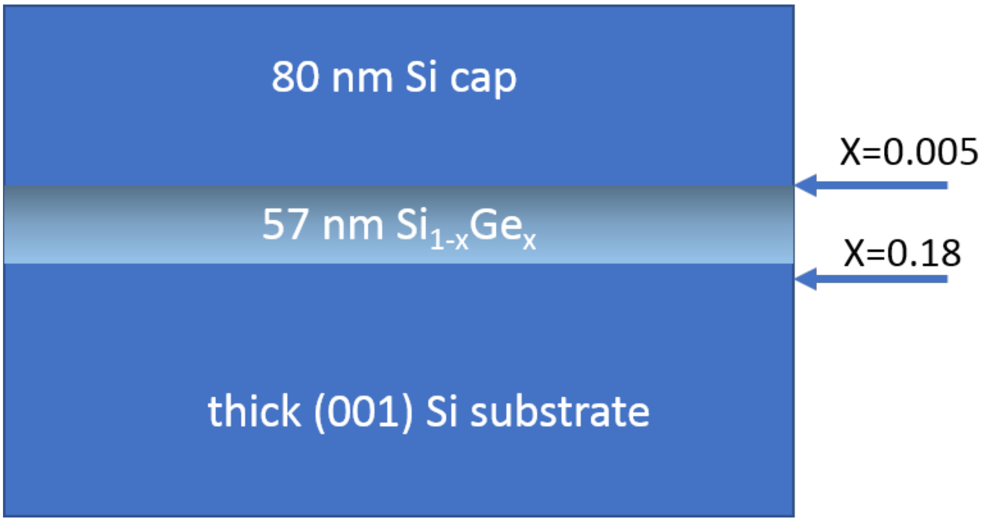
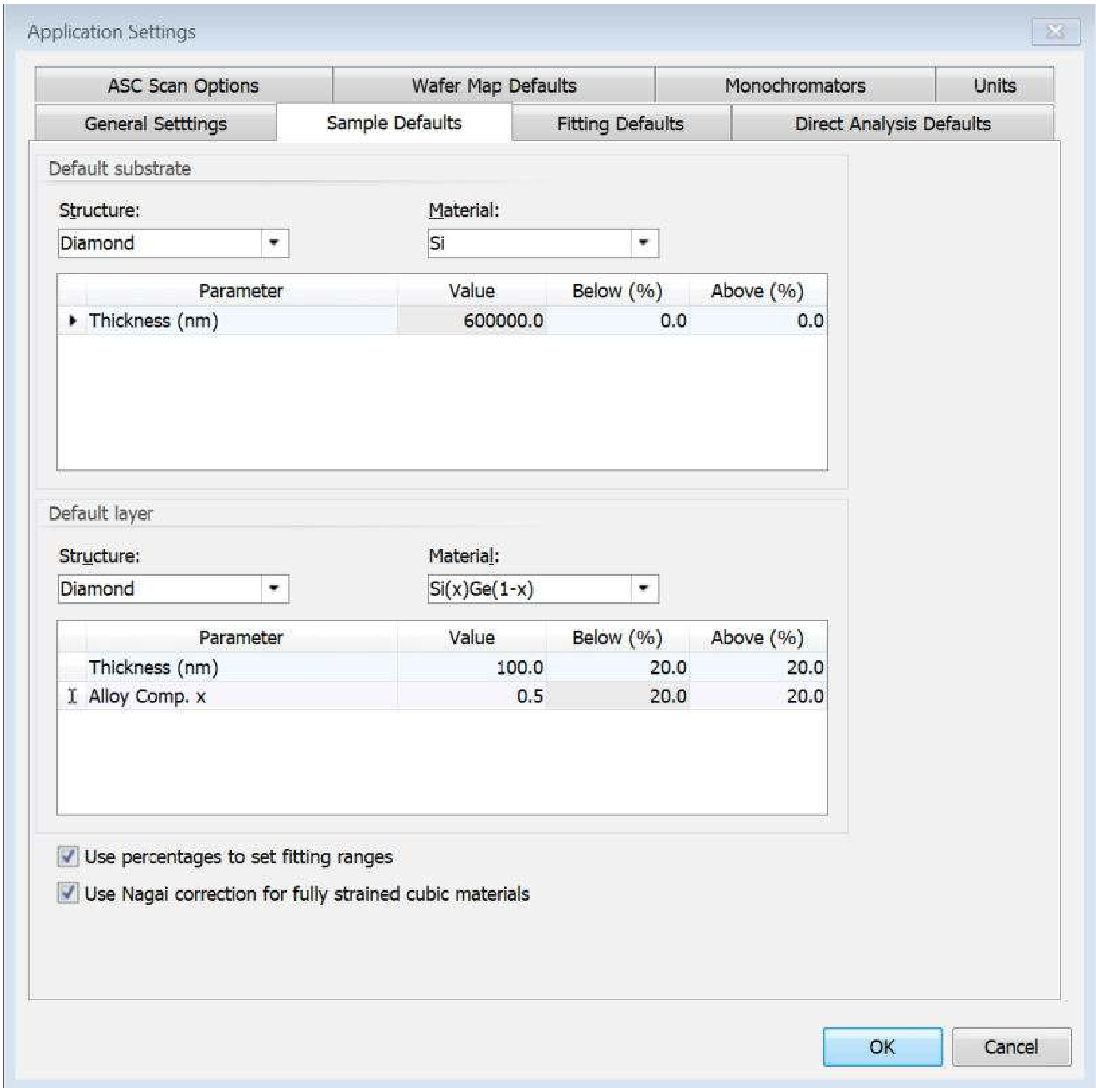


***Figure 4.1** Sample structure*

1. Start AMASS.
2. Go to **View > View as H.R. diffraction**.
3. Set the substrate as follows:
   a. Go to **Settings > Application Settings**.
   b. Go to the **Sample Defaults** tab.
   c. In the **Default substrate** frame, select **Diamond** from the **Structure** drop-down list.

   d. In the **Default substrate** frame, select **Si** from the **Material** drop-down list. The list only contains materials that are part of the chosen structure type.

4. Set the layer as follows:
   a. In the **Default layer** frame, select **Diamond** from the **Structure** drop-down list.
   b. In the **Default layer** frame, select **Si(x)Ge(1-x)** from the **Material** drop-down list.
   c. If applicable, change the default values for thickness and composition.
   d. If applicable, select the **Use percentages to set fitting ranges** check box. When this check box is selected, you can change the percentage values that will be used to set the fitting ranges.



Default substrate

Structure: Diamond

Material: Si

Parameter	Value	Below (%)	Above (%)
Thickness (nm)	600000.0	0.0	0.0

Default layer

Structure: Diamond

Material: Si(x)Ge(1-x)

Parameter	Value	Below (%)	Above (%)
Thickness (nm)	100.0	20.0	20.0
Alloy Comp. x	0.5	20.0	20.0

☑ Use percentages to set fitting ranges

☑ Use Nagai correction for fully strained cubic materials

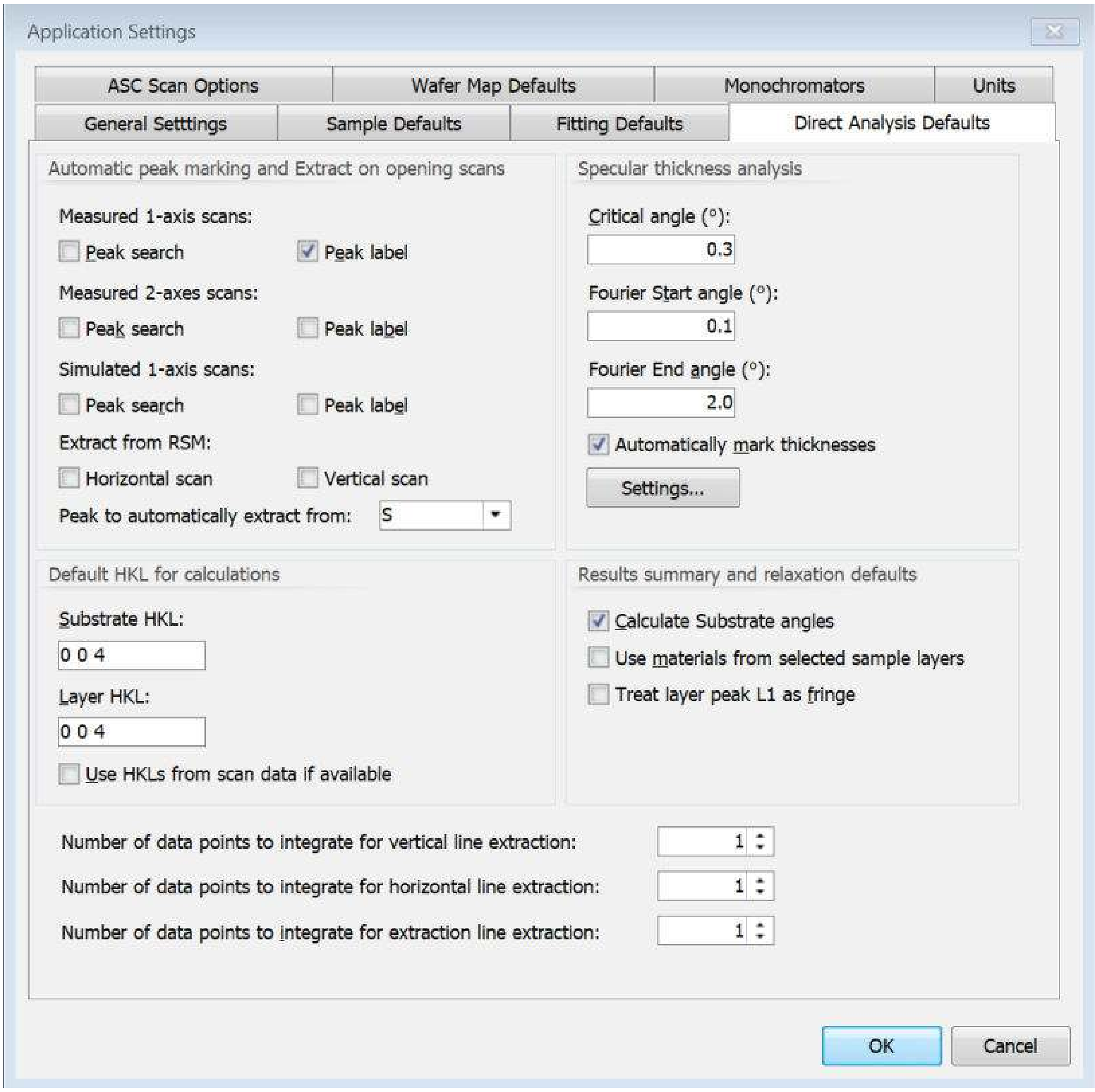
Figure 4.2 *Sample defaults for GeSi layer*

   e. Go to the **Direct Analysis Defaults** tab.
   f. In the **Substrate HKL** field, enter "0 0 4".

   NOTE: Make sure that you enter the value as 0, space, 0, space, 4.

g. In the **Layer HKL** field, enter "0 0 4"

NOTE: Make sure that you enter the value as 0, space, 0, space, 4.



Automatic peak marking and Extract on opening scans

Measured 1-axis scans:
☐ Peak search ☑ Peak label

Measured 2-axes scans:
☐ Peak search ☐ Peak label

Simulated 1-axis scans:
☐ Peak search ☐ Peak label

Extract from RSM:
☐ Horizontal scan ☐ Vertical scan

Peak to automatically extract from: S

Specular thickness analysis

Critical angle (°): 0.3

Fourier Start angle (°): 0.1

Fourier End angle (°): 2.0

☑ Automatically mark thicknesses

Default HKL for calculations

Substrate HKL: 0 0 4

Layer HKL: 0 0 4

☐ Use HKLs from scan data if available

Results summary and relaxation defaults

☑ Calculate Substrate angles
☐ Use materials from selected sample layers
☐ Treat layer peak L1 as fringe

Number of data points to integrate for vertical line extraction: 1

Number of data points to integrate for horizontal line extraction: 1

Number of data points to integrate for extraction line extraction: 1

Figure 4.3 Direct Analysis Defaults tab

5. Click **OK** to save the settings and close the window.
6. Go to **Sample > New Sample**. At the bottom of the screen, the **New Sample Editor** tab opens with the default material of the substrate.
7. Add the first layer:
    a. In the **Layers** pane, click **Add Layer**.
    b. In the **Layer Details** pane, expand **Grading Details**.
    c. In the **Grading Type** field, select **Linear**.
    d. In the **No. of Laminae** field, enter "5".
    e. In the **Value (x)** field of **Top Alloy Comp. x Details**, enter "0.995".
    f. In the **Value (x)** field of **Bottom Alloy Comp. x Details**, enter "0.82".
    g. In the **Value (nm)** field of **Thickness Details**, enter "57".

8. Add the second layer:
    a. In the **Layers** pane, click **Add Layer**.
    b. In the **Material** column, select **Si [Diamond]** from the drop-down list
    c. In the **Thickness (nm)** column, enter "8".
9. Save the sample:
    a. Go to **Sample > Save Sample As**.
    b. In the **File name** field, enter "Sample A.asamxl".
    c. Click **Save**.

4.3 Sample B (InP substrate)

This is the sample structure used for the sample file in this example:

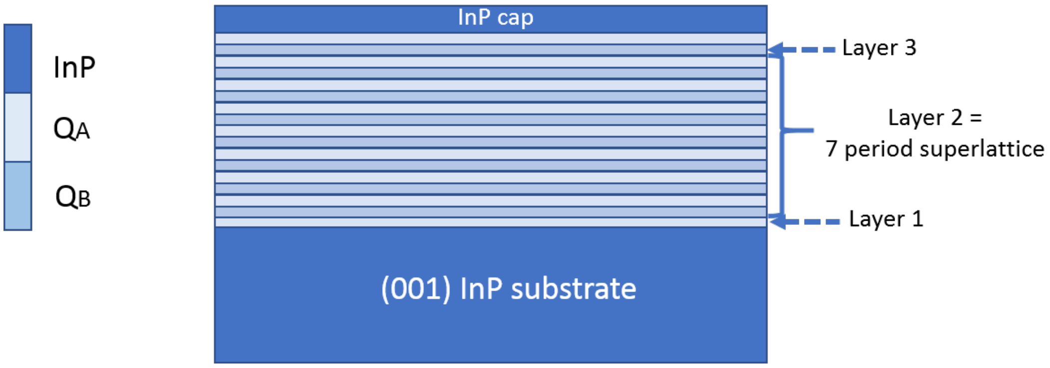


Figure 4.4 Device structure with 7 quantum wells on InP

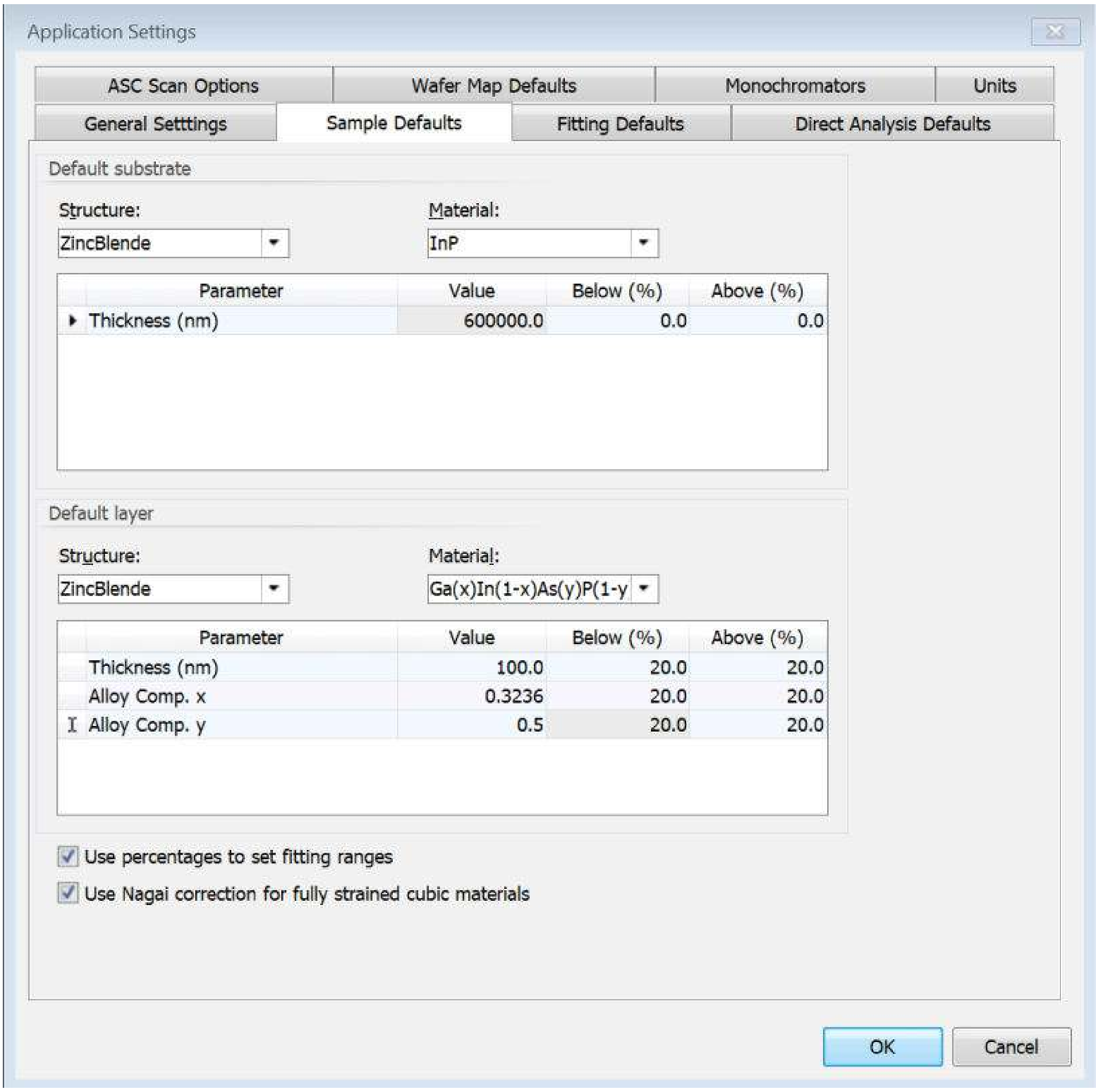
The sample has an (001) indium phosphide substrate and capping layer, with alternating layers of 2 different compositions of indium gallium phosphide arsenide ($Ga_xIn_{(1-x)}As_yP_{(1-y)}$). The x-values and y-values for the 2 quaternaries are: Q_A x=0.3236, y=0.5000; Q_B x=0.196, y=0.8000. To make the sample model, the sample must be divided into layers as shown on the right side of the figure.

Table 4.1 Layer thicknesses in microns

Layer	Material	Thickness
0	InP	250000
1	Q_A	10
2	7 periods	147
2.0	Q_B	7
2.1	Q_A	14
3	Q_B	7
4	Q_A	10
5	InP	100

1. Set the substrate as follows:
    a. Go to **Settings > Application Settings**.
    b. Go to the **Sample Defaults** tab.
    c. In the **Default substrate** frame, select **ZincBlende** from the **Structure** drop-down list.

   d. In the **Default substrate** frame, select **InP** from the **Material** drop-down list. The list only contains materials that are part of the chosen structure type.
   e. In the **Value** column of the **Thickness (nm)** row, enter "250000" (necessary for layer 0).
2. Set the layer as follows:
   a. In the **Default layer** frame, select **ZincBlende** from the **Structure** field.
   b. In the **Default layer** frame, select **Ga(x)In(1-x)As(y)P(1-y)** from the **Material** field.
   c. In the **Value** column of the **Thickness (nm)** row, enter 10" (necessary for layers 1 and 4).
   d. In the **Value** column of the **Alloy Comp. x** row, enter "0.3236" for the fraction of Ga.
   e. In the **Value** column of the **Alloy Comp. y** row, enter "0.5" for the fraction of As.
   f. If applicable, select the **Use percentages to set fitting ranges** check box. When this check box is selected, you can change the percentage values that will be used to set the fitting ranges.



Default substrate

Structure: ZincBlende

Material: InP

Parameter	Value	Below (%)	Above (%)
Thickness (nm)	600000.0	0.0	0.0

Default layer

Structure: ZincBlende

Material: Ga(x)In(1-x)As(y)P(1-y

Parameter	Value	Below (%)	Above (%)
Thickness (nm)	100.0	20.0	20.0
Alloy Comp. x	0.3236	20.0	20.0
Alloy Comp. y	0.5	20.0	20.0

☑ Use percentages to set fitting ranges

☑ Use Nagai correction for fully strained cubic materials

Figure 4.5 *Sample Defaults tab*

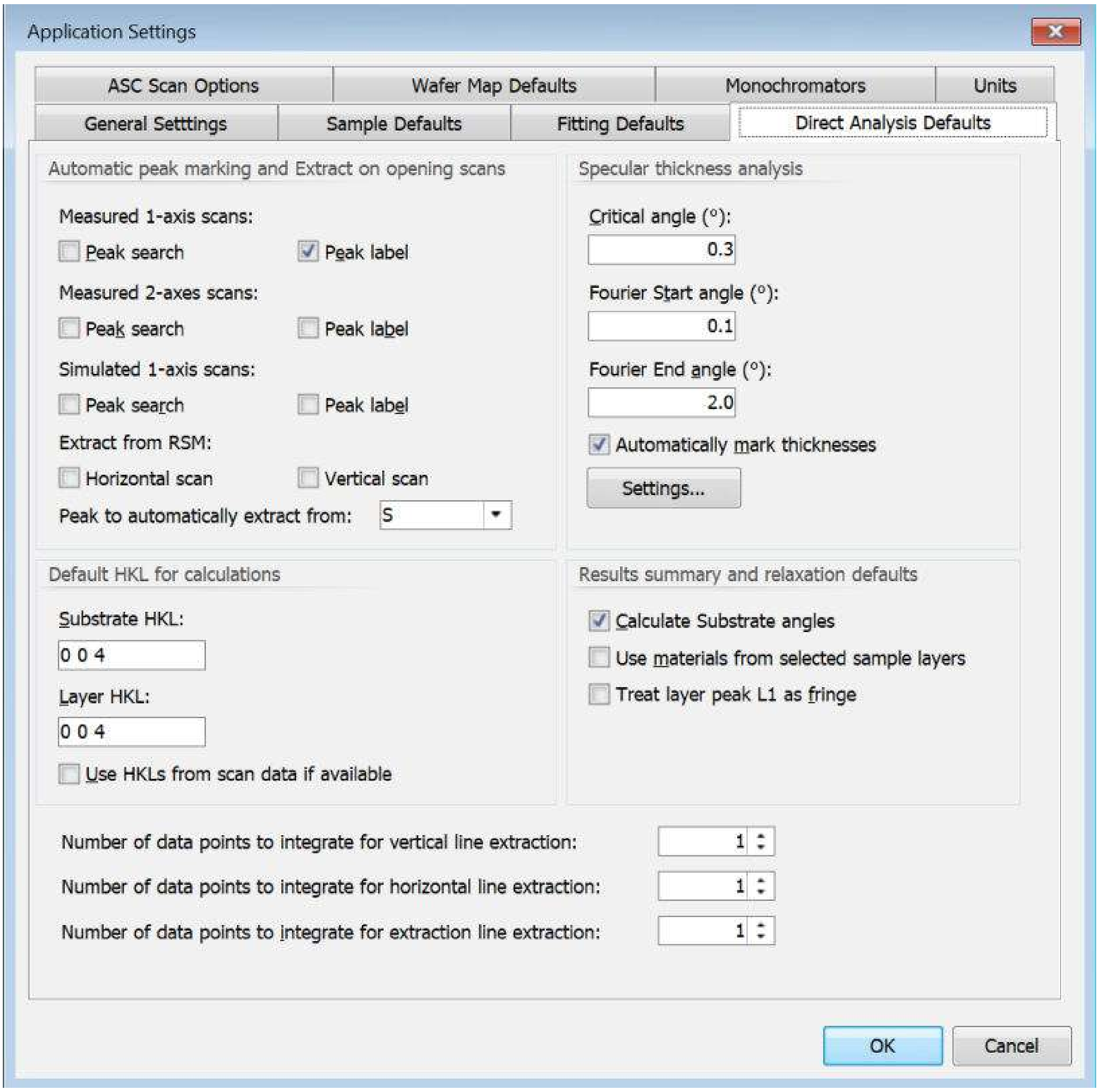
   g. Go to the **Direct Analysis Defaults** tab.

h. In the **Substrate HKL** field, enter "0 0 4".

   NOTE: Make sure that you enter the value as 0, space, 0, space, 4.

i. In the **Layer HKL** field, enter "0 0 4".

   NOTE: Make sure that you enter the value as 0, space, 0, space, 4.



Automatic peak marking and Extract on opening scans

Measured 1-axis scans:
☐ Peak search ☑ Peak label

Measured 2-axes scans:
☐ Peak search ☐ Peak label

Simulated 1-axis scans:
☐ Peak search ☐ Peak label

Extract from RSM:
☐ Horizontal scan ☐ Vertical scan

Peak to automatically extract from: S

Specular thickness analysis

Critical angle (°): 0.3

Fourier Start angle (°): 0.1

Fourier End angle (°): 2.0

☑ Automatically mark thicknesses

Default HKL for calculations

Substrate HKL: 0 0 4

Layer HKL: 0 0 4

☐ Use HKLs from scan data if available

Results summary and relaxation defaults

☑ Calculate Substrate angles
☐ Use materials from selected sample layers
☐ Treat layer peak L1 as fringe

Number of data points to integrate for vertical line extraction: 1

Number of data points to integrate for horizontal line extraction: 1

Number of data points to integrate for extraction line extraction: 1

Figure 4.6 Direct Analysis Defaults tab

3. Click **OK** to save the settings and close the window.
4. Go to **Sample > New Sample**. At the bottom of the screen, the **New Sample Editor** tab opens with the default material of the substrate.
5. In the **Layers** pane, click **Add Layer** to add layer 1.
6. Add layer 2 as follows:
   a. In the **Layers** pane, click **Add Superlattice**.
   b. Select **Layer No. 2 Superlattice**.
   c. In the **Number of repeats** field of the **Superlattice Details** pane, enter "7".

7. A default zinc blende layer has been entered as the first layer of the superlattice (SL Repeat unit 0). We must add a second layer (SL repeat unit 1) to the superlattice. Do as follows:
    a. Select **SL Repeat Unit 0**.
    b. In the **Layers** pane, click **Add Layer**.
8. Edit the composition and thickness of SL repeat layer 0 and the thickness of SL repeat unit 1:
    a. In the **Thickness (nm)** field of **SL Repeat Unit 0**, enter "7".
    b. In the **Alloy Comp. x** field, enter "0.196" for Ga.
    c. In the **Alloy Comp. y** field, enter "0.5" for As.
    d. In the **Thickness (nm)** field of **SL Repeat Unit 1**, enter "14".
9. Use copy and paste to add layer 3 and layer 4 as they are the same as layer 2.0 and layer 1:
    a. Right-click **Rep. Unit No. 0** and select **Copy Layer**.
    b. Right-click **Layer No. 2** and select **Paste as Next Layer**.
    c. Right-click **Layer No. 1** and select **Copy Layer**.
    d. Right-click **Layer No. 3** and select **Paste as Next Layer**.
10. Add InP cap as layer 5:
    a. In the **Layers** pane, click **Add Layer**.
    b. From the **Material** drop-down list, select **InP [ZincBlende]**.
    c. In the **Thickness (nm)** field, enter "100".
11. Save the sample:
    a. Go to **Sample > Save Sample As**.
    b. In the **File name** field, enter "Sample B.asamxl".
    c. Click **Save**.

4.3.1 Set up links

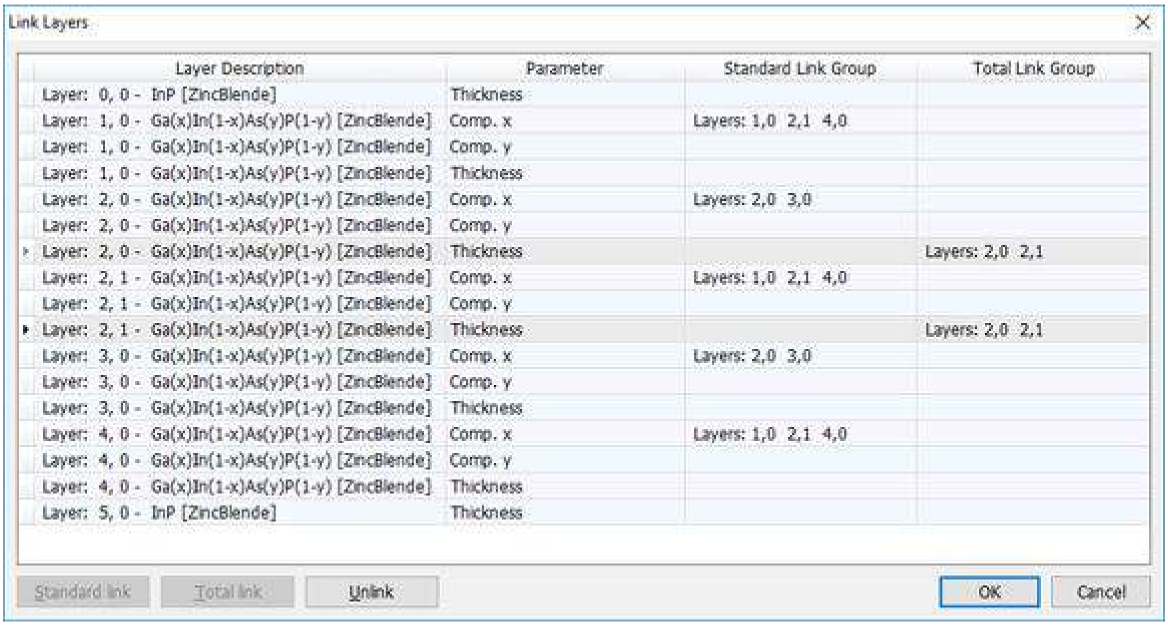
These links will be set up for this sample:

- Standard links between compositions x of all the layers of composition Q_A.
- Standard links between compositions x of all the layers of composition Q_B.
- Total link for the layer thickness of layers 2.0 and 2.1.

When these links have been set up, the Ga composition x of all the Q_A layers and all the Q_B layers will all change together when one of the layers is edited. The combined thickness of layers 2.0 and 2.1 will stay constant when the thickness of either layer is edited. These links are saved in the sample file and will be active when edited manually and when automatic fitting is used.

1. In the **Layers** pane, click **Link layers**.
2. Press **Ctrl** and then select these layers:
    - **Layer: 1, 0 Comp. x**
    - **Layer: 2, 1 Comp. x**
    - **Layer: 4, 0 Comp. x**
3. Click **Standard link** to make a link between these layers.
4. Select these layers:
    - **Layer: 2, 0 Comp. x**
    - **Layer: 3, 0 Comp. x**

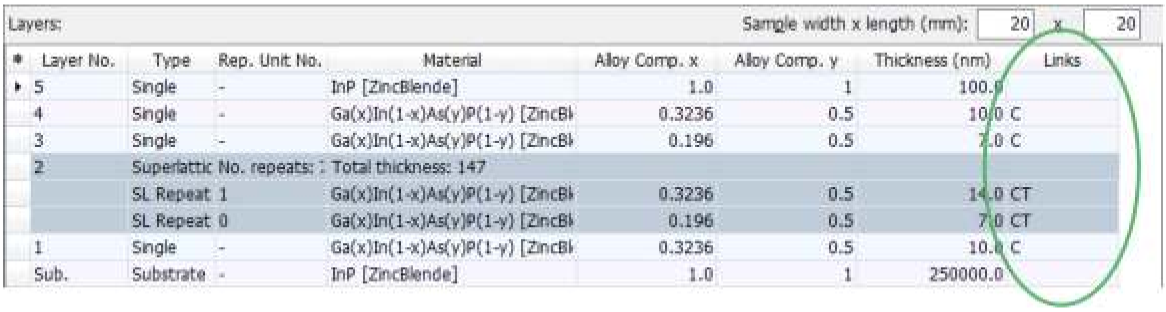
5. Click **Standard link**.
6. Select these layers:
   - **Layer: 2, 0 Thickness**
   - **Layer: 2, 1 Thickness**
7. Click **Total link**.



Layer Description	Parameter	Standard Link Group	Total Link Group
Layer: 0, 0 - InP [ZincBlende]	Thickness		
Layer: 1, 0 - Ga(x)In(1-x)As(y)P(1-y) [ZincBlende]	Comp. x	Layers: 1,0 2,1 4,0	
Layer: 1, 0 - Ga(x)In(1-x)As(y)P(1-y) [ZincBlende]	Comp. y		
Layer: 1, 0 - Ga(x)In(1-x)As(y)P(1-y) [ZincBlende]	Thickness		
Layer: 2, 0 - Ga(x)In(1-x)As(y)P(1-y) [ZincBlende]	Comp. x	Layers: 2,0 3,0	
Layer: 2, 0 - Ga(x)In(1-x)As(y)P(1-y) [ZincBlende]	Comp. y		
Layer: 2, 0 - Ga(x)In(1-x)As(y)P(1-y) [ZincBlende]	Thickness		Layers: 2,0 2,1
Layer: 2, 1 - Ga(x)In(1-x)As(y)P(1-y) [ZincBlende]	Comp. x	Layers: 1,0 2,1 4,0	
Layer: 2, 1 - Ga(x)In(1-x)As(y)P(1-y) [ZincBlende]	Comp. y		
Layer: 2, 1 - Ga(x)In(1-x)As(y)P(1-y) [ZincBlende]	Thickness		Layers: 2,0 2,1
Layer: 3, 0 - Ga(x)In(1-x)As(y)P(1-y) [ZincBlende]	Comp. x	Layers: 2,0 3,0	
Layer: 3, 0 - Ga(x)In(1-x)As(y)P(1-y) [ZincBlende]	Comp. y		
Layer: 3, 0 - Ga(x)In(1-x)As(y)P(1-y) [ZincBlende]	Thickness		
Layer: 4, 0 - Ga(x)In(1-x)As(y)P(1-y) [ZincBlende]	Comp. x	Layers: 1,0 2,1 4,0	
Layer: 4, 0 - Ga(x)In(1-x)As(y)P(1-y) [ZincBlende]	Comp. y		
Layer: 4, 0 - Ga(x)In(1-x)As(y)P(1-y) [ZincBlende]	Thickness		
Layer: 5, 0 - InP [ZincBlende]	Thickness		

Figure 4.7 *Link Layers window*

8. Click **OK**. A new column **Links** is added to the sample table to show which parameters of which layers are linked.



Sample width x length (mm): 20 x 20

Layer No.	Type	Rep. Unit No.	Material	Alloy Comp. x	Alloy Comp. y	Thickness (nm)	Links
5	Single	-	InP [ZincBlende]	1.0	1	100.0	
4	Single	-	Ga(x)In(1-x)As(y)P(1-y) [ZincBl	0.3236	0.5	10.0	C
3	Single	-	Ga(x)In(1-x)As(y)P(1-y) [ZincBl	0.196	0.5	7.0	C
2	Superlattic	No. repeats:	Total thickness: 147				
	SL Repeat	1	Ga(x)In(1-x)As(y)P(1-y) [ZincBl	0.3236	0.5	14.0	CT
	SL Repeat	0	Ga(x)In(1-x)As(y)P(1-y) [ZincBl	0.196	0.5	7.0	CT
1	Single	-	Ga(x)In(1-x)As(y)P(1-y) [ZincBl	0.3236	0.5	10.0	C
Sub.	Substrate	-	InP [ZincBlende]	1.0	1	250000.0	

Figure 4.8 *Sample Data window for Sample B*

9. Save the sample:
   a. Go to **Sample > Save Sample As**.
   b. In the **File name** field, enter "Sample B.asamxl".
   c. Click **Save**.

4.4 Sample C (sapphire substrate)

This is the sample structure used for the sample file in this example:

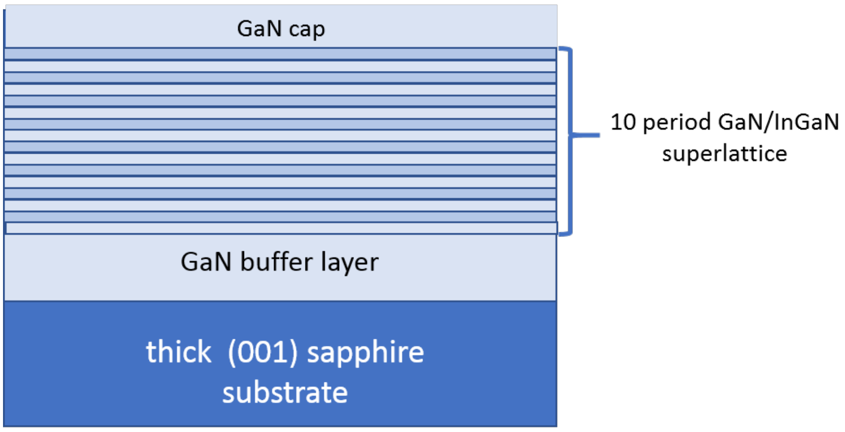
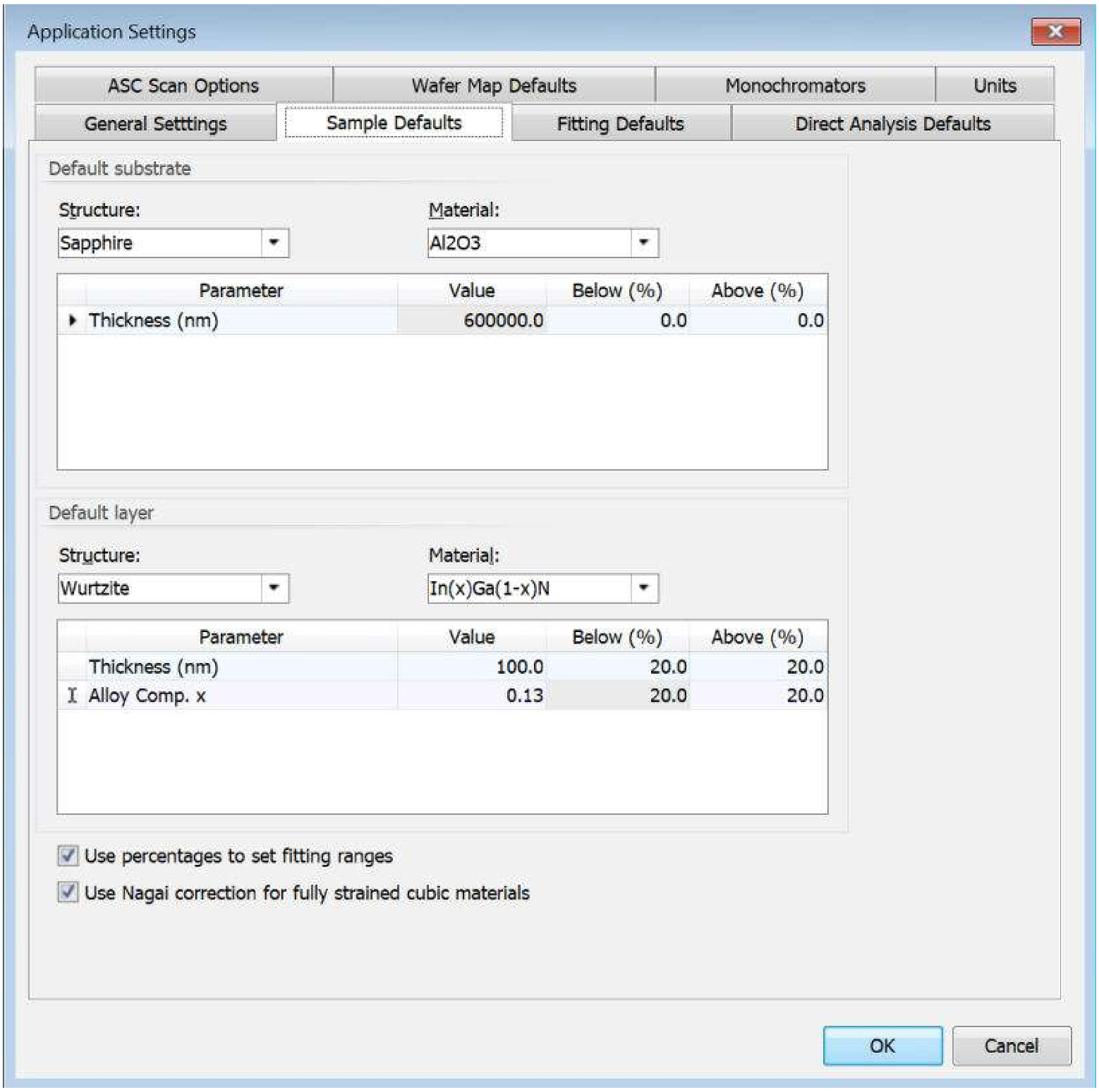


Figure 4.9 Sample with sapphire substrate

For this sample, the interface between the sapphire and the GaN buffer layer is assumed as totally relaxed.

1. Set the substrate as follows:
    a. Go to **Settings > Application Settings**.
    b. Go to the **Sample Defaults** tab.
    c. In the **Default substrate** frame, select **Sapphire** from the **Structure** drop-down list.
    d. In the **Default substrate** frame, select **Al2O3** from the **Material** drop-down list. The list only contains materials that are part of the chosen structure type. In this case, only **Al2O3** is possible.
2. Set the layer as follows:
    a. In the **Default layer** frame, select **Wurtzite** from the **Structure** drop-down list.
    b. In the **Default layer** frame, select **In(x)Ga(1-x)N** from the **Material** drop-down list.
    c. In the **Value** column of the **Thickness (nm)** row, enter "100".
    d. In the **Value** column of **Alloy Comp. x**, enter "0.13".



Default substrate

Structure: Sapphire

Material: Al2O3

Parameter	Value	Below (%)	Above (%)
Thickness (nm)	600000.0	0.0	0.0

Default layer

Structure: Wurtzite

Material: In(x)Ga(1-x)N

Parameter	Value	Below (%)	Above (%)
Thickness (nm)	100.0	20.0	20.0
Alloy Comp. x	0.13	20.0	20.0

☑ Use percentages to set fitting ranges

☑ Use Nagai correction for fully strained cubic materials

Figure 4.10 Sample Defaults tab

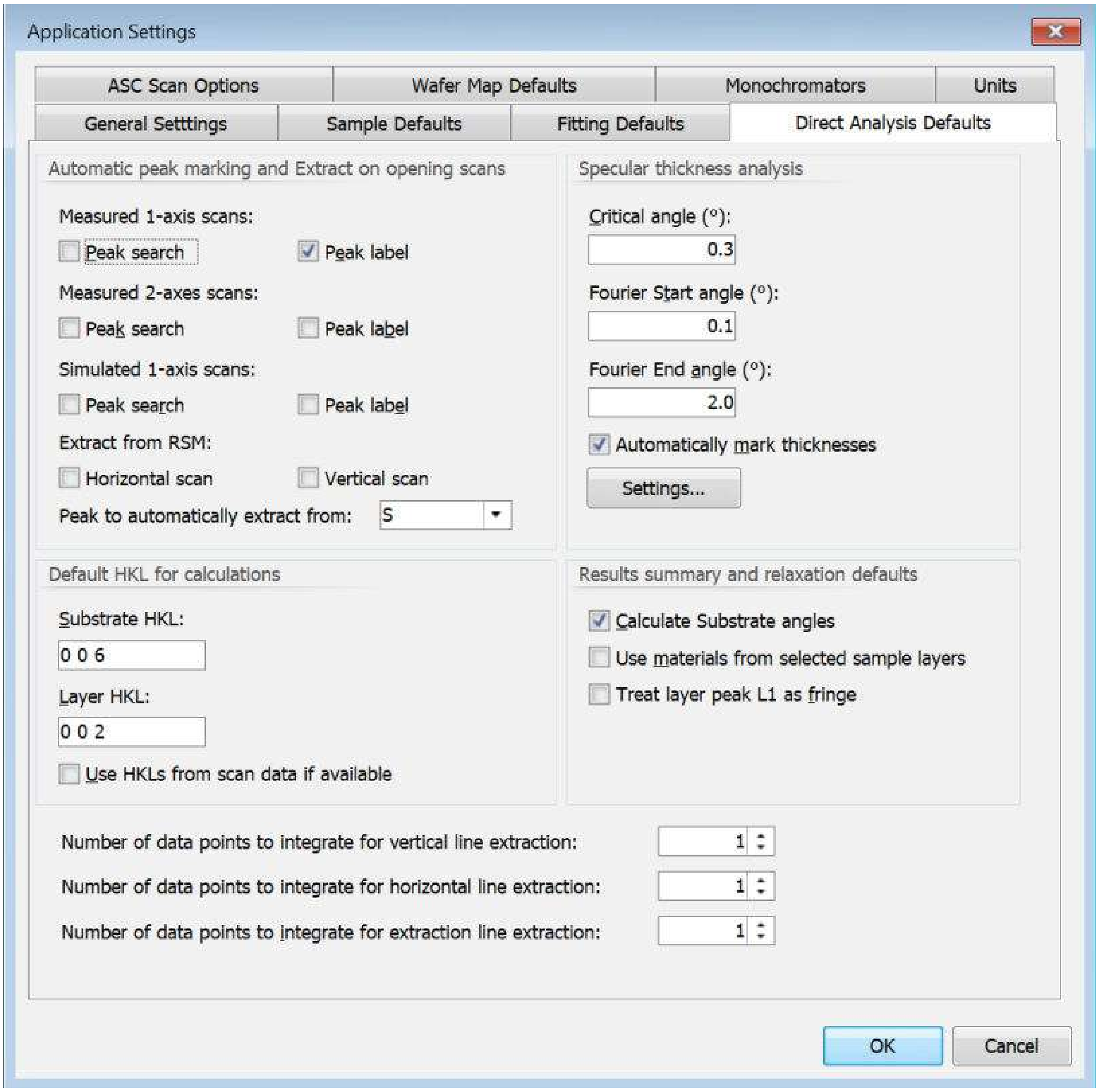
e. Go to the **Direct Analysis Defaults** tab.

f. In the **Substrate HKL** field, enter "0 0 6".

NOTE: Make sure that you enter the value as 0, space, 0, space, 6.

g. In the **Layer HKL** field, enter "0 0 2"

NOTE: Make sure that you enter the value as 0, space, 0, space, 2.



Automatic peak marking and Extract on opening scans

Measured 1-axis scans:
☐ Peak search ☑ Peak label

Measured 2-axes scans:
☐ Peak search ☐ Peak label

Simulated 1-axis scans:
☐ Peak search ☐ Peak label

Extract from RSM:
☐ Horizontal scan ☐ Vertical scan

Peak to automatically extract from: S

Specular thickness analysis

Critical angle (°): 0.3
Fourier Start angle (°): 0.1
Fourier End angle (°): 2.0
☑ Automatically mark thicknesses

Default HKL for calculations

Substrate HKL: 0 0 6
Layer HKL: 0 0 2
☐ Use HKLs from scan data if available

Results summary and relaxation defaults

☑ Calculate Substrate angles
☐ Use materials from selected sample layers
☐ Treat layer peak L1 as fringe

Number of data points to integrate for vertical line extraction: 1
Number of data points to integrate for horizontal line extraction: 1
Number of data points to integrate for extraction line extraction: 1

Figure 4.11 Direct Analysis Defaults tab

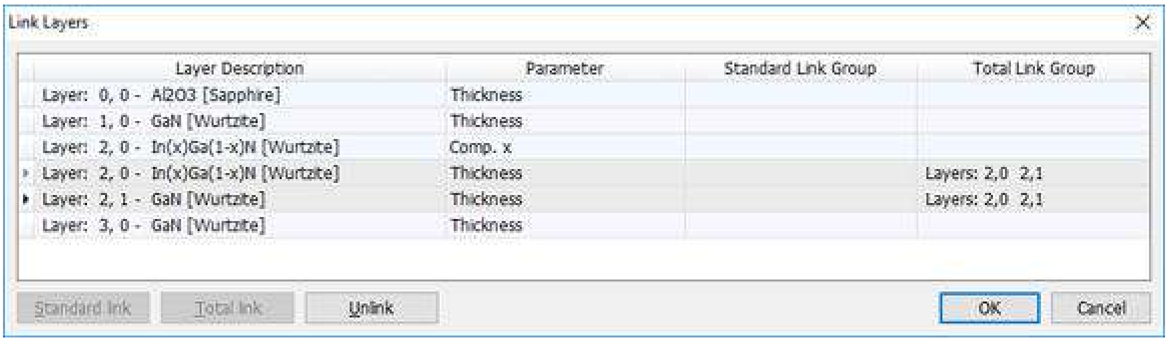
3. Click **OK** to save the settings and close the window.
4. Go to **Sample > New Sample**. At the bottom of the screen, the **New Sample Editor** tab opens with the default material of the substrate.
5. Enter the fully relaxed GaN buffer layer which is 1.5 microns thick:
   a. In the **Layers** pane, click **Add Layer**. A 0.1 micron $In_{0.5}GaN_{0.5}N$ layer is added as we set in the defaults.
   b. From the **Material** drop-down list, select **GaN [Wurtzite]**.
   c. In the **Thickness (nm)** field, enter "1500".
   d. In the **HR Parameters** field of **Layer Details**, click the arrow.
   e. Clear the **Couple Y direction relaxation to X direction** check box.
   f. Click **OK**.
   g. In the **Layer Details** pane, expand **Relaxation Details** and **Relaxation Y Details**.
   h. In the both **Value (%)** fields, enter "100".

6. Enter the superlattice which contains 10 repeats of 2.5 nm of $In_{0.13}$ $Ga_{0.87}N$ plus 7 nm of GaN:
    a. In the **Layers** pane, click **Add Superlattice**.
    b. Select **Layer No. 2**.
    c. In the **Number of repeats** field, enter "10".
7. A default wurtzite layer has been entered as the first layer of the superlattice (layer 2.0). We must add a second layer to the superlattice:
    a. Select **SL Repeat unit 0**.
    b. In the **Layers** pane, click **Add Layer**.
    c. In the **Alloy Comp. x** field of **SL Repeat unit 0**, make sure that "0.13" is shown.
    d. In the **Thickness (nm)** field, enter "2.5".
    e. In the **Relax X, Y(%)** field, enter "0".
    f. From the **Material** drop-down list of **SL Repeat unit 1**, select **GaN [Wurtzite]**.
    g. In the **Thickness (nm)** field, enter "7.0".
    h. In the **Relax (%)** field, enter "0".
8. Add the 50 nm GaN capping layer:
    a. Select **Layer No. 2**.
    b. In the **Layers** pane, click **Add Layer**.
    c. From the **Material** drop-down list, select **GaN [Wurtzite]**.
    d. In the **Thickness (nm)** field, enter "50".
    e. In the **Relax (%)** fields, enter "0".
9. Save the sample:
    a. Go to **Sample > Save Sample As**.
    b. In the **File name** field, enter "Sample C.asamxl".
    c. Click **Save**.

4.4.1 Set up links

For this sample, 1 total link can be added to fix the superlattice period. This link is saved in the sample file and will be active when edited manually and when automatic fitting is used. Refer to Chapter 8.

1. In the **Layers** pane, click **Link layers**.
2. Press `Ctrl` and then select these layers:
    - **Layer: 2, 0 Thickness**
    - **Layer: 2, 1 Thickness**
3. Click **Total link**.



Layer Description	Parameter	Standard Link Group	Total Link Group
Layer: 0, 0 - Al2O3 [Sapphire]	Thickness		
Layer: 1, 0 - GaN [Wurtzite]	Thickness		
Layer: 2, 0 - In(x)Ga(1-x)N [Wurtzite]	Comp. x		
Layer: 2, 0 - In(x)Ga(1-x)N [Wurtzite]	Thickness		Layers: 2,0 2,1
Layer: 2, 1 - GaN [Wurtzite]	Thickness		Layers: 2,0 2,1
Layer: 3, 0 - GaN [Wurtzite]	Thickness		

Figure 4.12 *Link Layers window*

4. Click **OK**.
5. Save the sample:
    a. Go to **Sample > Save Sample As**.
    b. In the **File name** field, enter "Sample C.asamxl".
    c. Click **Save**.

4.5 Sample D (a-plane GaN)

This is the sample structure used for the sample file in this example:

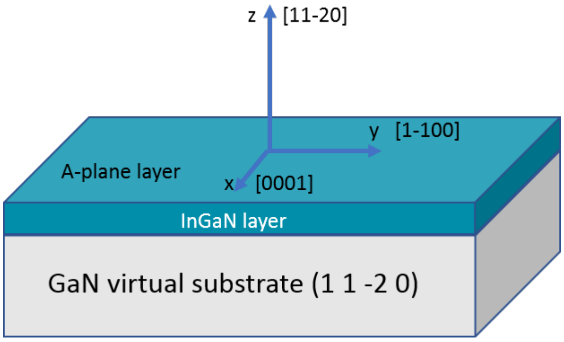
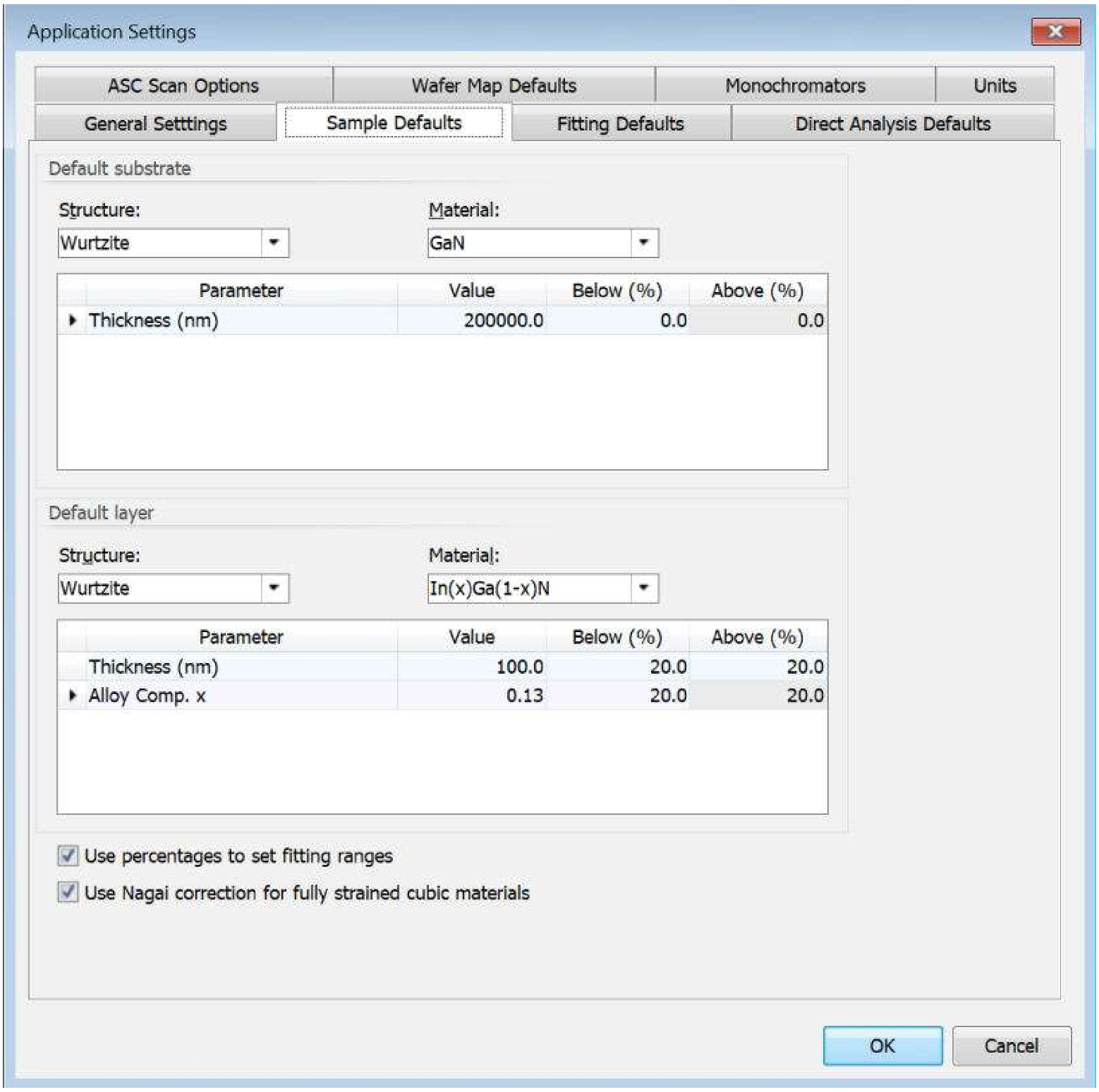


Figure 4.13 *A-plane GaN sample*

For this sample the relaxation along the x-directions and y-directions are different. The sample substrate is a GaN virtual substrate. It is assumed to be equivalent to a totally relaxed buffer layer on any substrate. A single partially relaxed InGaN layer is on top of the GaN.

1. Set the substrate as follows:
    a. Go to **Settings > Application Settings**.
    b. Go to the **Sample Defaults** tab.
    c. In the **Default substrate** frame, select **Wurtzite** from the **Structure** drop-down list.
    d. In the **Default substrate** frame, select **GaN** from the **Material** drop-down list. The list only contains materials that are part of the chosen structure type.
    e. In the **Value** column of the **Thickness (nm)** row, enter "200000".
2. Set the layer as follows:
    a. In the **Default layer** frame, select **Wurtzite** from the **Structure** drop-down list.
    b. In the **Default layer** frame, select **In(x)Ga(1-x)N** from the **Material** drop-down list.
    c. In the **Value** column of the **Thickness (nm)** row, enter "100".



Default substrate

Structure: Wurtzite

Material: GaN

Parameter	Value	Below (%)	Above (%)
Thickness (nm)	200000.0	0.0	0.0

Default layer

Structure: Wurtzite

Material: In(x)Ga(1-x)N

Parameter	Value	Below (%)	Above (%)
Thickness (nm)	100.0	20.0	20.0
Alloy Comp. x	0.13	20.0	20.0

☑ Use percentages to set fitting ranges

☑ Use Nagai correction for fully strained cubic materials

Figure 4.14 Sample Defaults tab

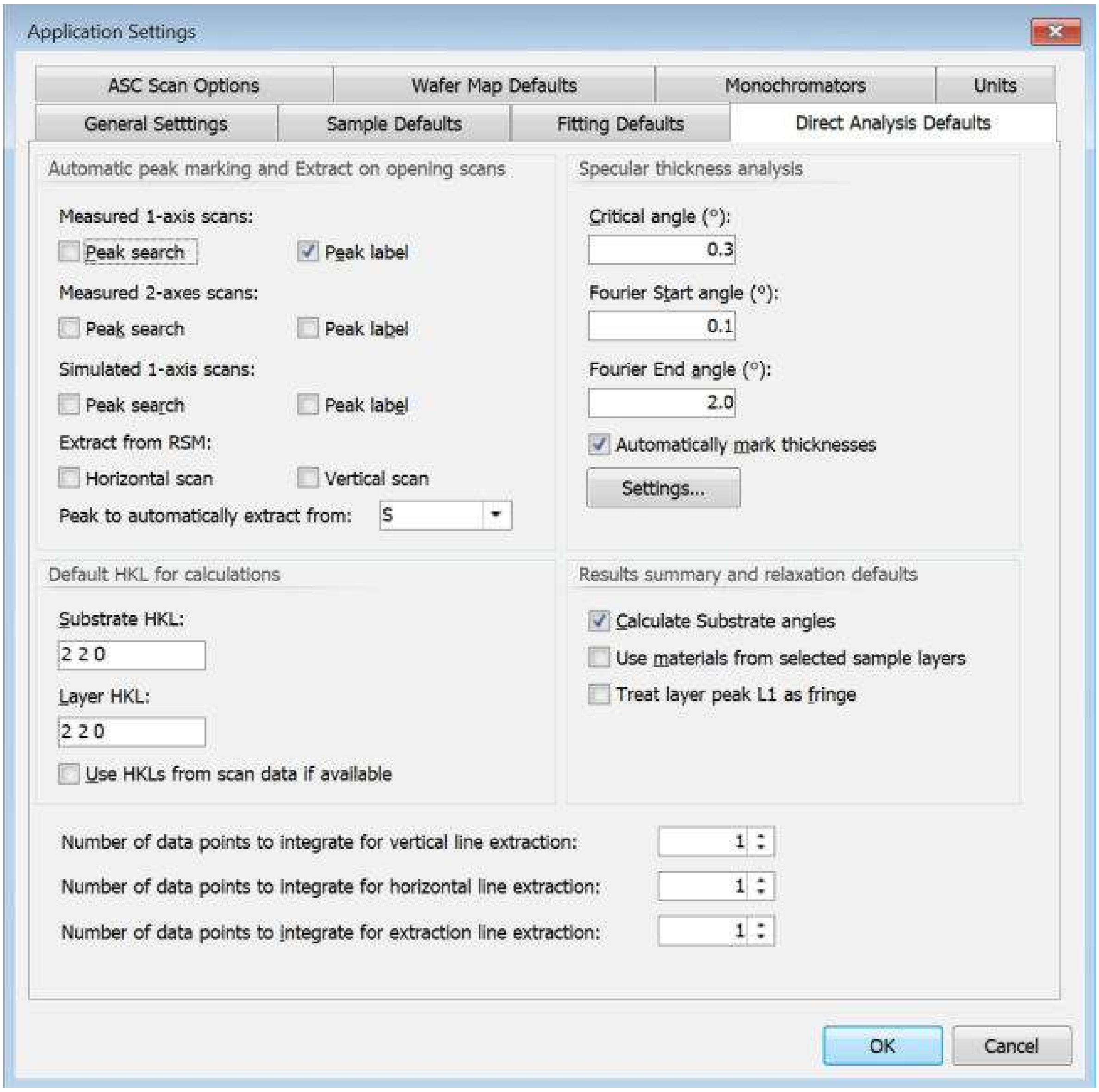
d. Go to the **Direct Analysis Defaults** tab.

e. In the **Substrate HKL** field, enter "2 2 0".

NOTE: Make sure that you enter the value as 2, space, 2, space, 0.

f. In the **Layer HKL** field, enter "2 2 0"

NOTE: Make sure that you enter the value as 2, space, 2, space, 0.



Automatic peak marking and Extract on opening scans

Measured 1-axis scans:
☐ Peak search ☑ Peak label

Measured 2-axes scans:
☐ Peak search ☐ Peak label

Simulated 1-axis scans:
☐ Peak search ☐ Peak label

Extract from RSM:
☐ Horizontal scan ☐ Vertical scan

Peak to automatically extract from: S

Specular thickness analysis

Critical angle (°): 0.3

Fourier Start angle (°): 0.1

Fourier End angle (°): 2.0

☑ Automatically mark thicknesses

Default HKL for calculations

Substrate HKL: 2 2 0

Layer HKL: 2 2 0

☐ Use HKLs from scan data if available

Results summary and relaxation defaults

☑ Calculate Substrate angles
☐ Use materials from selected sample layers
☐ Treat layer peak L1 as fringe

Number of data points to integrate for vertical line extraction: 1

Number of data points to integrate for horizontal line extraction: 1

Number of data points to integrate for extraction line extraction: 1

Figure 4.15 Direct Analysis Defaults tab

3. Click **OK** to save the settings and close the window.
4. Go to **Sample > New Sample**. At the bottom of the screen, the **New Sample Editor** tab opens with the default material of the substrate. The default substrate is wurtzite, the default material is GaN and the default thickness is 2.0000000.
5. In the **HR Parameters** field of **Layer Details**, click the arrow.
6. In the **Primary HKL or nearest surface normal direction** field, enter "1 1 0".

   NOTE: Make sure that you enter the value as 1, space, 1, space, 0.

7. In the **Simulation reflection (HKL)** field, enter "2 2 0".

   NOTE: Make sure that you enter the value as 2, space, 2, space, 0.

8. Click **OK**.
9. In the **Layers** pane, click **Add Layer**.
10. From the **Material** drop-down list, select **In(x)Ga(1-x)N [Wurtzite]**.

11. In the **Alloy Comp. x** field, enter "0.1".
12. In the **HR Parameters** field of **Layer Details**, click the arrow.
13. In the **Primary HKL or nearest surface normal direction** field, enter "1 1 0".

    NOTE: Make sure that you enter the value as 1, space, 1, space, 0.

14. In the **Perpendicular distortion calculation** field, select **Hexagonal a plane**.
15. Clear the **Couple Y direction relaxation to X direction** check box.
16. In the **Simulation reflection (HKL)** field, enter "2 2 0".

    NOTE: Make sure that you enter the value as 2, space, 2, space, 0.

17. Click **OK**.
18. In the **Layer Details** pane, expand **Relaxation Details**.
19. In the **Value (%)** field, enter "50" for the relaxation of the 0001 planes.
20. In the **Layer Details** pane, expand **Relaxation Y Details**.
21. In the **Value (%)** field, enter "40" for the relaxation of the 1-100 planes.
22. Save the sample:
    a. Go to **Sample > Save Sample As**.
    b. In the **File name** field, enter "Sample D.asamxl".
    c. Click **Save**.

CHAPTER 5 USE GRAPHICS WITH AREA SCANS

5.1 Introduction

This chapter gives 3 examples on how to manipulate area scan data. The files used in the examples are recorded from layered materials.

The first example uses data collected from a sample which has a layer of SBTN (=$SrBi_2(Ta_{0.7}Nb_{0.3})_2O_9$) on a (100) Si substrate coated with layers of silicon dioxide, titanium and platinum. We will project a 2theta-omega/chi map as a powder scan.

The second and third examples use data collected from a sample which has an InGaAs/GaAs superlattice on a gallium arsenide (GaAs) substrate. We will merge 2 area scans and find the average composition of the superlattice and the parallel mismatch between the superlattice and substrate from the merged reciprocal space map.

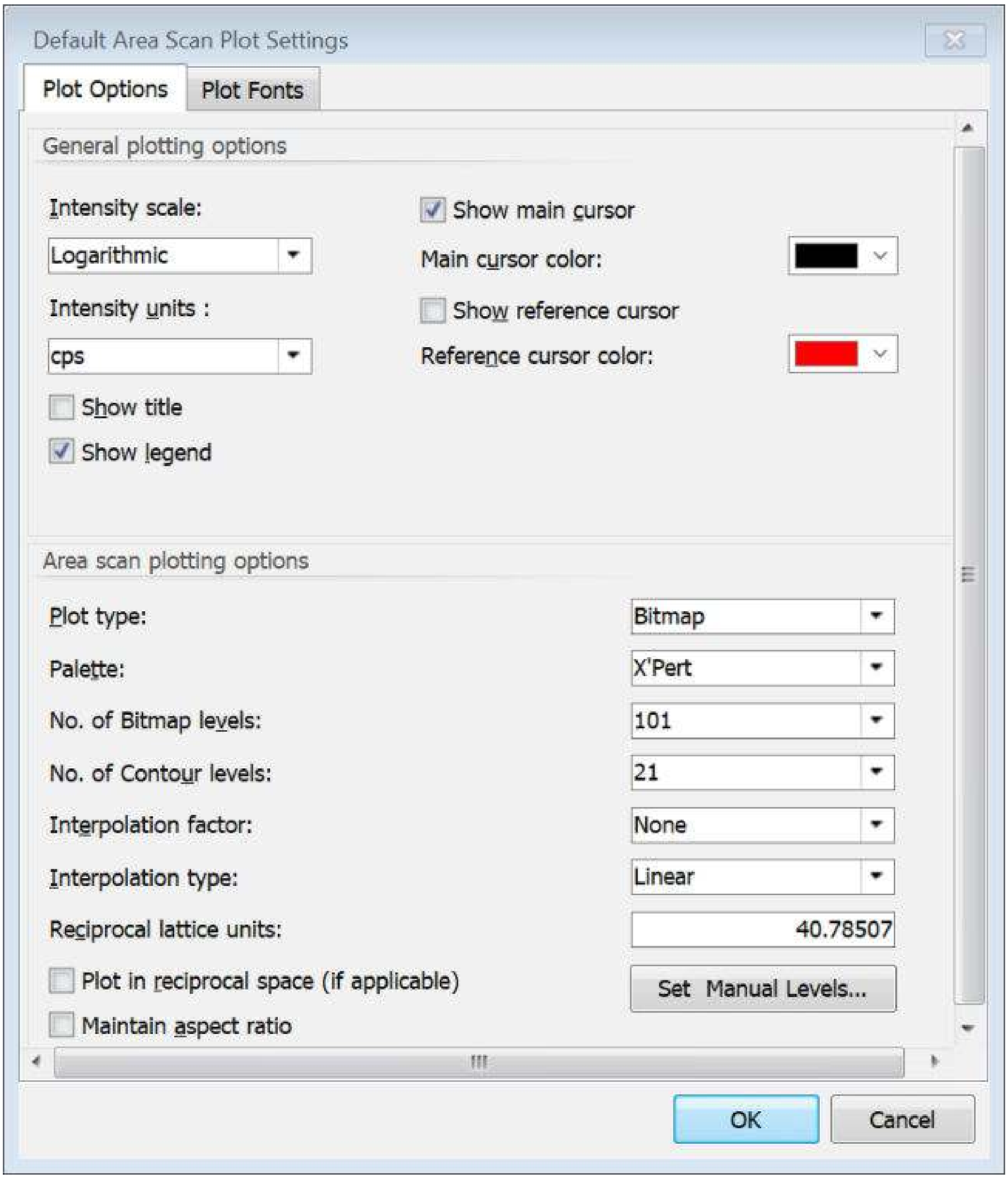
5.2 Project an area scan

This section gives information about how to select plot options for an area scan and how to project a scan. The data used is file "SBTN fibre.A00". [1]

1. Start AMASS.
2. Go to **Settings > Default Area Scan Plot Settings**.
3. Use these settings:

---

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



Intensity scale: Logarithmic

Intensity units : cps

☐ Show title

☑ Show legend

☑ Show main cursor

Main cursor color: ■

☐ Show reference cursor

Reference cursor color: 🟥

Plot type: Bitmap

Palette: X'Pert

No. of Bitmap levels: 101

No. of Contour levels: 21

Interpolation factor: None

Interpolation type: Linear

Reciprocal lattice units: 40.78507

☐ Plot in reciprocal space (if applicable)

☐ Maintain aspect ratio

Figure 5.1 Default Area Scan Plot Settings window

4. Go to **File > Open Scan(s)**.
5. Go to **C:\Users\User.Name\Documents\PANalytical\AMASS\Examples**.
6. Select "SBTN fibre.A00".
7. Click **Open**.

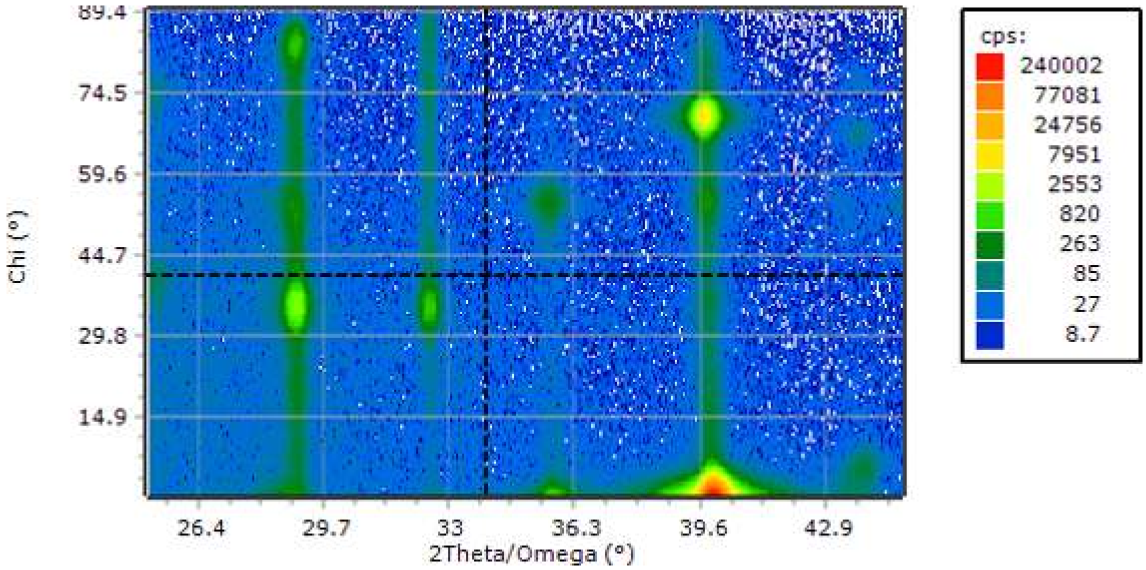


Figure 5.2 SBTN fibre.A00 plotted in absolute degrees

This area map is a set of 2theta-omega scans recorded for chi values between 0 and 90 degrees. The thin film has a fiber texture. The intensity for each reflection is divided along vertical lines in the plot. When all the intensity is projected onto the horizontal axis, a 2theta-omega scan is made which would be recorded from a polycrystalline sample of the same material. This scan can be used to examine the phases.

8. Go to **Tools > 2-axes Scan Tools > Project to X Axis** to project the map. The projected scan is in the next available graph that contains 1-axis data. The scan name is "SBTN fibre_PROJ_#1.ascnxl".

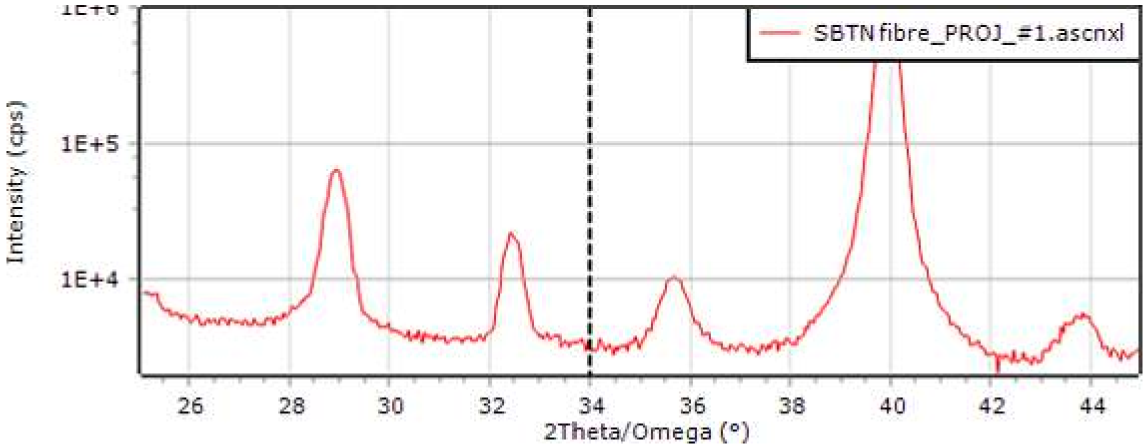
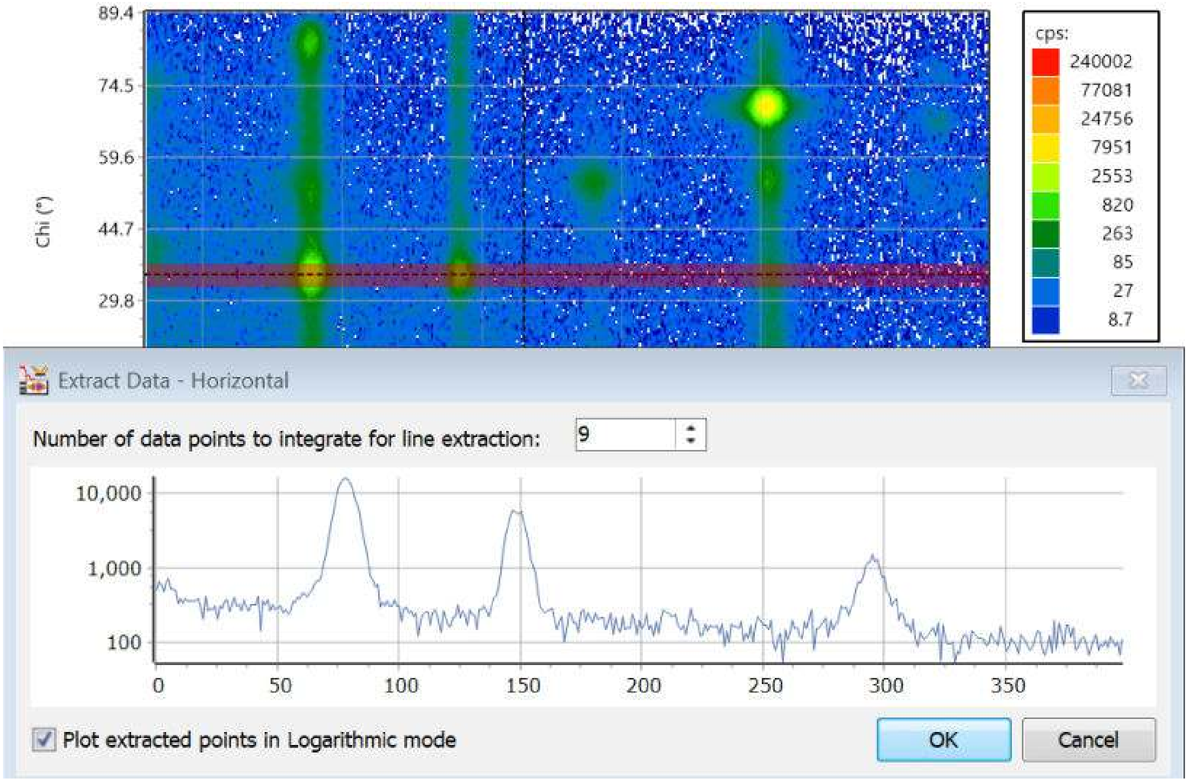


Figure 5.3 Projected scan with logarithmic intensity scaling

The projected data is not automatically saved. You can save it with a project or as a single scan.

9. To extract integrated vertical or horizontal scans from an area map, do as follows:
   a. In the **Scan List** pane, select the map.
   b. Move the cursor line to the line of interest. If the cursor line is not shown, click .
   c. Go to **Tools > 2-axes Scan Tools > Extract Horizontal Scan** or **Tools > 2-axes Scan Tools > Extract Vertical Scan**.
   d. Enter the number of data points for the integration. The integration width is shown in the main graph.



Number of data points to integrate for line extraction: 9

☑ Plot extracted points in Logarithmic mode

Figure 5.4 Extract Data - Horizontal window

A preview of the extracted data is shown in the window. If you change the integration width, the shown scan is immediately updated.

e. Click **OK** to confirm the extraction. The data are then added to the next available main graph that contains 1-axis data.

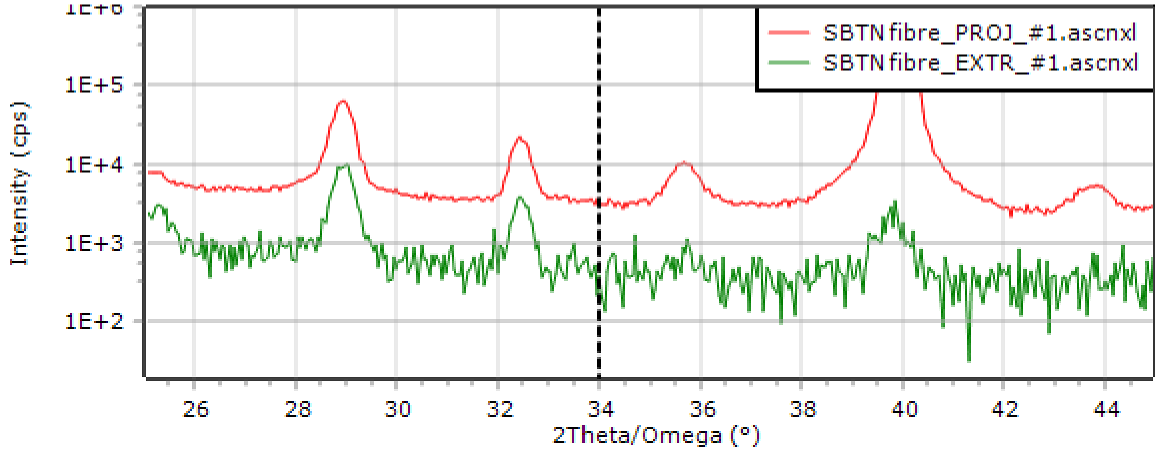
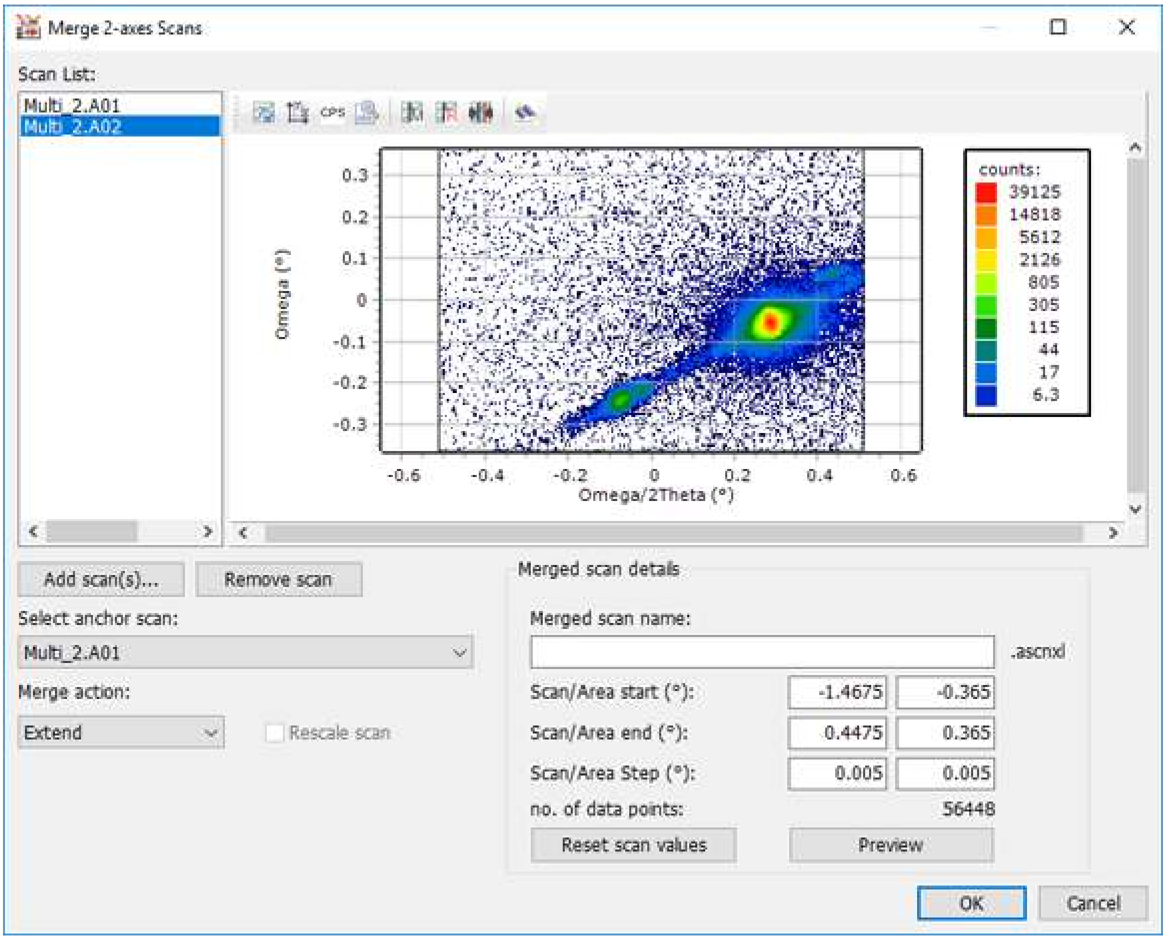


Figure 5.5 Extracted horizontal scan

5.3 Merge area scans

This example gives information about how to merge area scans and then use the merged data to find the parallel mismatch and the average composition of a partially relaxed superlattice on (001) GaAs. The data used are the files "Multi_2.A01" and "Multi_2.A02". These are reciprocal space maps of the (4 4 4) reflection from the InGaAs/GaAs multilayer and the (4 4 4) reflection from the (001) gallium arsenide (GaAs) substrate.

1. Go to **Tools > 2-axes Scan Tools > Merge 2-axes Scans**.
2. Click **Add scan(s)**.
3. Go to **C:\Users\User.Name\Documents\PANalytical\AMASS\Examples**.
4. Select "Multi_2.A01" and "Multi_2.A02".
5. Click **Open**.



Scan List:
Multi_2.A01
Multi_2.A02

Select anchor scan: Multi_2.A01

Merge action: Extend

☐ Rescale scan

Merged scan details

Merged scan name: .ascnxl

Scan/Area start (°): -1.4675 -0.365

Scan/Area end (°): 0.4475 0.365

Scan/Area Step (°): 0.005 0.005

no. of data points: 56448

Figure 5.6 Merge 2-axes Scans window

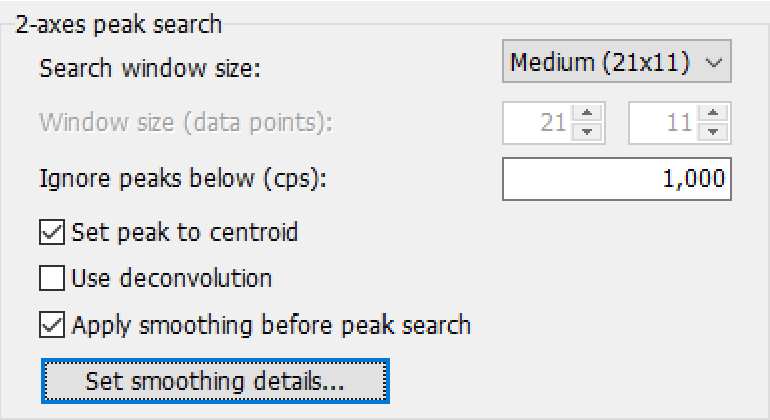
The scans are shown in the **Scan List**. Click on the scan name to toggle between the scans.

6. In the **Merged scan name** field, enter a name for the merged scan.
7. Click **Preview**. The graph shows the merged data.
8. Click **OK** to accept the merged data. The merged data will be loaded to one of the main graphs. The projected data is not automatically saved. You can save it with a project or as scan data.
9. Continue with measure parallel mismatch and average composition of a superlattice. Refer to Section 5.4. Do not close AMASS.

5.4 Measure parallel mismatch and average composition of a superlattice

This example gives information about how to mark and label peaks in an area scan and use the peak positions of the substrate and layer to find the parallel mismatch and the average composition of a superlattice. The data from the previous section is used.

1. Click to open the **Area Scan Plot Settings** window.
2. From the **Plot type** drop-down list, select **Bitmap**.
3. From the **Palette** drop-down list, select **X'Pert**.
4. Select the **Plot in reciprocal space (if applicable)** and **Maintain aspect ratio** check boxes.
5. Click **OK**.
6. Set up parameters for the peak search:
   a. Go to the **2-axes Peak Search Details** tab.
   b. Use these settings:



2-axes peak search

Search window size: Medium (21x11)

Window size (data points): 21 11

Ignore peaks below (cps): 1,000

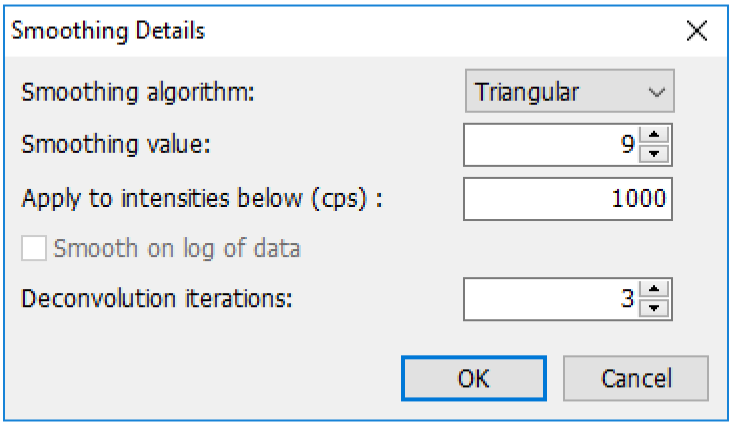
☑ Set peak to centroid

☐ Use deconvolution

☑ Apply smoothing before peak search

Figure 5.7 2-axes peak search details

   c. Click **Set smoothing details**.
   d. Use these settings:



Smoothing Details

Smoothing algorithm: Triangular

Smoothing value: 9

Apply to intensities below (cps) : 1000

☐ Smooth on log of data

Deconvolution iterations: 3

Figure 5.8 Smoothing details

7. In the **Scan List** pane, select the scan.
8. Press F9 to do the peak search. The plot must show as follows:

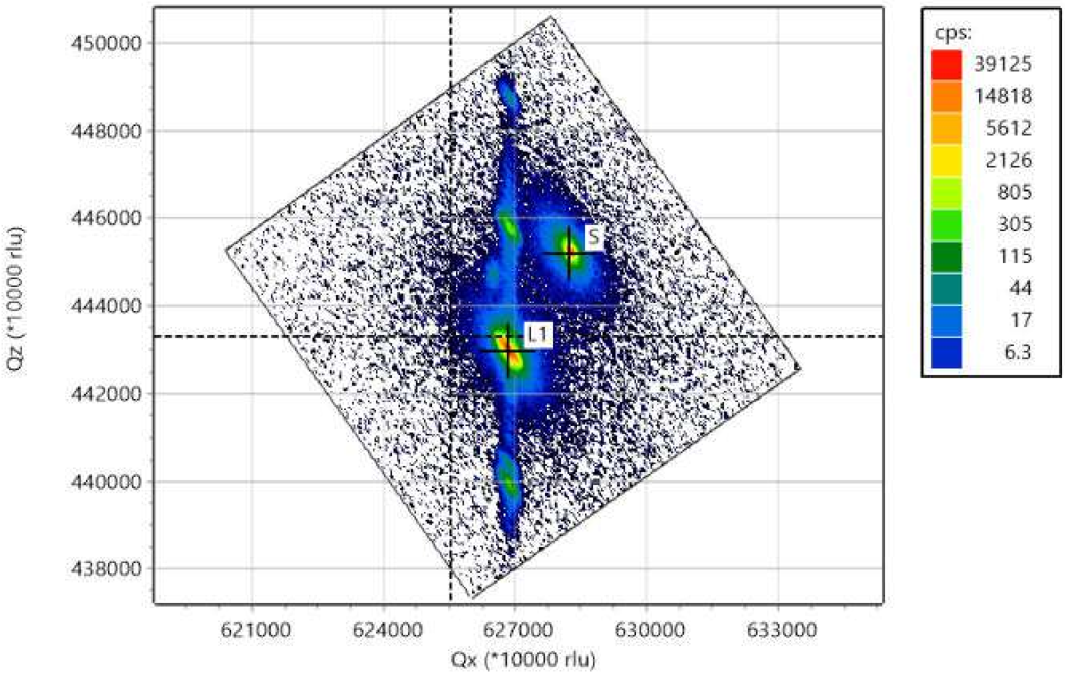
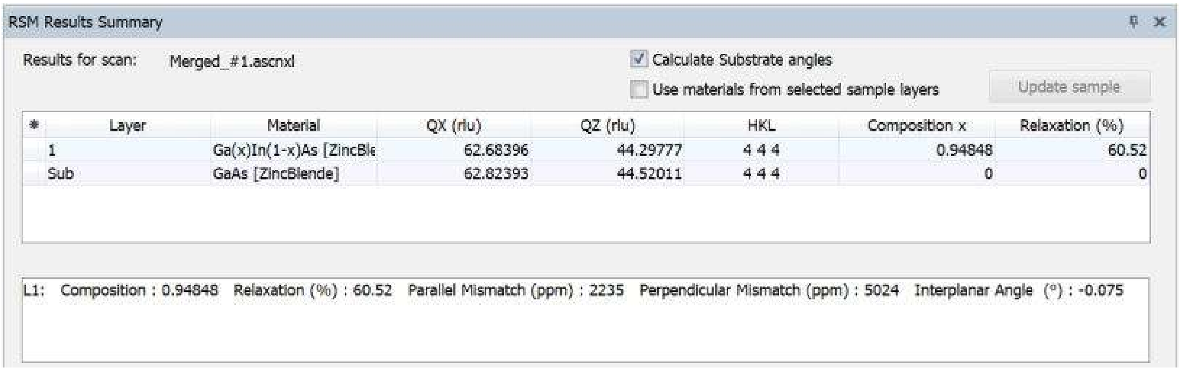


Figure 5.9 Marked peak positions

9. Manually label the substrate and layer peak:
   a. Go to the **Peaks Found** tab.
   b. For the peak with the highest intensity, select **Layer** from the **Peak Type** drop-down list.
   c. For the peak with the second highest intensity, select **Substrate** from the **Peak Type** drop-down list. The peaks are labeled "S" and "L".
10. Find the average composition, relaxation and parallel mismatch of the Ga(x)In(1-x)GaAs/GaS superlattice:
    a. Go to the **RSM Results Summary** tab.
    b. For the substrate, select **GaAs** from the **Material** drop-down list.
    c. For layer 1, select **Ga(x)In(1-x)As** from the **Material** drop-down list.
    d. In the **HKL** column, enter "4 4 4" for the substrate and layer 1.

    NOTE: Make sure that you enter the value as 4, space, 4, space, 4.

    The values for the Ga composition, the relaxation and parallel d-spacing mismatch (fractional differences in d-spacings) to the substrate surface are given. If the d-value for the substrate is known, this information can be used to find the in-plane lattice parameters of the layer unit cell.



Results for scan: Merged_#1.ascnxl

☑ Calculate Substrate angles

☐ Use materials from selected sample layers

*	Layer	Material	QX (rlu)	QZ (rlu)	HKL	Composition x	Relaxation (%)
	1	Ga(x)In(1-x)As [ZincBl	62.68396	44.29777	4 4 4	0.94848	60.52
	Sub	GaAs [ZincBlende]	62.82393	44.52011	4 4 4	0	0

L1: Composition : 0.94848 Relaxation (%) : 60.52 Parallel Mismatch (ppm) : 2235 Perpendicular Mismatch (ppm) : 5024 Interplanar Angle (°) : -0.075

Figure 5.10 *RMS Results Summary tab*

11. Close AMASS.

CHAPTER 6 FIND COMPOSITION AND RELAXATION FROM ROCKING CURVES

6.1 Introduction

This chapter gives information about how to find the composition and percentage relaxation of a layer from 4 rocking curves. The 4 curves are supplied from a gallium indium arsenide (In(x)Ga(1-x)As) layer on a (001) GaAs substrate.

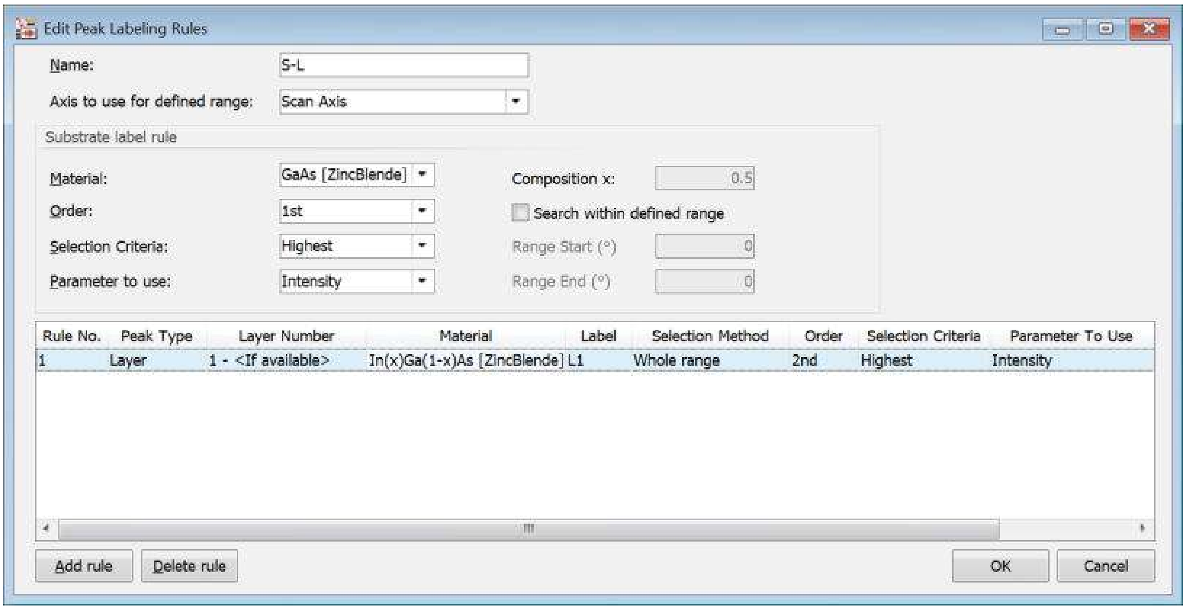
The rocking curves are for 004 and 224 reflections with the [110] direction horizontal with phi = 90 for scans with file names that end with "a", and phi = -90 for scans with file names that end with "b". All 4 rocking curves show 2 peaks - the weaker peak is from the layer in all curves.

The 4 scans are the optimum set necessary to calculate relaxation from rocking curves. They are 2 symmetrical reflections, measured before and after a 180 rotation in phi. There are 2 rocking curves that use the same asymmetrical reflection, 1 with low angle of incidence and 1 with high angle of incidence and phi rotated by 180. For more information about approximations with fewer rocking curves, refer to the AMASS Help.

The procedure given 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.

6.2 Set the defaults

1. Start AMASS.
2. Go to **View > View as H.R. Diffraction**.
3. Go to the **1-axis Peak Search Details** tab.
4. Select **Set peak to center**.
5. In the **Ignore peaks below (cps)** field, enter "500". This is set just above the background level.
6. Make a new rule:
    a. Click **Add**.
    b. In the **Name** field, enter "S-L".
    c. Click **Add rule**. A line is added to the grid.
    d. Use these settings:



Name: S-L

Axis to use for defined range: Scan Axis

Substrate label rule

Material: GaAs [ZincBlende]

Order: 1st

Selection Criteria: Highest

Parameter to use: Intensity

Composition x: 0.5

☐ Search within defined range

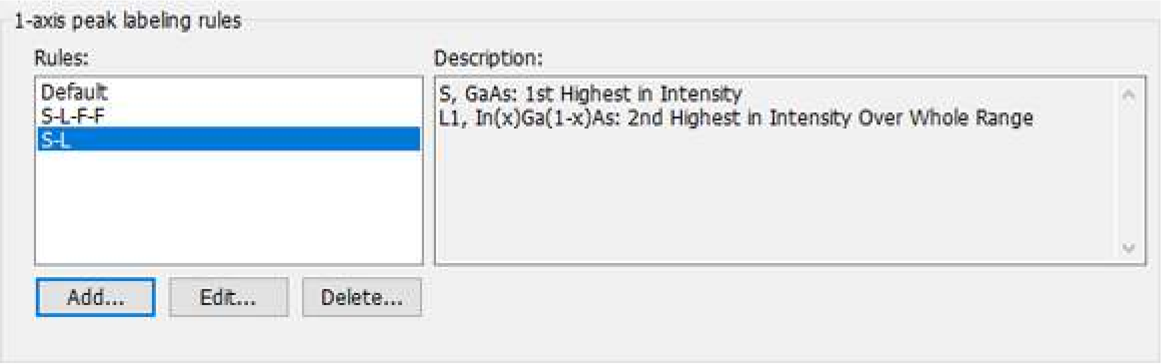
Range Start (°) 0

Range End (°) 0

Rule No.	Peak Type	Layer Number	Material	Label	Selection Method	Order	Selection Criteria	Parameter To Use
1	Layer	1 - <If available>	In(x)Ga(1-x)As [ZincBlende]	L1	Whole range	2nd	Highest	Intensity

Figure 6.1 Edit Peak Labeling Rules window

e. Click **OK**. The **1-axis Peak Search Details** tab is shown with these peak labeling parameters set. Peaks will be found and labeled in each measured scan as it is loaded.



1-axis peak labeling rules

Rules:

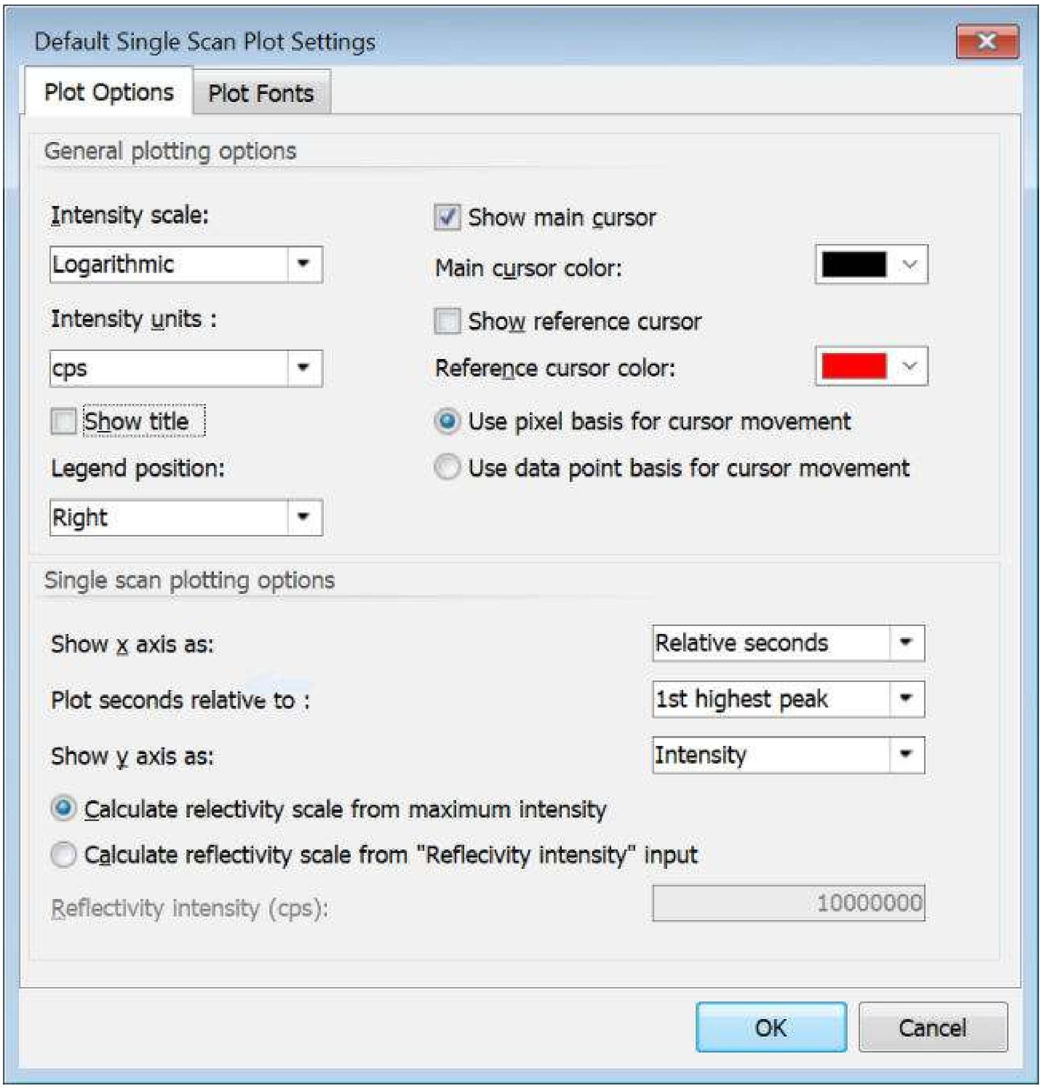
Default
S-L-F-F
S-L

Description:

S, GaAs: 1st Highest in Intensity
L1, In(x)Ga(1-x)As: 2nd Highest in Intensity Over Whole Range

Figure 6.2 Peak labeling parameters

7. Set the plot options:
   a. Go to **Settings > Default Single Scan Plot Settings**.
   b. From the **Intensity scale** drop-down list, select **Logarithmic**.
   c. From the **Intensity units** drop-down list, select **cps**.
   d. From the **Show x axis** as drop-down list, select **Relative seconds**.
   e. From the **Plot seconds relative to** drop-down list, select **1st highest peak**.



General plotting options

Intensity scale: Logarithmic

Intensity units : cps

☐ Show title

Legend position: Right

☑ Show main cursor

Main cursor color: ⬛

☐ Show reference cursor

Reference cursor color: 🟥

● Use pixel basis for cursor movement

○ Use data point basis for cursor movement

Single scan plotting options

Show x axis as: Relative seconds

Plot seconds relative to : 1st highest peak

Show y axis as: Intensity

● Calculate relectivity scale from maximum intensity

○ Calculate reflectivity scale from "Reflecivity intensity" input

Reflectivity intensity (cps): 10000000

Figure 6.3 Default Single Scan Plot Settings window

8. Click **OK**.

6.3 Show and print results

1. Go to **File > Open Scan(s)**.
2. Go to **C:\Users\User.Name\Documents\PANalytical\AMASS\Examples**.
3. Select "GaInAs004a.d00", "GaInAs004b.d00", "GaInAs224a.d00" and "GaInAs224b.d00".
4. Click **Open**.

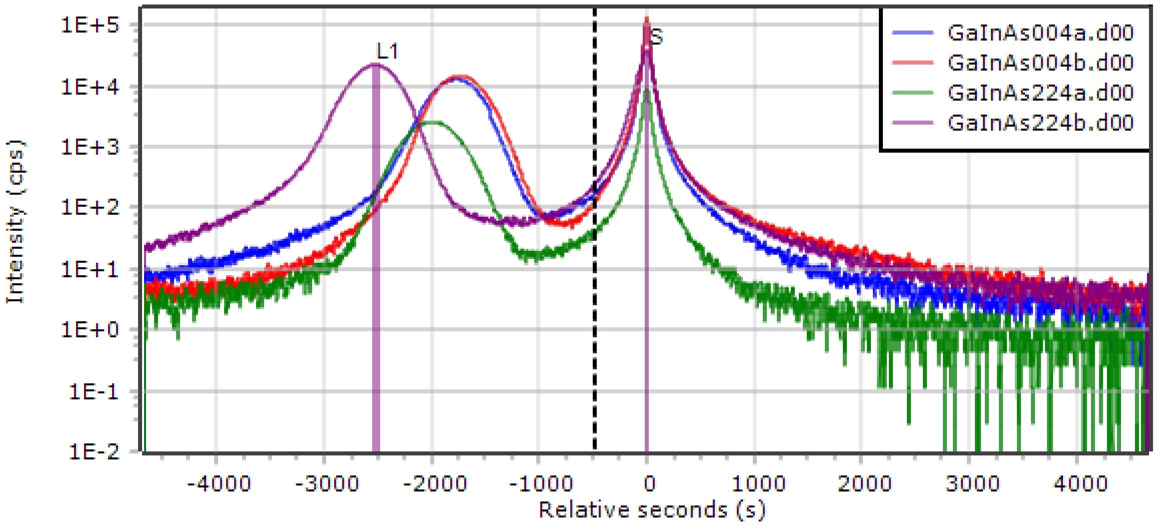
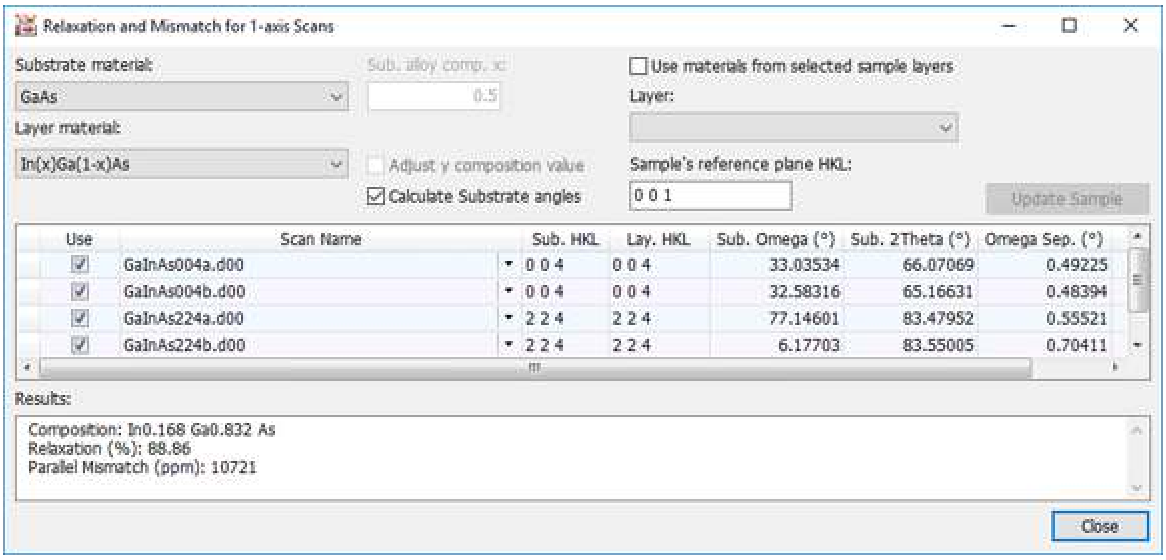


Figure 6.4 The 4 measured scans with the marked peaks

5. Go to **Tools > 1-axis Scan Tools > Relaxation and Mismatch for 1-axis Scans**. The 4 measured rocking curves are now shown in the graph. The **Relaxation and Mismatch for 1-axis Scans** window shows the calculated composition, relaxation and parallel mismatch of the layer.



Substrate material: GaAs
Sub. alloy comp. x: 0.5
Layer material: In(x)Ga(1-x)As
☐ Adjust y composition value
☑ Calculate Substrate angles
☐ Use materials from selected sample layers
Layer:
Sample's reference plane HKL: 0 0 1

Use	Scan Name	Sub. HKL	Lay. HKL	Sub. Omega (°)	Sub. 2Theta (°)	Omega Sep. (°)
☑	GaInAs004a.d00	0 0 4	0 0 4	33.03534	66.07069	0.49225
☑	GaInAs004b.d00	0 0 4	0 0 4	32.58316	65.16631	0.48394
☑	GaInAs224a.d00	2 2 4	2 2 4	77.14601	83.47952	0.55521
☑	GaInAs224b.d00	2 2 4	2 2 4	6.17703	83.55005	0.70411

Results:

```
Composition: In0.168 Ga0.832 As
Relaxation (%): 88.86
Parallel Mismatch (ppm): 10721
```

Figure 6.5 The 4 measured scans with relaxation and composition

6. If you want to change the combination of scans, select or clear the **Use** check boxes next to the scan names. Relaxation and composition can be calculated from 3 curves or 2 curves (which must include 1 asymmetrical scan).
7. Go to **Report > Report Setup**.
8. In the **Available report items** field, select the item that you want to include in the report. **One Axis Relaxation and Mismatch** must be included.
9. Click >.
10. Go back to step 2 until you have added all the items that you want to include in the report.
11. Click **OK**.
12. If you want to print the report, go to **Report > Print Report**.

13. If you want to save the report, go to **Report > Save Report To File As** and select the format that you want to save the report as.

6.4 Analyze your own data

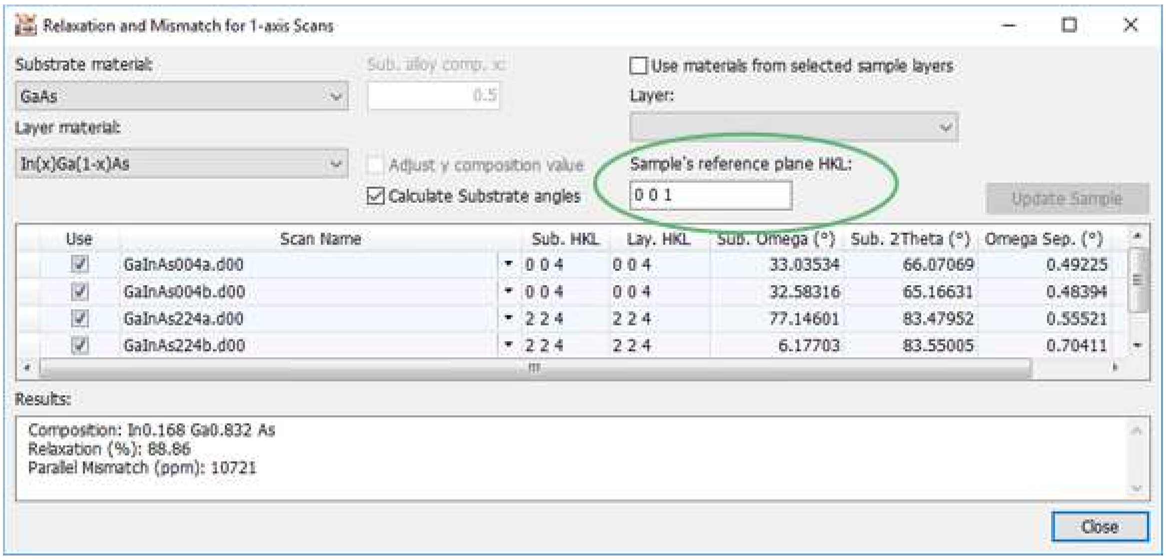
The previous sections gave information about how to calculate the composition and relaxation from 4 rocking curves with the default sample structure. This section gives procedures that can be necessary when you want to analyze your own data.

6.4.1 Edit HKL values

The mismatch, composition and relaxation calculations need 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 give the necessary information:

1. Go to **File > Open Scan(s)**.
2. Select the scan that you want to open.
3. Click **Open**.
4. Go to **Tools > 1-axis Scan Tools > Relaxation and Mismatch for 1-axis Scans**.
5. In the **Sample's reference plane HKL** field, enter the correct HKL information.

   NOTE: Make sure that you enter the value as <h>, space, <k>, space, <l>.



Substrate material: GaAs
Sub. alloy comp. x: 0.5
Layer material: In(x)Ga(1-x)As
☐ Adjust y composition value
☑ Calculate Substrate angles
☐ Use materials from selected sample layers
Layer:
Sample's reference plane HKL: 0 0 1

Use	Scan Name	Sub. HKL	Lay. HKL	Sub. Omega (°)	Sub. 2Theta (°)	Omega Sep. (°)
☑	GaInAs004a.d00	0 0 4	0 0 4	33.03534	66.07069	0.49225
☑	GaInAs004b.d00	0 0 4	0 0 4	32.58316	65.16631	0.48394
☑	GaInAs224a.d00	2 2 4	2 2 4	77.14601	83.47952	0.55521
☑	GaInAs224b.d00	2 2 4	2 2 4	6.17703	83.55005	0.70411

Results:

```
Composition: In0.168 Ga0.832 As
Relaxation (%): 88.86
Parallel Mismatch (ppm): 10721
```

Figure 6.6 *Scan Information window*

6. Click **OK**.

6.4.2 Use your own sample file

You can use your own sample file instead of the default sample file.

1. Go to **File > Open Scan(s)**.
2. Select the scan that you want to open.
3. Click **Open**.
4. Go to **Sample > Open Sample**.

5. Select your sample file.
6. Click **Open**.
7. Go to **Tools > 1-axis Scan Tools > Relaxation and Mismatch for 1-axis Scans**.
8. Select the **Use materials from selected sample layers** check box.
9. From the **Layer** drop-down list, select the layer that you want to use.

6.4.3 Use the results to update the sample file

You can transfer the values calculated in relaxation and mismatch for 1-axis scans to the sample file when the results are shown in the results pane. Do as follows:

1. Go to **Tools > 1-axis Scan Tools > Relaxation and Mismatch for 1-axis Scans**.
2. Click **Update Sample**. The original parameters of the selected layer is overwritten.

CHAPTER 7 FIND COMPOSITION AND RELAXATION FROM MAPS

7.1 Introduction

This chapter gives information about how to find the composition and percentage relaxation of a layer from 4 diffraction space maps. The 4 curves are supplied from a gallium indium arsenide (Ga_{1}-$_{x}In_{x}As$) layer on a (001) GaAs substrate.

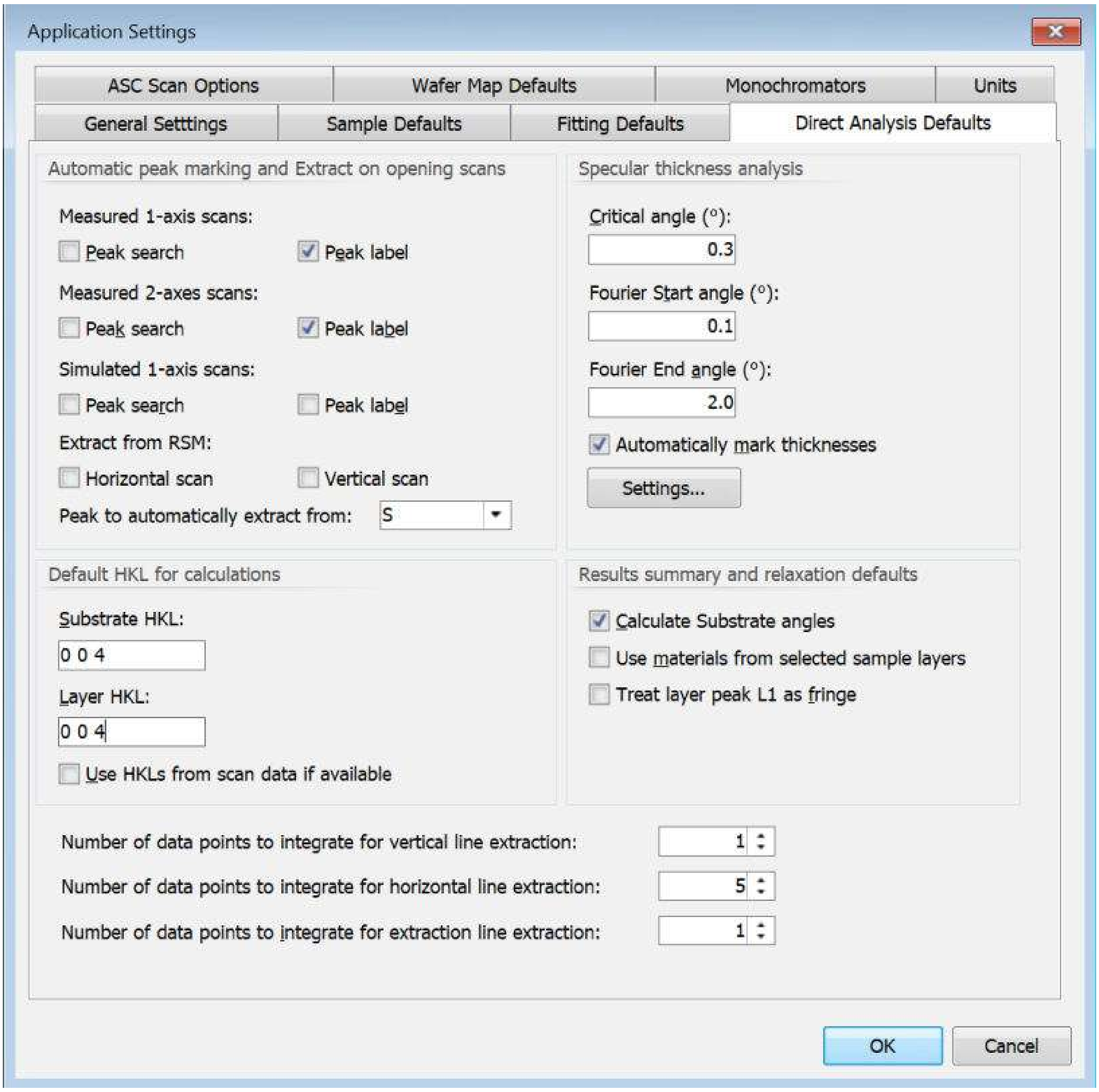
All 4 maps show 2 peaks - the weaker peak is from the layer in every map. The set of maps consists of a symmetrical 004 and an asymmetrical 444 reflection recorded in 2 orthogonal reciprocal lattice planes which are normal to the substrate surface. The pair of maps with phi = 0 have file names that end with "a", the pair of maps with phi = 90 have file names that end with "b".

The 4 maps given can be used to calculate the 3 layer unit cell parameters. With 1 pair of maps you can calculate the unit cell in 1 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 and the relaxation is the same in the orthogonal direction.

The procedure given 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.

7.2 Set the defaults

1. Start AMASS.
2. Click 📈 to view details for HR diffraction.
3. Go to **Settings > Application Settings**.
4. Go to the **Direct Analysis Defaults** tab.
5. In the **Automatic peak marking on opening scans** frame, select the **Peak label** check box for **Measured 2-axis scans**.



Automatic peak marking and Extract on opening scans

Measured 1-axis scans:

☐ Peak search ☑ Peak label

Measured 2-axes scans:

☐ Peak search ☑ Peak label

Simulated 1-axis scans:

☐ Peak search ☐ Peak label

Extract from RSM:

☐ Horizontal scan ☐ Vertical scan

Peak to automatically extract from: S

Specular thickness analysis

Critical angle (°): 0.3

Fourier Start angle (°): 0.1

Fourier End angle (°): 2.0

☑ Automatically mark thicknesses

Settings...

Default HKL for calculations

Substrate HKL: 0 0 4

Layer HKL: 0 0 4

☐ Use HKLs from scan data if available

Results summary and relaxation defaults

☑ Calculate Substrate angles

☐ Use materials from selected sample layers

☐ Treat layer peak L1 as fringe

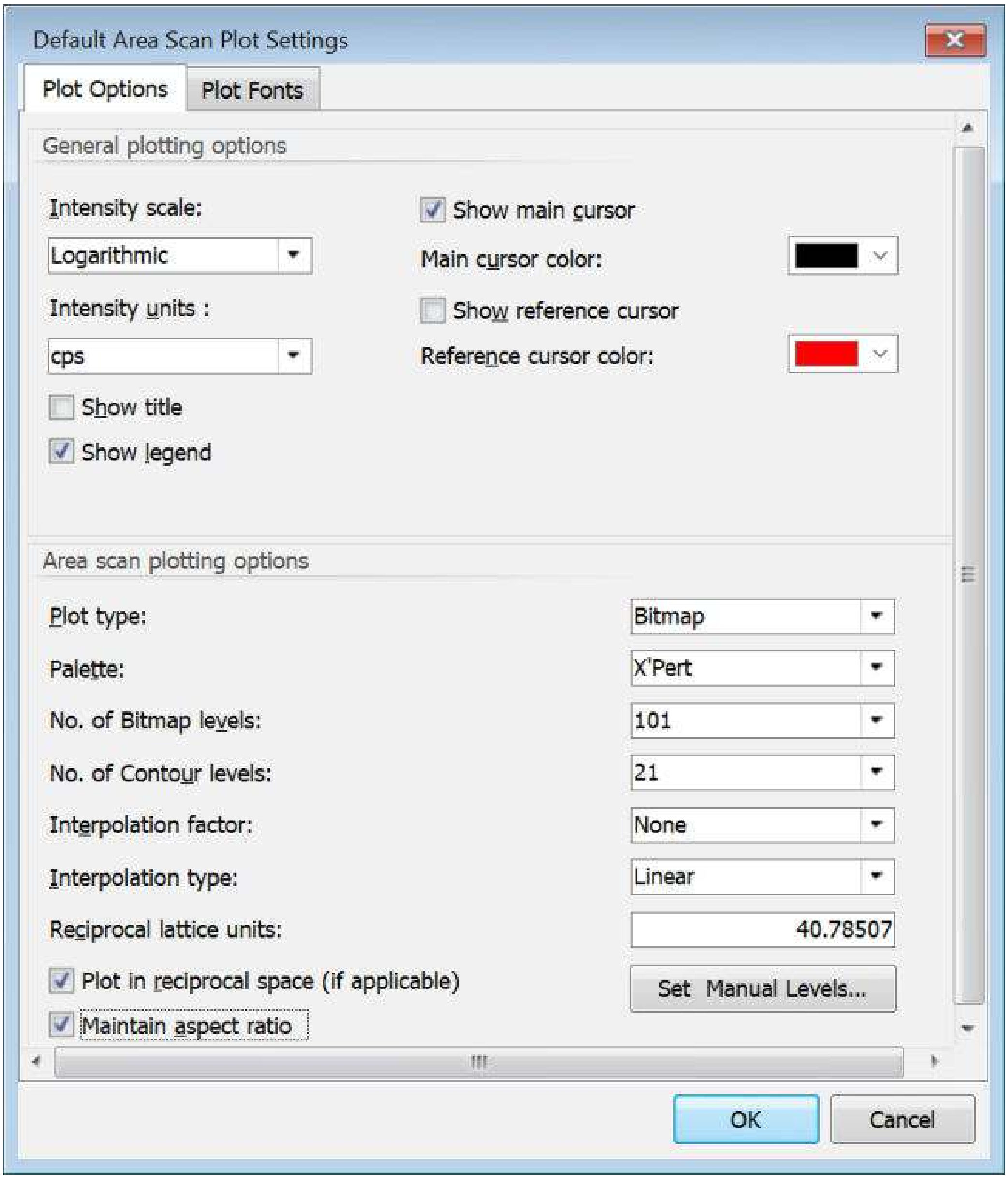
Number of data points to integrate for vertical line extraction: 1

Number of data points to integrate for horizontal line extraction: 5

Number of data points to integrate for extraction line extraction: 1

Figure 7.1 Direct Analysis Defaults window

6. Click **OK** to save the settings and close the window.
7. Set the plot options:
    a. Go to **Settings > Default Area Scan Plot Settings**.
    b. From the **Intensity scale** drop-down list, select **Logarithmic**.
    c. From the **Plot type** drop-down list, select **Bitmap**.
    d. Select the **Plot in reciprocal space (if applicable)** check box.



Intensity scale: Logarithmic

Intensity units : cps

☐ Show title

☑ Show legend

☑ Show main cursor

Main cursor color: ■

☐ Show reference cursor

Reference cursor color: 🟥

Plot type: Bitmap

Palette: X'Pert

No. of Bitmap levels: 101

No. of Contour levels: 21

Interpolation factor: None

Interpolation type: Linear

Reciprocal lattice units: 40.78507

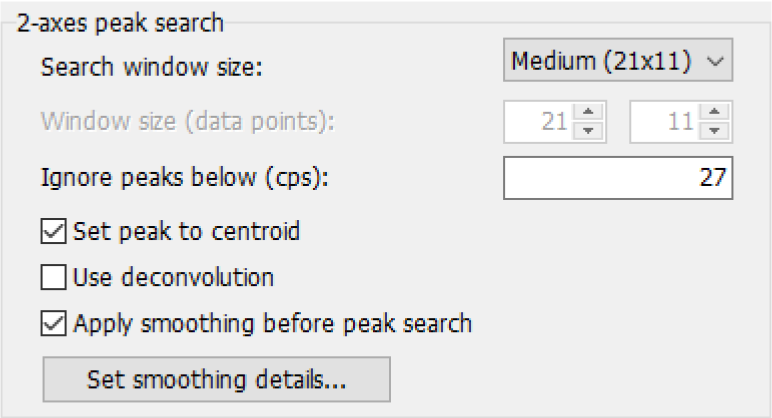
☑ Plot in reciprocal space (if applicable)

☑ Maintain aspect ratio

Figure 7.2 Default Single Scan Plot Settings window

e. Click **OK**.

8. Go to the **2-axis Peak Search Details** tab.
9. Use these settings:



2-axes peak search

Search window size: Medium (21x11)

Window size (data points): 21 11

Ignore peaks below (cps): 27

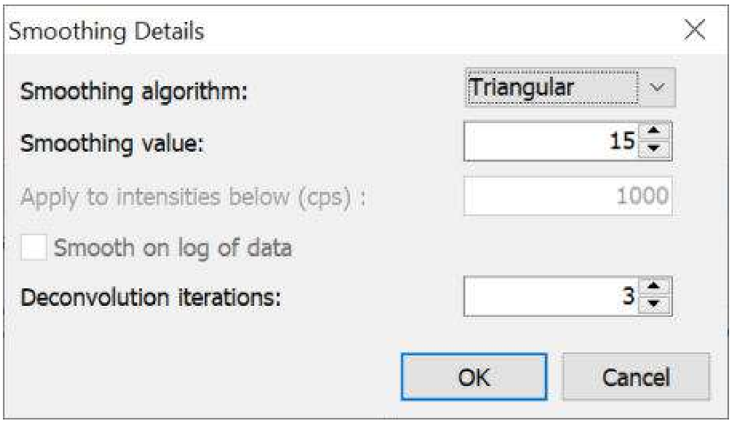
☑ Set peak to centroid

☐ Use deconvolution

☑ Apply smoothing before peak search

Figure 7.3 2-axes peak search frame

10. Set the smoothing details:
    a. Click **Set smoothing details**.
    b. Use these settings:



Smoothing Details

Smoothing algorithm: Triangular

Smoothing value: 15

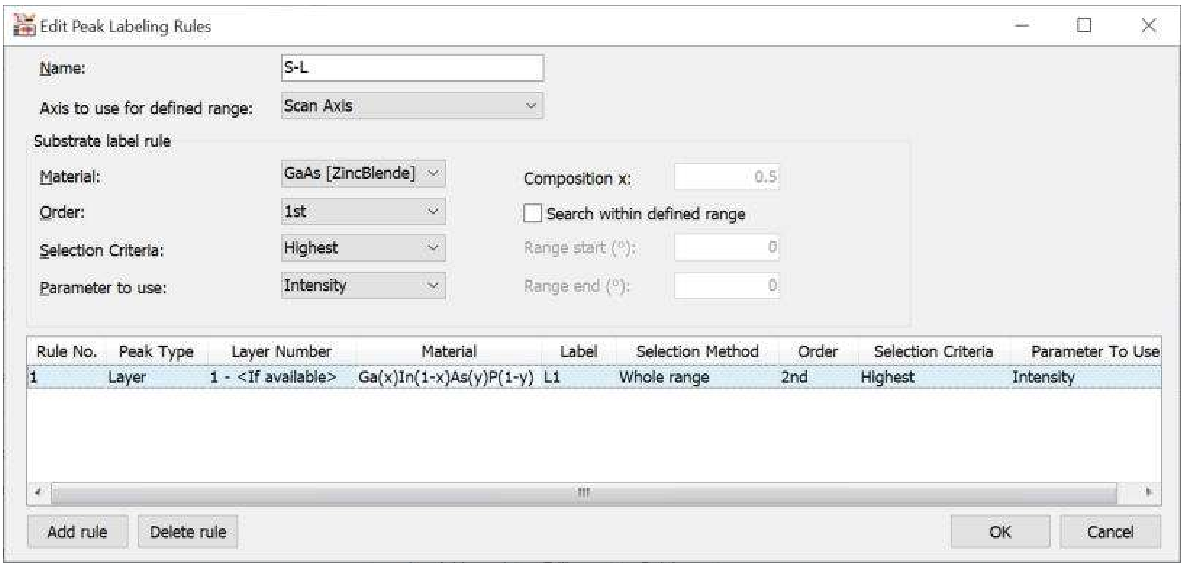
Apply to intensities below (cps) : 1000

☐ Smooth on log of data

Deconvolution iterations: 3

Figure 7.4 Smoothing Details window

    c. Click **OK**.
11. Make a new rule:
    a. Click **Add**.
    b. In the **Name** field, enter "S-L".
    c. Click **Add rule**. A line is added to the grid.
    d. Use these settings:



Name: S-L

Axis to use for defined range: Scan Axis

Substrate label rule

Material: GaAs [ZincBlende]

Order: 1st

Selection Criteria: Highest

Parameter to use: Intensity

Composition x: 0.5

☐ Search within defined range

Range start (°): 0

Range end (°): 0

Rule No.	Peak Type	Layer Number	Material	Label	Selection Method	Order	Selection Criteria	Parameter To Use
1	Layer	1 - <If available>	Ga(x)In(1-x)As(y)P(1-y)	L1	Whole range	2nd	Highest	Intensity

Figure 7.5 Edit Peak Labeling Rules window

e. Click **OK**. When a measured scan is loaded, peak positions are marked with crosses. The substrate and layer peaks are marked "S" and "L" respectively.

7.3 Show and print results

1. Go to **File > Open Scan(s)**.
2. Go to **C:\Users\User.Name\Documents\PANalytical\AMASS\Examples**.
3. Select "Map004a.a00", "Map004b.a00", "Map444a.a00" and "Map444b.a00".
4. Click **Open**. Each map will be shown in one of the graphs.
5. Make sure that the marked and labeled peaks are shown in each map.

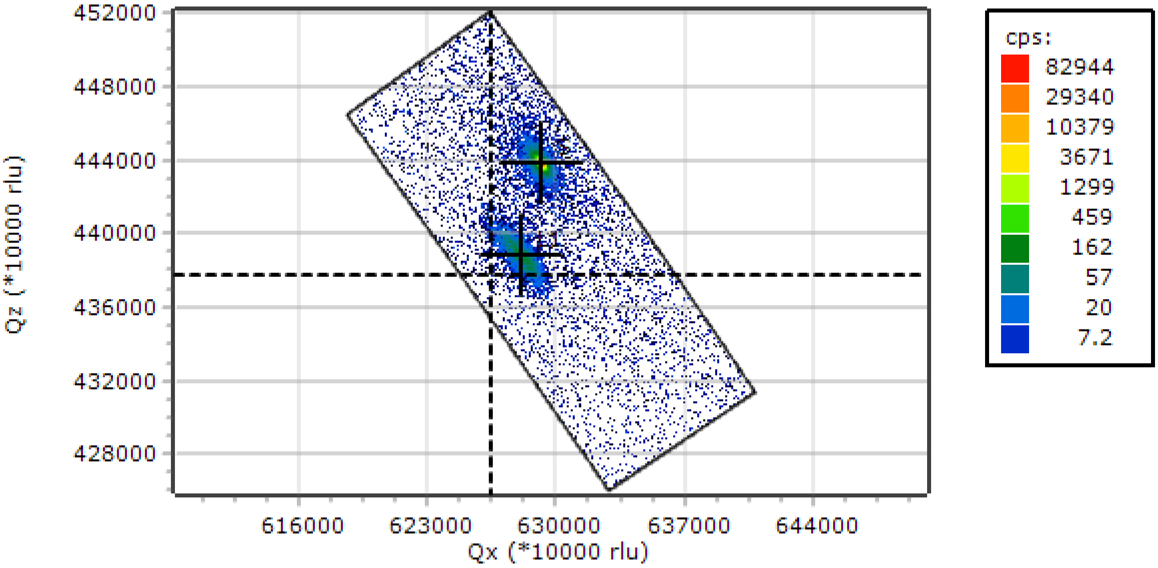
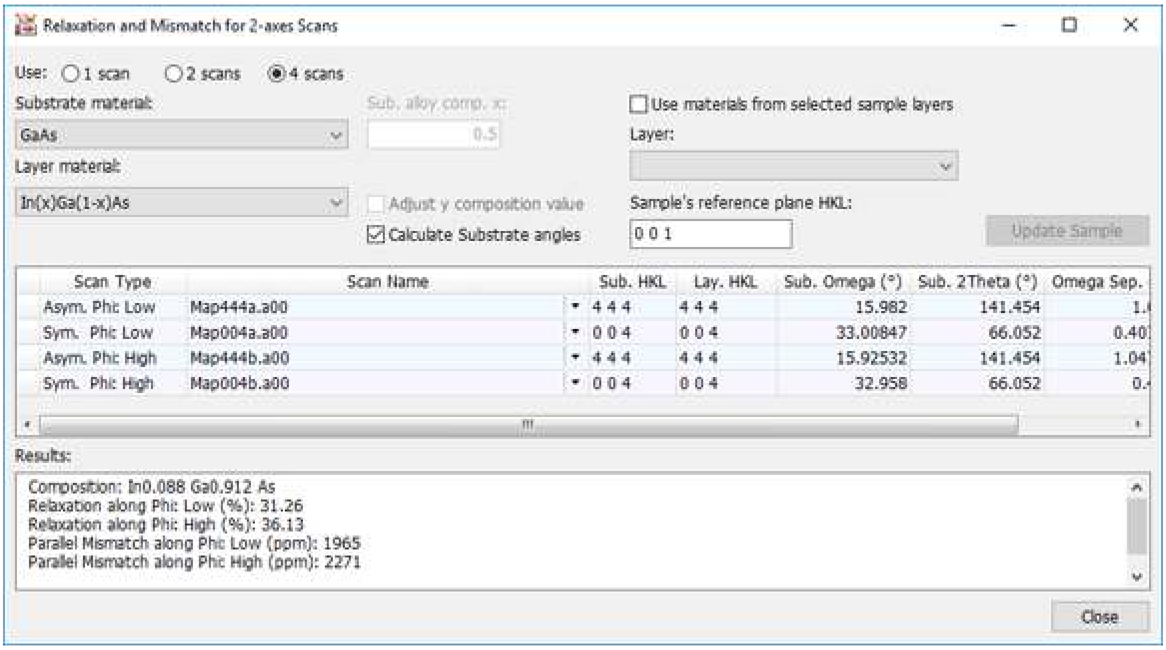


Figure 7.6 The 4 measured scan shown with the marked peaks

6. Go to **Tools > 2-axis Scan Tools > Relaxation and Mismatch for 2-axis Scans**. The 4 measured maps are now shown in the graph. The results value which shown are related to the **Calculate Substrate angles** check box. If the check box is not selected, the Bragg angles are calculated from the 2theta positions of the peaks. If the check box is selected, the expected

position of the substrate peak is calculated from the layer lattice parameter stored in the database and the wavelength. The layer angles are calculated from substrate peak position and the measured peak separations.



Use: ○ 1 scan ○ 2 scans ● 4 scans

Substrate material: GaAs

Layer material: In(x)Ga(1-x)As

☐ Adjust y composition value

☑ Calculate Substrate angles

☐ Use materials from selected sample layers

Sample's reference plane HKL: 0 0 1

Scan Type	Scan Name	Sub. HKL	Lay. HKL	Sub. Omega (°)	Sub. 2Theta (°)	Omega Sep.
Asym. Phi: Low	Map444a.a00	4 4 4	4 4 4	15.982	141.454	1.
Sym. Phi: Low	Map004a.a00	0 0 4	0 0 4	33.00847	66.052	0.40
Asym. Phi: High	Map444b.a00	4 4 4	4 4 4	15.92532	141.454	1.04
Sym. Phi: High	Map004b.a00	0 0 4	0 0 4	32.958	66.052	0.

Results:

```
Composition: In0.088 Ga0.912 As
Relaxation along Phi: Low (%): 31.26
Relaxation along Phi: High (%): 36.13
Parallel Mismatch along Phi: Low (ppm): 1965
Parallel Mismatch along Phi: High (ppm): 2271
```

Figure 7.7 The 4 measured scans with relaxation and composition

7. If you want to change the number of scans used in the calculation, use the radio buttons above the scan names in the **Relaxation and Mismatch for 2-axes Scans** window.
8. Go to **Report > Report Setup**.
9. In the **Available report items** field, select the item that you want to include in the report. **Two Axes Relaxation and Mismatch** must be included.
10. Click >.
11. Go back to step 2 until you have added all the items that you want to include in the report.
12. Click **OK**.
13. If you want to print the report, go to **Report > Print Report**.
14. If you want to save the report, go to **Report > Save Report To File As** and select the format that you want to save the report as.

CHAPTER 8 MAKE SIMULATIONS AND USE AUTOMATIC FITTING OF ROCKING CURVES

8.1 Introduction

This chapter shows the simulation and fitting functionality. You must have an HR Option License next to the AMASS Basic License. If you do not have the HR Option License you cannot do a simulation and automatic fitting.

8.2 Simulate with the Simulate Setup tab

This section gives you instructions to simulate a rocking curve with the **Simulation Setup** tab. It is possible to edit parameters on the different tabs of the **Sample Details** tab to make the fit between a simulated curve and a measured curve better.

The sample structure used is a SiGe heterojunction bipolar transistor (HBT) with 2 discrete SiGe layers and a Si cap. Use the measured scan "SiGe.d00" in your Documents folder: **...\PANalytical \AMASS\Examples**.

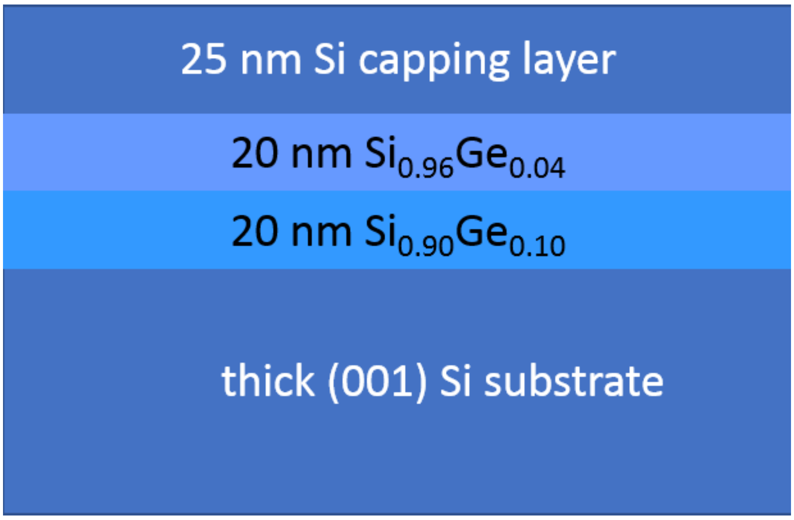


Figure 8.1 The SiGe HBT structure with 2 SiGe layers

8.2.1 Set the defaults

1. Start AMASS.
2. Go to **View > View as H.R. Diffraction**.
3. Set the substrate as follows:
   a. Go to **Settings > Application Settings**.
   b. Go to the **Sample Defaults** tab.
   c. In the **Default substrate** frame, select **Diamond** from the **Structure** drop-down list.

   d. In the **Default substrate** frame, select **Si** from the **Material** drop-down list. The list only contains materials that are part of the chosen structure type.

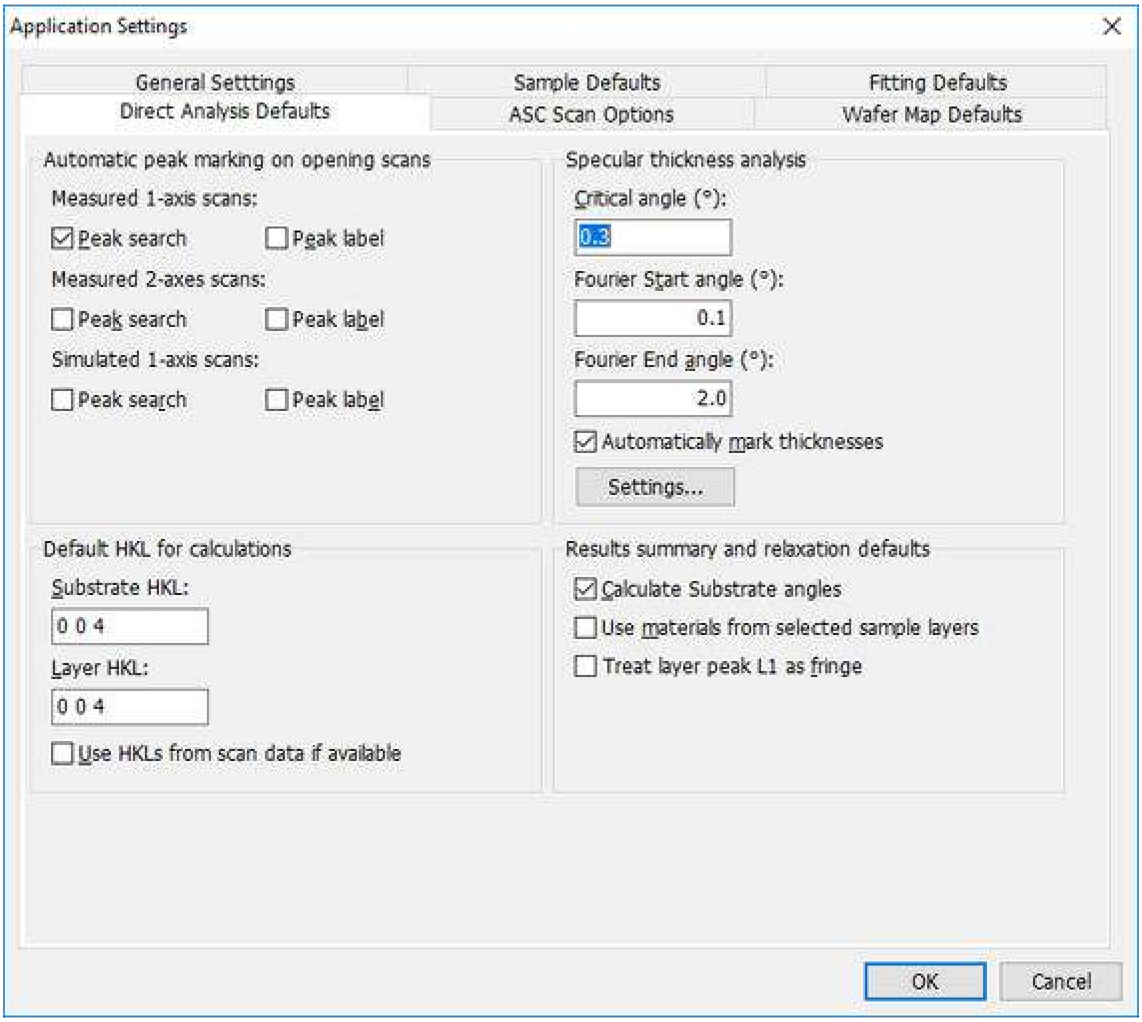
4. Set the layer as follows:
   a. In the **Default layer** frame, select **Diamond** from the **Structure** drop-down list.
   b. In the **Default layer** frame, select **Si(x)Ge(1-x)** from the **Material** drop-down list.
   c. If applicable, change the default values for thickness and composition.
   d. If applicable, select the **Use percentages to set fitting ranges** check box. When this check box is selected, you can change the percentage values that will be used to set the fitting ranges.
   e. Go to the **Direct Analysis Defaults** tab.
   f. In the **Substrate HKL** field, enter "0 0 4".

      NOTE: Make sure that you enter the value as 0, space, 0, space, 4.

   g. In the **Layer HKL** field, enter "0 0 4"

      NOTE: Make sure that you enter the value as 0, space, 0, space, 4.

5. In the **Automatic peak marking on opening scans** frame, select the **Peak search** check box for **Measured 1-axis scans**.



Automatic peak marking on opening scans

Measured 1-axis scans:
☑ Peak search ☐ Peak label

Measured 2-axes scans:
☐ Peak search ☐ Peak label

Simulated 1-axis scans:
☐ Peak search ☐ Peak label

Specular thickness analysis

Critical angle (°): 0.3

Fourier Start angle (°): 0.1

Fourier End angle (°): 2.0

☑ Automatically mark thicknesses

Default HKL for calculations

Substrate HKL: 0 0 4

Layer HKL: 0 0 4

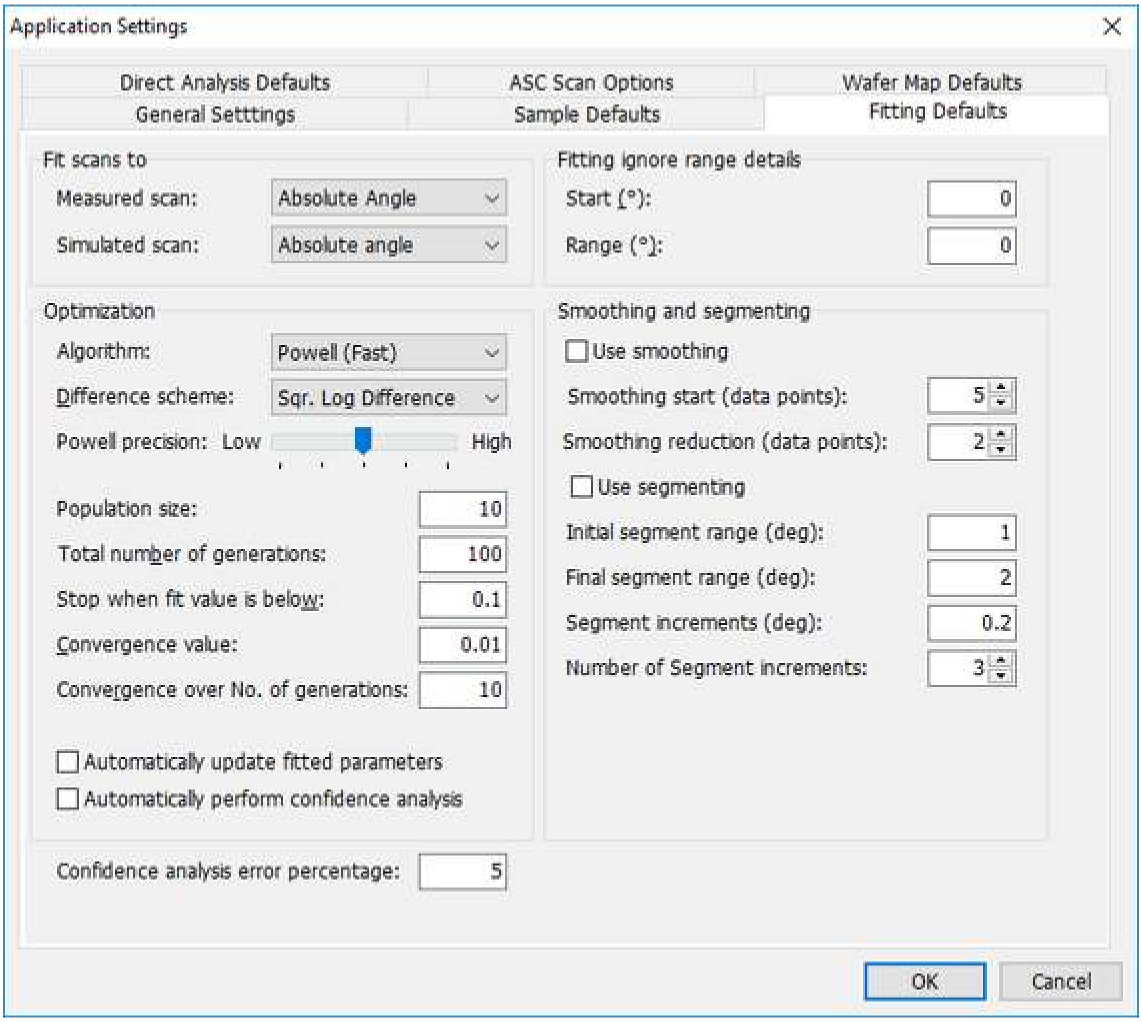
☐ Use HKLs from scan data if available

Results summary and relaxation defaults

☑ Calculate Substrate angles
☐ Use materials from selected sample layers
☐ Treat layer peak L1 as fringe

Figure 8.2 Direct Analysis Defaults tab

6. Go to the **Fitting Defaults** tab.
7. From the **Algorithm** drop-down list, select **Powell (Fast)**.
8. From the **Difference scheme** drop-down list, select **Sqr. Log Difference**.
9. Clear the **Automatically update fitted parameters** check box.
10. In the **Confidence analysis error percentage**, enter "5".



Fit scans to
Measured scan: Absolute Angle
Simulated scan: Absolute angle

Fitting ignore range details
Start (°): 0
Range (°): 0

Optimization
Algorithm: Powell (Fast)
Difference scheme: Sqr. Log Difference
Powell precision: Low – High
Population size: 10
Total number of generations: 100
Stop when fit value is below: 0.1
Convergence value: 0.01
Convergence over No. of generations: 10
☐ Automatically update fitted parameters
☐ Automatically perform confidence analysis

Smoothing and segmenting
☐ Use smoothing
Smoothing start (data points): 5
Smoothing reduction (data points): 2
☐ Use segmenting
Initial segment range (deg): 1
Final segment range (deg): 2
Segment increments (deg): 0.2
Number of Segment increments: 3

Confidence analysis error percentage: 5

Figure 8.3 Fitting Defaults tab

11. Click **OK**.

8.2.2 Make a new sample

1. Load the experimental scan:
    a. Go to **File > Open Scan(s)**.
    b. Go to **C:\Users\User.Name\Documents\PANalytical\AMASS\Examples**.
    c. Select "SiGe.d00".
    d. Click **Open**.
2. Go to **Sample > New Sample**. The grid currently shows the default material for the substrate as set in **Settings > Application Defaults**. If necessary, this can be edited.

3. Add the first layer:
   a. In the **Layers** pane, click **Add Layer**. The substrate layer moves down 1 row and the new layer is the top row. The material is Si(x)Ge(1-x) as set in the defaults.
   b. In the **Alloy Comp. x** field, enter "0.9".
   c. In the **Thickness (nm)** field, enter "20".
4. Add other layers to the sample:
   a. Select **Layer No. 1** in the grid.
   b. In the **Layers** pane, click **Add Layer**.
   c. In the **Alloy Comp. x** field, enter "0.96".
   d. In the **Thickness (nm)** field, enter "20".
   e. In the **Layers** pane, click **Add Layer**.
   f. From the **Material** drop-down list, select **Si [Diamond]**.
   g. In the **Thickness (nm)** field, enter "25".
   h. In the **Sample length (mm)** field, enter "100".
5. Save the sample:
   a. Go to **Sample > Save Sample As**.
   b. In the **File name** field, enter a file name.
   c. Click **Save**.

8.2.3 Do the simulation

1. Set the default single scan options:
   a. Go to **Settings > Default Single Scan Plot Settings**.
   b. From the **Intensity scale** drop-down list, select **Logarithmic**.
   c. From the **Intensity units** drop-down list, select **cps**.
   d. In the **Show x axis as** field, select the correct setting:
      - Select **Relative seconds** if you want to plot in seconds.
      - Select **Absolute angle (deg)** if you want to plot in degrees.
   e. If you selected **Relative seconds**, select an option from the **Plot seconds relative to** drop-down list. The option **1st highest peak** is a good selection to start with.
   f. Click **OK** to close the window.
2. Go to the **Simulation Setup** tab.
3. Select the **Normalise intensity** check box.
4. Click ... of **Primary wavelength (A)**.
5. Select the correct wavelength. In this example, **CuKa**.
6. Click **OK**.
7. Press F2 to start the simulation. A red line shows on the graph.
8. In the **Scan List** pane, select the filename of the opened scan.
9. Click **Use selected scan's values** to adjust the start and end values.
10. Press F2 again.

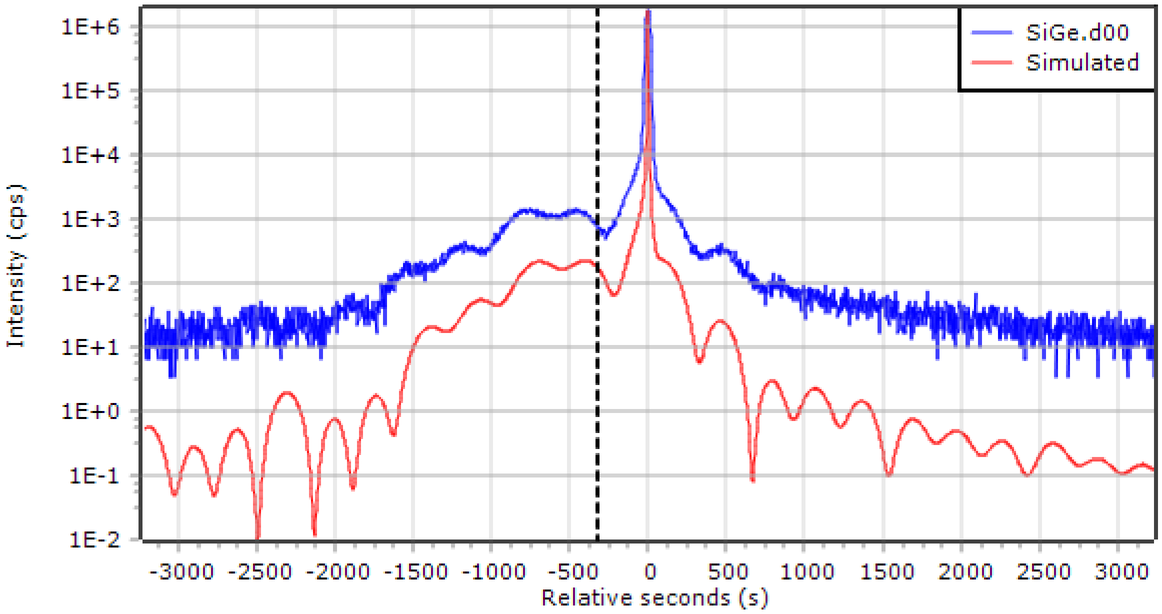


Figure 8.4 Rocking curve scan and simulation

11. Make sure that the instrument parameters are correct:
    a. In the **Simulation Setup** tab, select **Ge 220 Asym** from the **Monochromator** drop-down list.
    b. In the **Value** column of the **Background (cps)** row, enter "10".
    c. In the **Beam width (mm)** field, enter "1.4".
12. Press F2 again. The simulated curve now matches the measured curve better, but the peaks of the SiGe layers are **not** well matched.

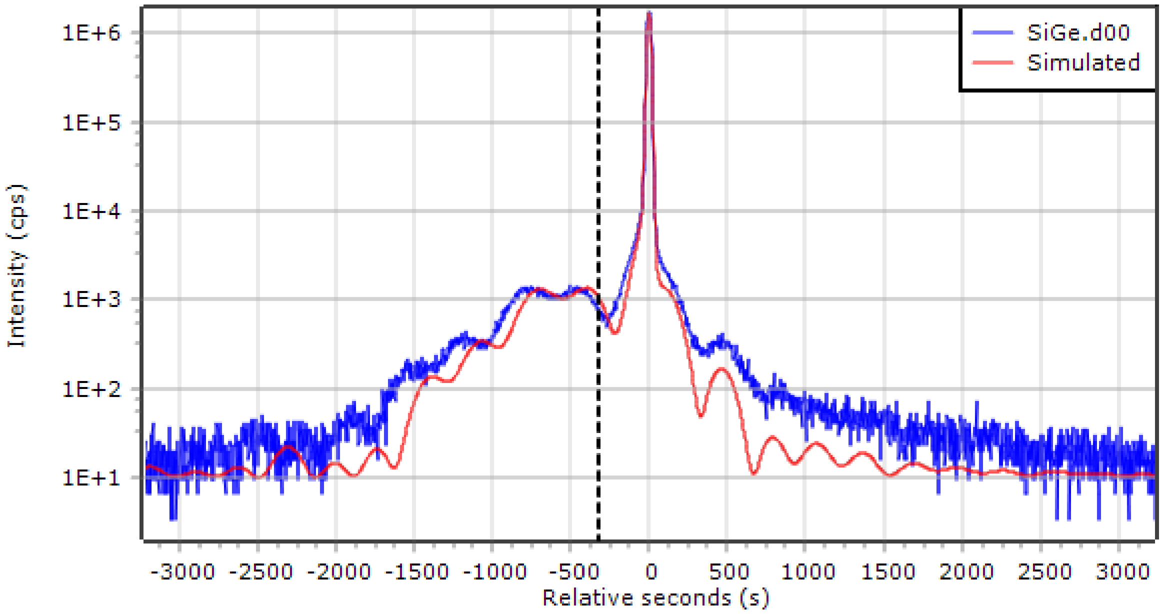


Figure 8.5 Simulated rocking curve

13. If you want to make the simulation better, manually edit the sample model.

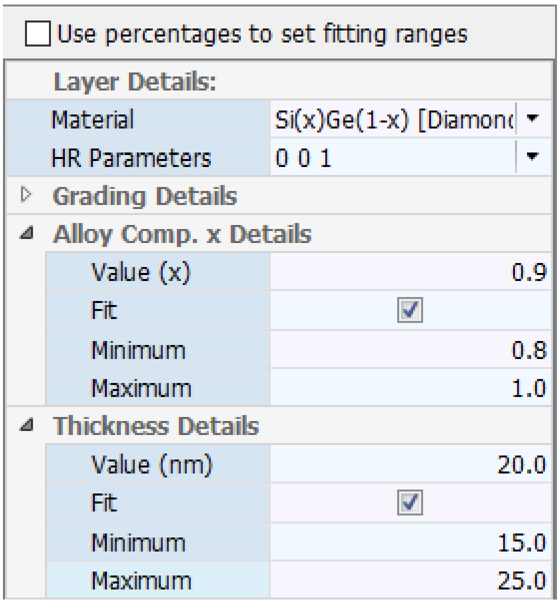
8.3 Fit with the Fitting Setup tab

Automatic fitting can be used to get a match between the measured and simulated curve. We use 2 examples:

- A SiGe HBT structure with 2 discrete SiGe layers
- A GaN/GaInN superlattice on a sapphire substrate.

8.3.1 Fit SiGe HBT with 2 discrete SiGe layers

1. Select the layer and convolution parameters to fit and its ranges:
   a. Go to the **Sample Details** tab.
   b. Select **Layer No. 1**.
   c. Clear the **Use percentages to set fitting ranges** check box.
   d. Use these settings:



☐ Use percentages to set fitting ranges

Layer Details:
Material: Si(x)Ge(1-x) [Diamonc
HR Parameters: 0 0 1

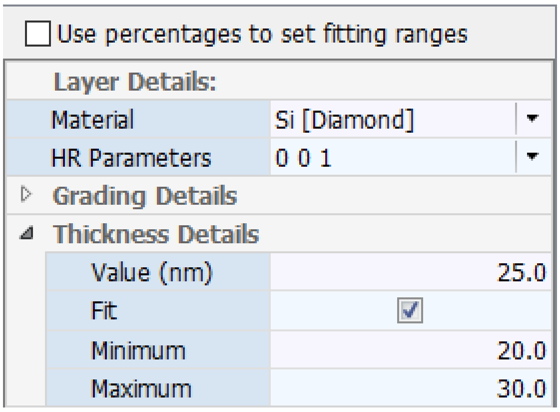
Grading Details

Alloy Comp. x Details
Value (x): 0.9
Fit: ☑
Minimum: 0.8
Maximum: 1.0

Thickness Details
Value (nm): 20.0
Fit: ☑
Minimum: 15.0
Maximum: 25.0

Figure 8.6 Settings for layers 1 and 2

   e. Do steps b to d again for **Layer No. 2** with the same settings.
   f. Select **Layer No. 3**.
   g. Use these settings:



☐ Use percentages to set fitting ranges

Layer Details:

Material	Si [Diamond]
HR Parameters	0 0 1

Grading Details

Thickness Details

Value (nm)	25.0
Fit	☑
Minimum	20.0
Maximum	30.0

Figure 8.7 Settings for layer 3

2. Select convolution parameters and its ranges for fittings:
   a. Go to the **Simulation Setup** tab.
   b. Clear the **Use percentages to set fitting ranges** check box.
   c. In the **Min.** field of the **Background (cps)** row, enter "2".
   d. In the **Max.** field of the **Background (cps)** row, enter "15".
3. Set up the fitting parameters:
   a. Go to the **Fitting Setup** tab.
   b. From the **Measured scan** drop-down list, select **1st highest peak**.
   c. From the **Simulated scan** drop-down list, select **Substrate**.
   d. Select the **Use smoothing** check box.
   e. In the **Smoothing start (data points)** field, enter "20".
   f. In the **Smoothing reduction (data points)** field, enter "10".
4. Press F3 to start the fit. During fitting, only 2 curves are shown in the graphics area and the difference plot. These are the smoothed measured curve and the current simulated curve. The progress of the fitting is shown in the **Fitting Results** tab. At the end of the fitting, the final simulated curve is shown together with the measured and the initially simulated scan. Scans that were previously loaded in the same window will also be shown.

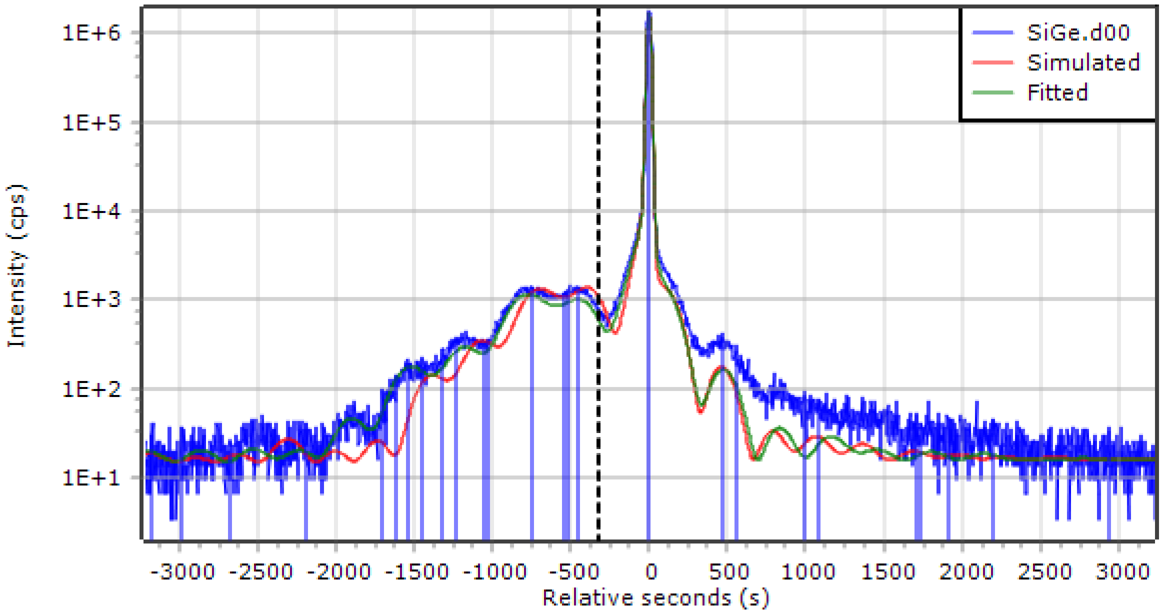
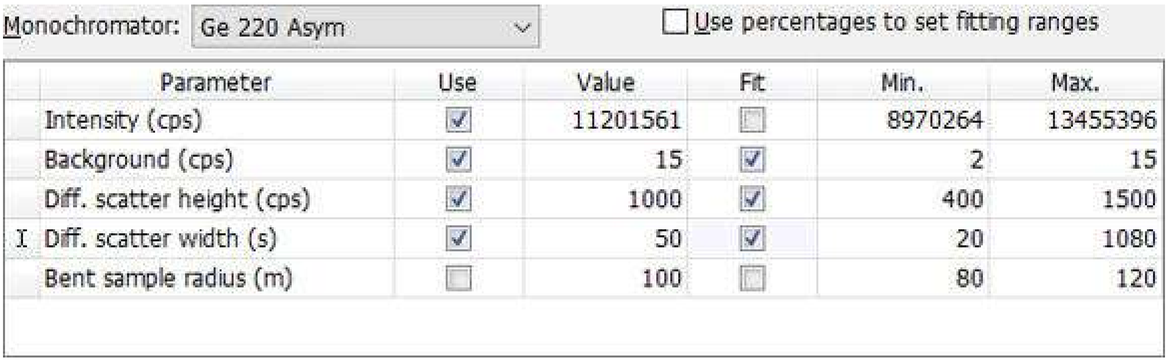


Figure 8.8 Simulated and fitted curve

The fitted curve now matches the peak positions of the measured data, but there are still differences in the intensities. Some of the values are highlighted when they are close to, but not equal to the limit. It is not necessary to change these values.

5. To make the fit better, add diffuse scattering parameters to the fit parameters:
   a. Go to the **Simulation Setup** tab.
   b. Use these settings:



Monochromator: Ge 220 Asym

☐ Use percentages to set fitting ranges

Parameter	Use	Value	Fit	Min.	Max.
Intensity (cps)	☑	11201561	☐	8970264	13455396
Background (cps)	☑	15	☑	2	15
Diff. scatter height (cps)	☑	1000	☑	400	1500
Diff. scatter width (s)	☑	50	☑	20	1080
Bent sample radius (m)	☐	100	☐	80	120

Figure 8.9 Diffuse scattering parameters

6. Press F3 to start the fit. The fitted curve now correctly matches the experimental data.

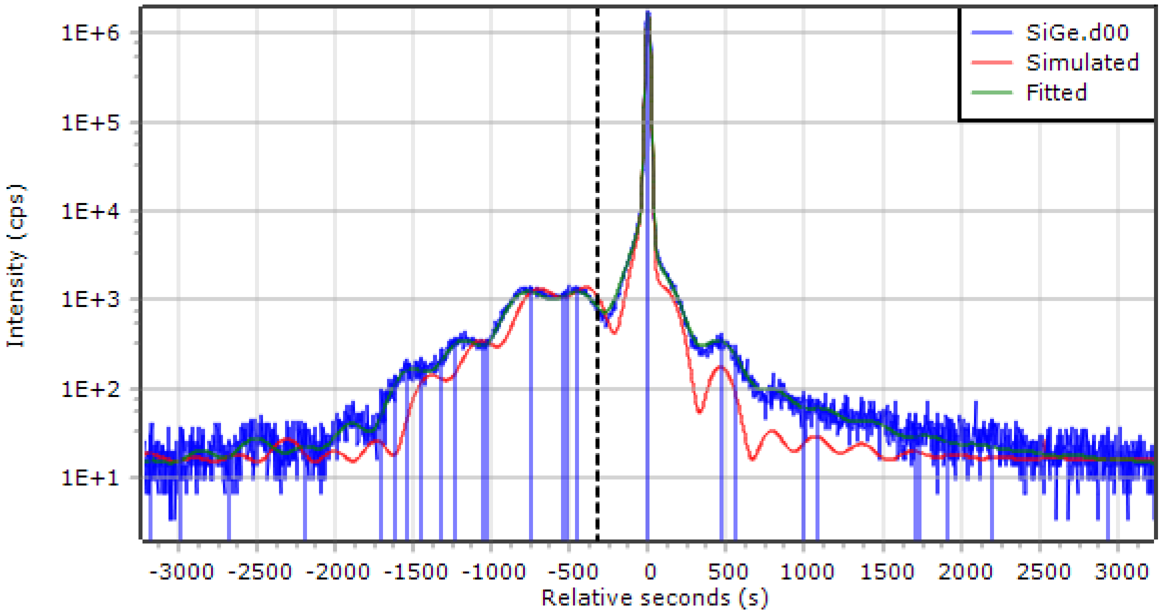


Figure 8.10 *Final fitted curve*

8.3.1.1 Confidence analysis

1. Go to **Simulation and Fitting > Perform Fitting Confidence Analysis**. The results of the confidence analysis are shown in the table of the **Fitting Results** tab. The columns **Low** and **High** show the calculated confidence ranges of each parameter based on the error percentage values set.


Fitting Results

Parameter	Initial Value	Current Value	Low	High	Min.	Max.
3, 0 - Si [Diamond]: Thic	25	22.5073	21.2688	23.7201	20	30
2, 0 - Si(x)Ge(1-x) [Diam	20	19.9121	18.6656	21.2313	15	25
2, 0 - Si(x)Ge(1-x) [Diam	0.96	0.9533	0.9472	0.95963	0.8	1
1, 0 - Si(x)Ge(1-x) [Diam	20	17.7077	16.6968	18.7207	15	25
1, 0 - Si(x)Ge(1-x) [Diam	0.9	0.88518	0.88075	0.88935	0.8	1
Background (cps)	15	8.9174	6.9703	11.0207	2	15
Diff. scatter height (cps)	1000	548.0758	460.6765	632.6861	400	1500
Diff. scatter width (sec)	50	313.2	286.3	341.2	20	1080

Figure 8.11 *Fitting results with confidence ranges*

2. If you want more information about a particular analysis, do as follows:
   a. Select the parameter.
   b. Go to **Simulation and Fitting > Plot Parameter's Fitting Confidence**.

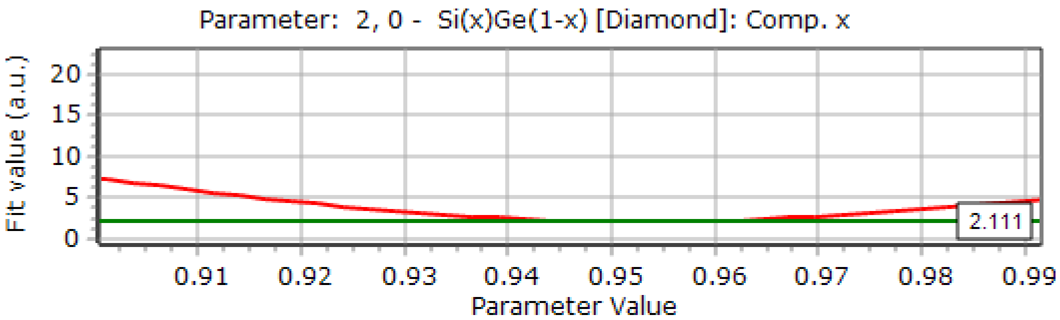


Figure 8.12 Fitting confidence plot with predefined error percentage line

The green horizontal line shows the predefined error percentage value. The cross sections with the red curve give the confidence range shown in the grid.

3. Save the project:
   a. Go to **File > Save Project As**.
   b. In the **File name** field, enter "HR_Fitting_Example1.aprjxl".
   c. Click **Save**.

8.3.1.2 Set up a report

1. Go to **Report > Report Setup**.
2. In the **Available report items** field, select the item that you want to include in the report.
3. Click >.
4. Go back to step 2 until you have added all the items that you want to include in the report.
5. Click **OK**.
6. If you want to print the report, go to **Report > Print Report**.
7. If you want to save the report, go to **Report > Save Report To File As** and select the format that you want to save the report as.

8.3.2 Fit a GaN/GaInN superlattice on a sapphire substrate

For this sample the interface between the sapphire and the GaN buffer layer is assumed to be totally relaxed.

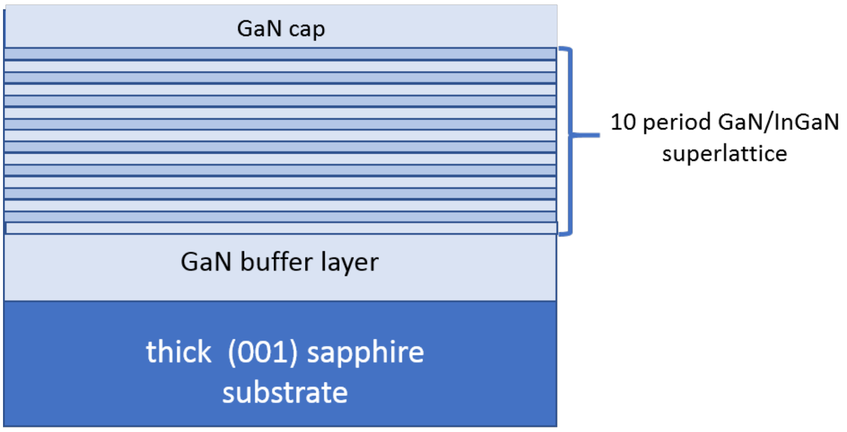


Figure 8.13 The sample structure for GaN.d00

To show automatic fitting for this sample, 2 files are supplied in the AMASS examples folder:

- GaN.d00, a measured rocking curve.
- GaN_MQW.aprjxl, a project file that contains the intended layer structure and necessary settings for fitting.

8.3.2.1 Do a simulation

1. Open the 2 files used in this example:
   a. Go to **File > Open Project**.
   b. Go to **C:\Users\User.Name\Documents\PANalytical\AMASS\Examples**.
   c. Select "GaN_MQW.aprjxl".
   d. Click **Open**.
   e. Go to **File > Open Scan(s)**.
   f. Select "GaN.d00".
   g. Click **Open**.
2. Press **F2** to start the simulation.

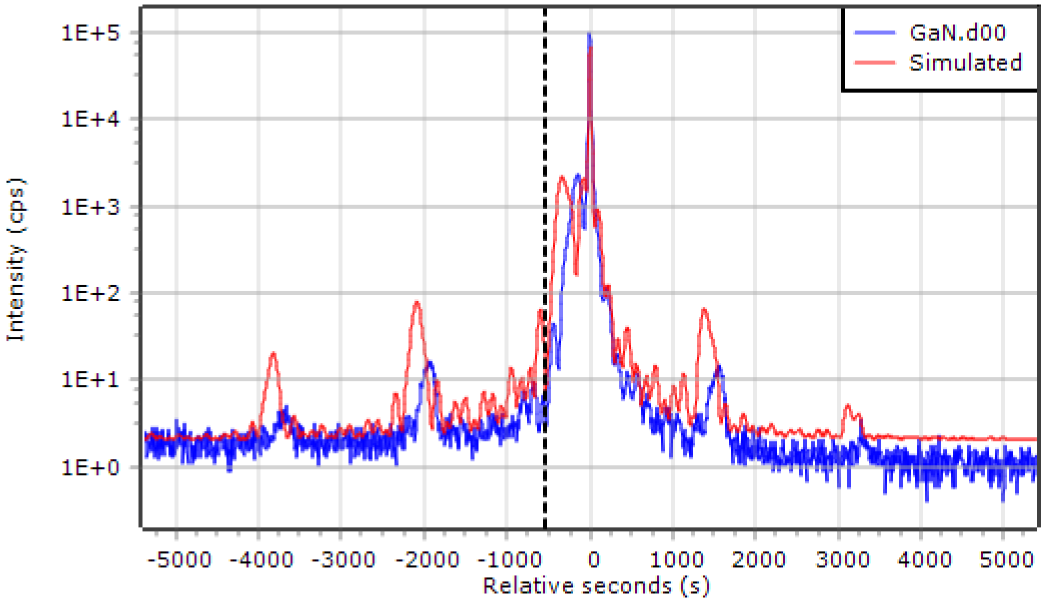
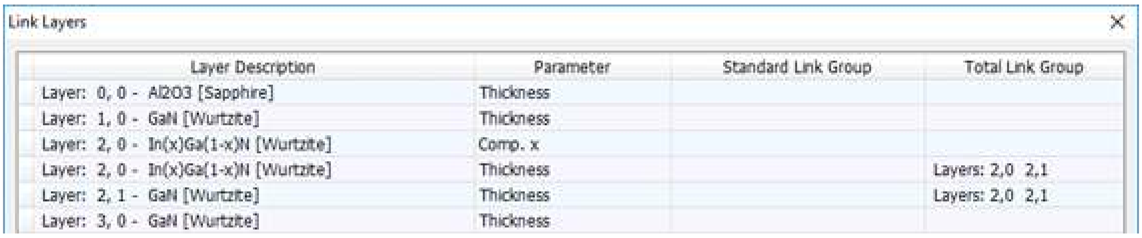


Figure 8.14 Loaded data and the first simulation

The first layer peak of the simulated scan is matched to the highest peak of the measured scan. This is because the sapphire peak is out of range of the measured scan. For this example, we use a sample file with a total link. If you want to see the information about this link, do as follows:

a. Go to the **Sample Details** tab.
b. In the **Layers** pane, click **Link layers**.



Layer Description	Parameter	Standard Link Group	Total Link Group
Layer: 0, 0 - Al2O3 [Sapphire]	Thickness		
Layer: 1, 0 - GaN [Wurtzite]	Thickness		
Layer: 2, 0 - In(x)Ga(1-x)N [Wurtzite]	Comp. x		
Layer: 2, 0 - In(x)Ga(1-x)N [Wurtzite]	Thickness		Layers: 2,0 2,1
Layer: 2, 1 - GaN [Wurtzite]	Thickness		Layers: 2,0 2,1
Layer: 3, 0 - GaN [Wurtzite]	Thickness		

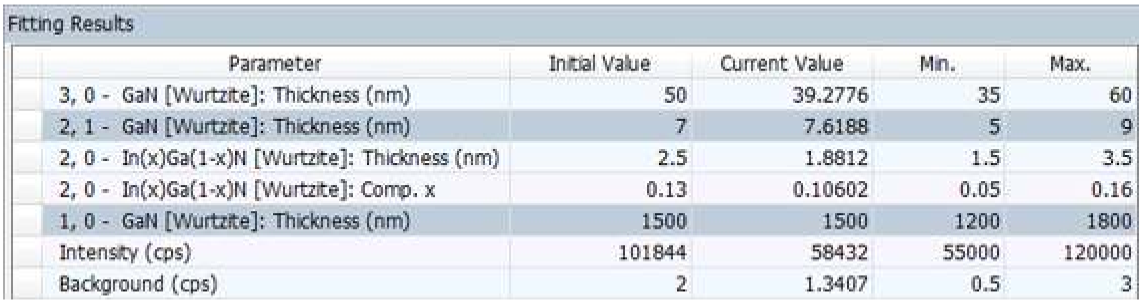
Figure 8.15 *Link Layers window*

There is a total link between the 2 layers of the superlattice. This has been done to get a good estimate of the period (the combined thickness of the 2 layers) from the satellite peak positions. In the sample file "GaN4.s00", the period was made the same as the estimated period and we **do not** want this to change during fitting.

c. Click **OK** to close the **Link Layers** window.

8.3.2.2 Fit sample parameters

1. Press F3 to start the fit. During fitting, only 2 curves are shown in the graphics area and the difference plot. These are the smoothed measured curve and the current simulated curve. The progress of the fitting is indicated in the **Fitting Results** tab.



Parameter	Initial Value	Current Value	Min.	Max.
3, 0 - GaN [Wurtzite]: Thickness (nm)	50	39.2776	35	60
2, 1 - GaN [Wurtzite]: Thickness (nm)	7	7.6188	5	9
2, 0 - In(x)Ga(1-x)N [Wurtzite]: Thickness (nm)	2.5	1.8812	1.5	3.5
2, 0 - In(x)Ga(1-x)N [Wurtzite]: Comp. x	0.13	0.10602	0.05	0.16
1, 0 - GaN [Wurtzite]: Thickness (nm)	1500	1500	1200	1800
Intensity (cps)	101844	58432	55000	120000
Background (cps)	2	1.3407	0.5	3

Figure 8.16 *Fitting Results*

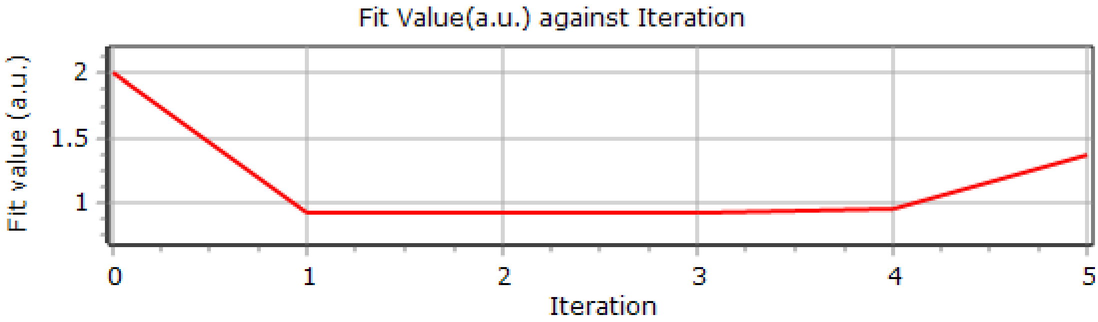


Figure 8.17 *Fitting plot*

2. Examine the values in the **Fitting Results** tab. If necessary, edit the values of all highlighted cells in the **Sample Details** tab so that they are no longer the same as the current value.
3. If you changed the values, press F3 to start the fit again.

   At the end of the fitting the final simulated curve is shown together with the measured and the initially simulated scan. Scans which were previously loaded in the same window will also be shown.

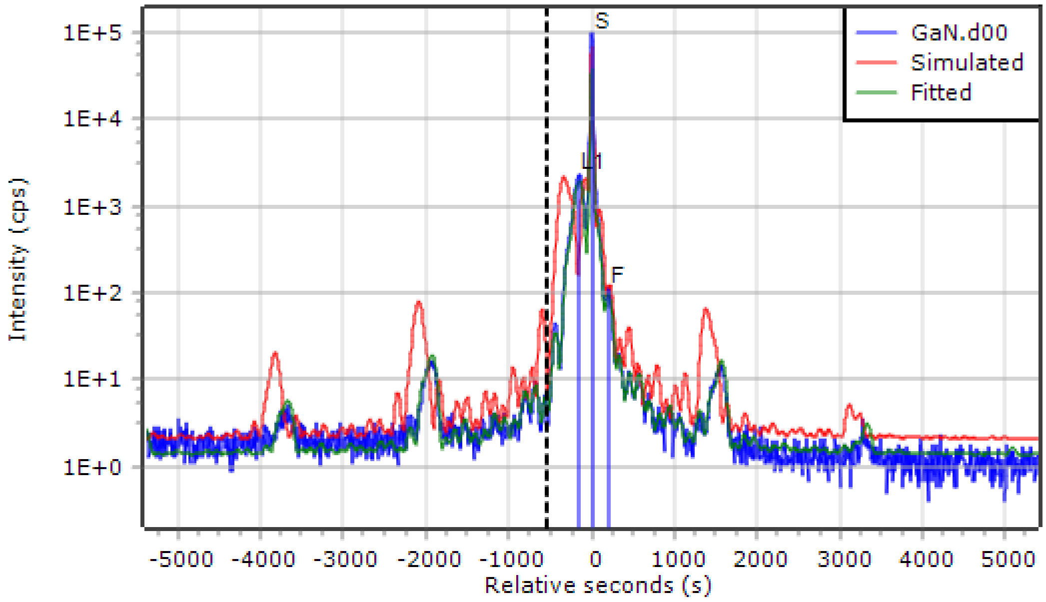


Figure 8.18 The fitted curve now matches the experimental data

8.3.2.3 Confidence analysis

1. Go to **Simulation and Fitting > Perform Fitting Confidence Analysis**. The results of the confidence analysis are shown in the table of the **Fitting Results** tab. The columns **Low** and **High** show the calculated confidence ranges of each parameter based on the error percentage values set.

Fitting Results

Parameter	Initial Value	Current Value	Low	High	Min.	Max.
3, 0 - GaN [Wurtzit	50	39.2776	37.7225	40.2941	35	60
2, 1 - GaN [Wurtzit	7	7.6188	5	9	5	9
2, 0 - In(x)Ga(1-x)N	2.5	1.8812	1.8242	1.9712	1.5	3.5
2, 0 - In(x)Ga(1-x)N	0.13	0.10602	0.10251	0.1105	0.05	0.16
1, 0 - GaN [Wurtzit	1500	1500	1200	1663.6292	1200	1800
Intensity (cps)	101844	58432	55000	66058	55000	120000
Background (cps)	2	1.3407	1.2367	1.4535	0.5	3

Figure 8.19 Fitting results with confidence ranges

2. If you want more information about a particular analysis, do as follows:
   a. Select the parameter.
   b. Go to **Simulation and Fitting > Plot Parameter's Fitting Confidence**.

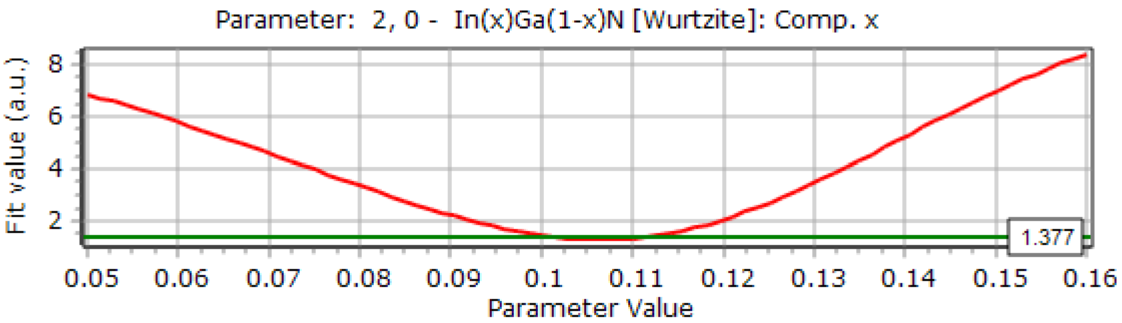


Figure 8.20 Fitting confidence plot with predefined error percentage line

The green horizontal line shows the predefined error percentage value. The cross sections with the red curve give the confidence range shown in the grid.

3. Save the project:
   a. Go to **File > Save Project As**.
   b. In the **File name** field, enter "HR_Fitting_Example2.aprjxl".
   c. Click **Save**.

8.3.2.4 Set up a report

1. Go to **Report > Report Setup**.
2. In the **Available report items** field, select the item that you want to include in the report.
3. Click >.
4. Go back to step 2 until you have added all the items that you want to include in the report.
5. Click **OK**.
6. If you want to print the report, go to **Report > Print Report**.
7. If you want to save the report, go to **Report > Save Report To File As** and select the format that you want to save the report as.

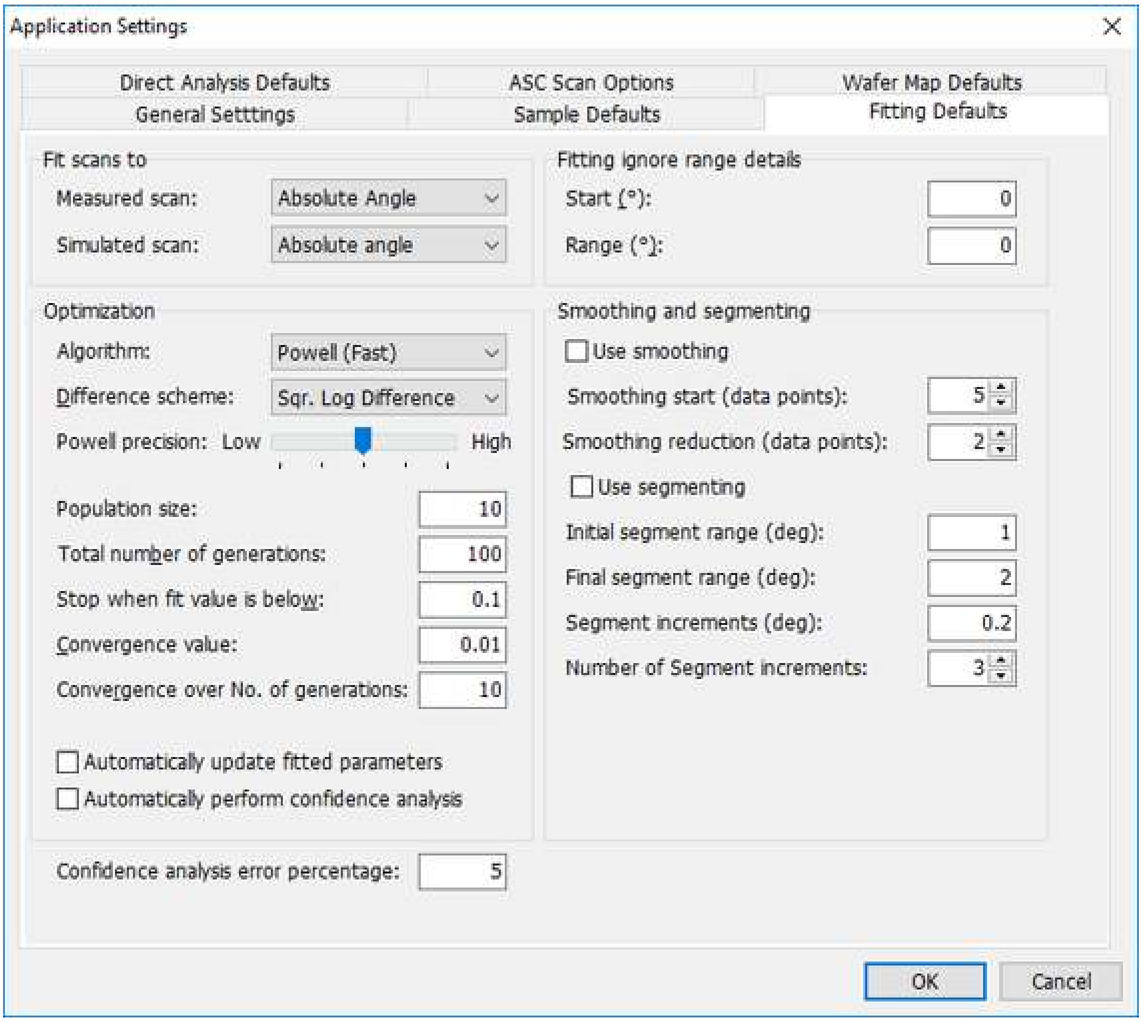
CHAPTER 9 MAKE SIMULATIONS AND USE AUTOMATIC FITTING OF SPECULAR REFLECTIVITY CURVES

9.1 Introduction

This chapter gives information about how to make a sample that contains a substrate and 2 single layers, and then do a simulation and fit the sample parameters.

9.2 Prepare the program

1. Start AMASS.
2. Go to **View > View as Reflectivity**.
3. Go to **Settings > Application Settings**.
4. Go to the **Fitting Defaults** tab.
5. From the **Algorithm** drop-down list, select **Powell (Fast)**.
6. From the **Difference scheme** drop-down list, select **Sqr. Log Difference**.
7. Clear the **Automatically update fitted parameters** check box.
8. In the **Confidence analysis error percentage**, enter "5".



Measured scan: Absolute Angle

Simulated scan: Absolute angle

Start (°): 0

Range (°): 0

Algorithm: Powell (Fast)

Difference scheme: Sqr. Log Difference

Powell precision: Low – High

Population size: 10

Total number of generations: 100

Stop when fit value is below: 0.1

Convergence value: 0.01

Convergence over No. of generations: 10

☐ Automatically update fitted parameters

☐ Automatically perform confidence analysis

Confidence analysis error percentage: 5

☐ Use smoothing

Smoothing start (data points): 5

Smoothing reduction (data points): 2

☐ Use segmenting

Initial segment range (deg): 1

Final segment range (deg): 2

Segment increments (deg): 0.2

Number of Segment increments: 3

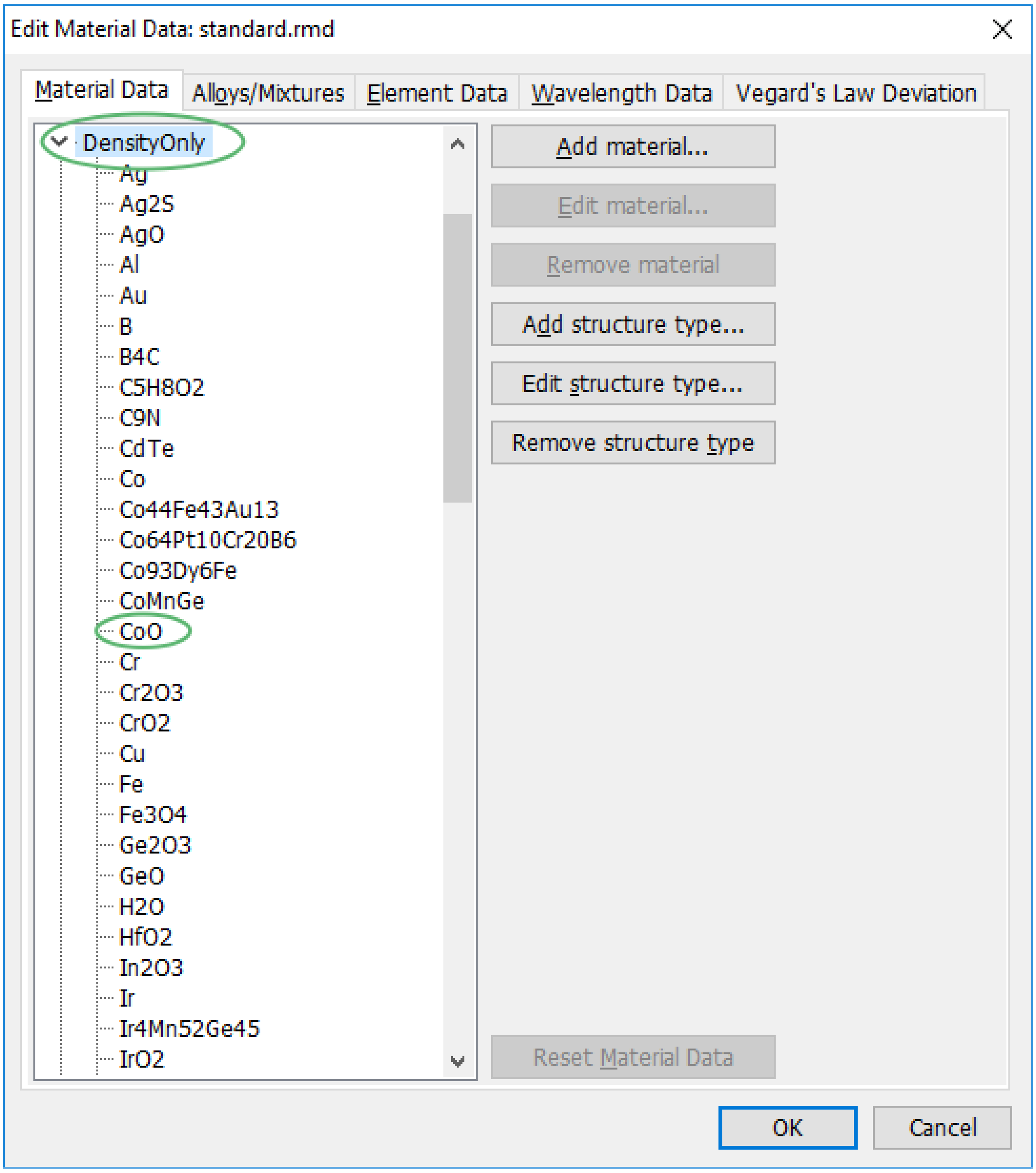
Figure 9.1 *Fitting Defaults tab*

9. Click **OK**.

9.2.1 Prepare materials in the material data file

The status bar shows "Standard.rmd" in the first box from the left to show that this is the current database.

1. Examine the available materials:
   a. Go to **Sample > Edit Material Data**.
   b. In the **DensityOnly** list, select **CoO**.



c. Click **Edit material**.

d. Make sure that the **Density (g/cm3)** value is correct:

- CoO, density = 6.45 g/cm3
- Fe3O4, density = 5.18 g/cm3
- SrTiO3, density = 5.1 g/cm3

e. Click **OK**.

f. Do steps b to e again for **Fe3O4** and **SrTiO3**.

g. Click **OK**.

h. If you get the message **Material data has changed. Do you want to save it?**, click **Yes** and then save the file.

2. If materials are missing, add them to the materials database:

a. Click **Add material**.

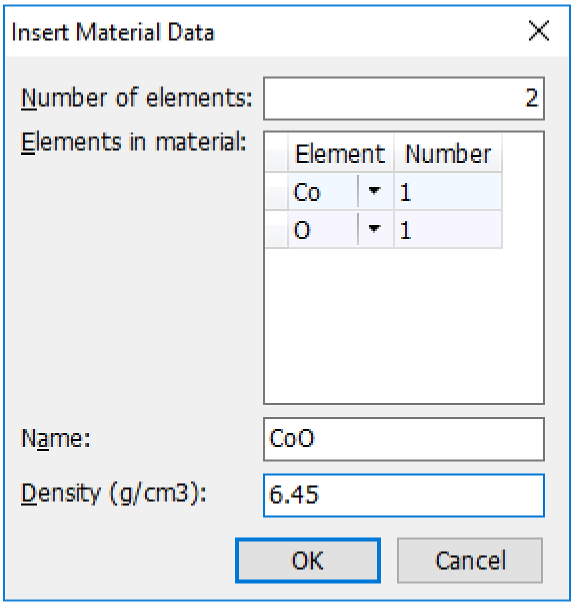
b. In the **Number of elements** field, enter "2".

c. From the first **Element** drop-down list, select the necessary element. In this example, **Co**.

d. From the second **Element** drop-down list, select the necessary element. In this example, **O**.

e. Click in the **Name** field to see the proposed material name. In this example, **CoO**.

f. In the **Density (g/cm3)** field, enter "6.45".



Number of elements: 2

Elements in material:

Element	Number
Co	1
O	1

Name: CoO

Density (g/cm3): 6.45

Figure 9.3 Insert Material Data window

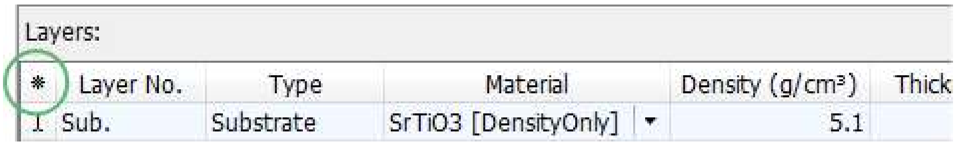
g. Click **OK**.

9.2.2 Make a new sample

1. Go to **Sample > New Sample**.
2. From the **Material** drop-down list, select **SrTiO3 [DensityOnly]**. If you want to see less material structures in the drop-down list, do as follows:
   a. In the **Extras** pane, click **Customize editor**.
   b. Clear the applicable check boxes.
   c. Click **OK**.
3. Make sure that the **Density (g/cm3)** is 5.1.
4. In the **Roughness (nm)** field, enter "1".

   There are 3 columns shown at the end of the grid: refractive index components **Delta**, **Beta** and **Elect. Density**. These values cannot be edited, because they are related to the selected wavelength selected on the **Simulation Setup** tab. If you do not want to see these columns, do as follows:

   a. Click * in the top left corner of the grid.



Layer No.	Type	Material	Density (g/cm³)	Thick
1 Sub.	Substrate	SrTiO3 [DensityOnly]	5.1	

Figure 9.4 Location of the asterisk button

   b. Clear the check boxes.

5. Add a layer to the sample:
    a. In the **Layers** pane, click **Add Layer**. The substrate layer moves down 1 row and the new layer is the top row.
    b. From the **Material** drop-down list, select **CoO [DensityOnly]**.
    c. Make sure that the **Density (g/cm3)** is 6.45.
    d. In the **Thickness (nm)** field, enter "40".
    e. In the **Roughness (nm)** field, enter "1".
6. Add the last layer to the sample:
    a. In the **Layers** pane, click **Add Layer**.
    b. From the **Material** drop-down list, select **Fe3O4 [DensityOnly]**.
    c. Make sure that the **Density (g/cm3)** is 5.18.
    d. In the **Thickness (nm)** field, enter "10".
    e. In the **Roughness (nm)** field, enter "1".
    f. In the **Sample length (mm)** field, enter "20".
7. Save the sample:
    a. Go to **Sample > Save Sample As**.
    b. In the **File Name** field, enter "Sample 1 for AG.asamxl".
    c. Click **Save**.

9.3 Set up the simulation

1. Go to **File > Open Scan(s)**.
2. Go to **C:\Users\User.Name\Documents\PANalytical\AMASS\Examples**.
3. Select "XRR-1.X00".
4. Click **Open**.

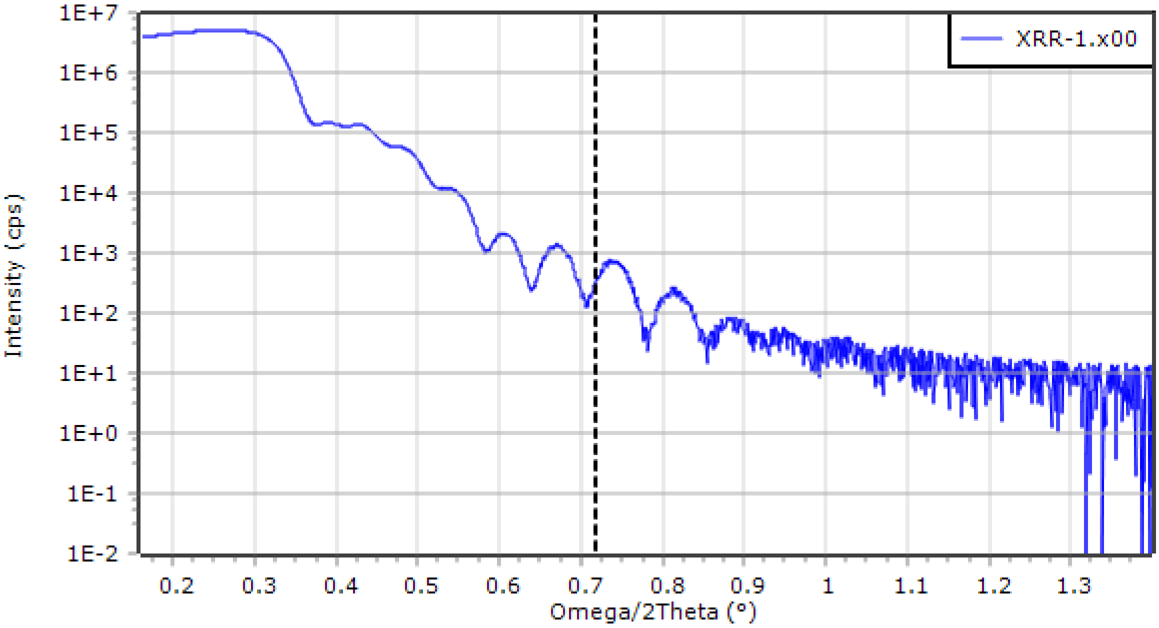


Figure 9.5 XRR scan data

5. Go to the **Simulation Setup** tab.

6. From the **Scan type** drop-down list, select **Specular: Omega/2Theta scan**.
7. Click **Use selected scan's values**. The **Start (deg)** and **End (deg)** fields will be updated with the values of the opened scan.
8. Select the **Normalise intensity** check box.
9. Click ... of **Primary wavelength (A)**.
10. Select the correct wavelength. In this example, **CuKa**.
11. Click **OK**.
12. Press F2 to start the simulation. A red line shows on the graph.
13. Make sure that the instrument parameters are correct:
    a. From the **Monochromator** drop-down list, select **Divergence**.
    b. In the **Value** field of **Background (cps)**, enter "5".
    c. In the **Value** field of **Divergence (°)**, enter "0.004".
    d. In the **Beam width (mm)** field, enter "0.1".
    e. Select the **Use sample and beam details** check box.
    f. Press F2 to start the simulation.

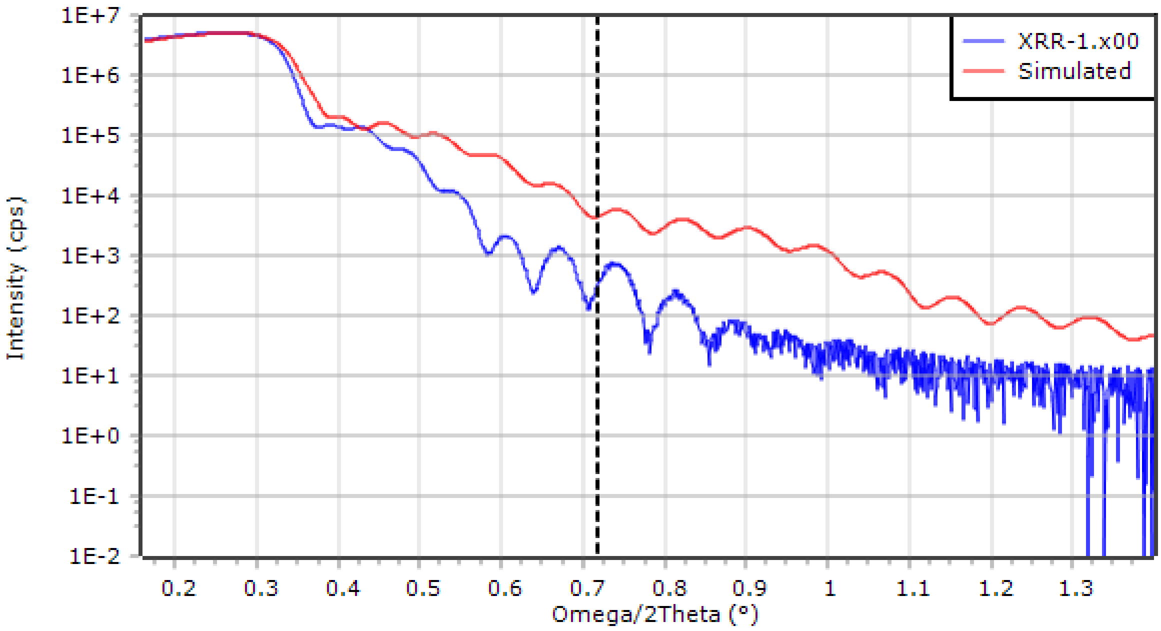


Figure 9.6 Simulated specular reflectivity curve

9.4 Fit sample parameters

9.4.1 Set the defaults

In this part of the exercise, the fitting parameters are set for the program and the cursor is moved to the end of the initial fitting scan range.

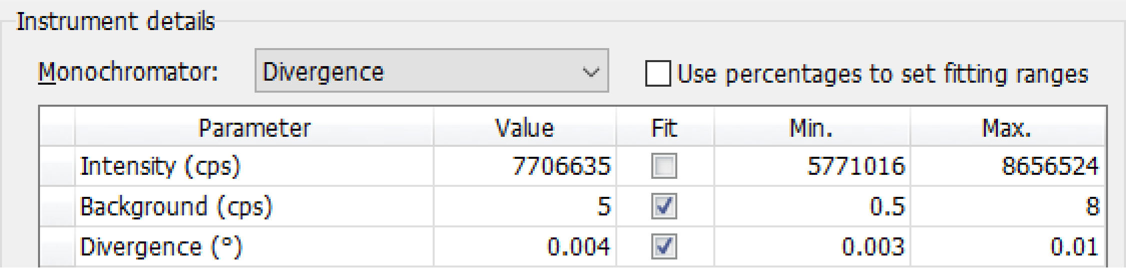
1. Move the cursor line to approximately 0.8°.
2. Right-click and then select **Use Cursor Position to Set Segment Increments**.
3. Go to the **Fitting Setup** tab.
4. From the **Algorithm** drop-down list, select **Powell (Fast)**.

5. From the **Difference scheme** drop-down list, select **Sqr. Log Difference**.
6. Make sure that the **Automatically update fitted parameters** is cleared.
7. Select these check boxes:
   - **Use smoothing**
   - **Use segmenting**
8. Go to the **Sample Details** tab.
9. Clear the **Use percentages to set fitting ranges** check box.
10. Select the substrate.
11. In the **Layer Details** pane, clear the **Fit** check boxes in **Density Details** and **Thickness Details**.
12. Use these settings:

Table 9.1 Roughness and thickness values

Layer	Parameter	Minimum	Maximum
2,0	Thickness	5	15
2,0	Roughness	0.5	2.5
1,0	Thickness	35	48
1,0	Roughness	0.5	2.2
Substrate	Roughness	0.5	1.5

13. Go to the **Simulation Setup** tab.
14. Use these settings:



Instrument details

Monochromator: Divergence

☐ Use percentages to set fitting ranges

Parameter	Value	Fit	Min.	Max.
Intensity (cps)	7706635	☐	5771016	8656524
Background (cps)	5	☑	0.5	8
Divergence (°)	0.004	☑	0.003	0.01

Figure 9.7 Instrument details settings

15. Press F3 to start the fitting. Examine the green line, it must stay close to the blue line. If it does not, the fitting parameters must be changed. For example, increase the minimum and maximum ranges, try another difference scheme, or try another fitting method (genetic algorithm).

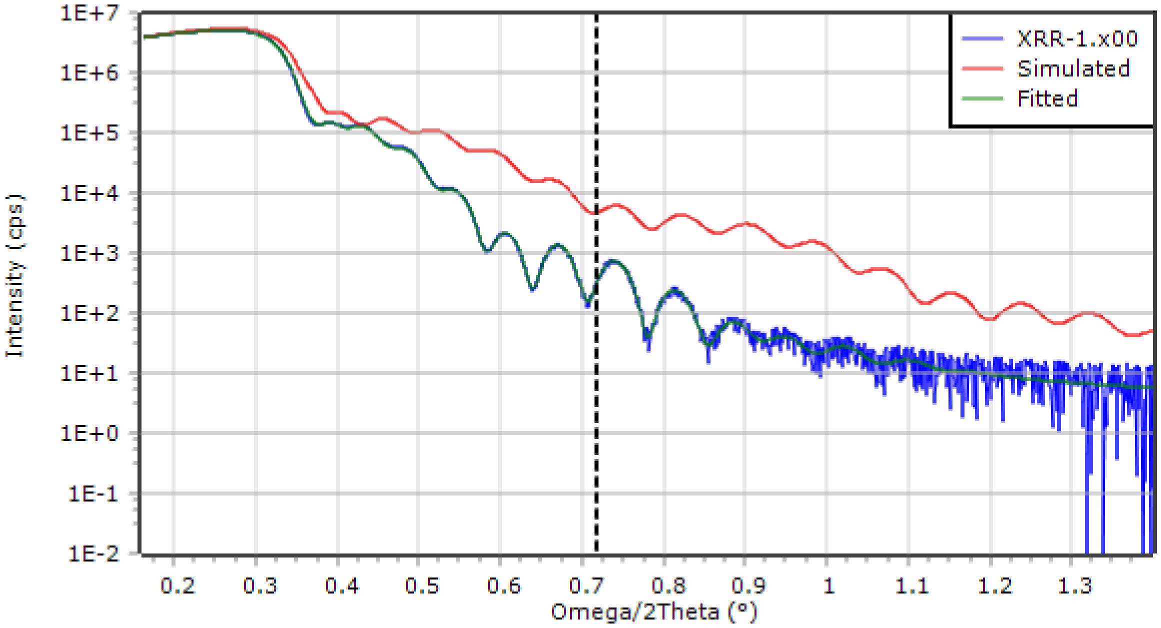
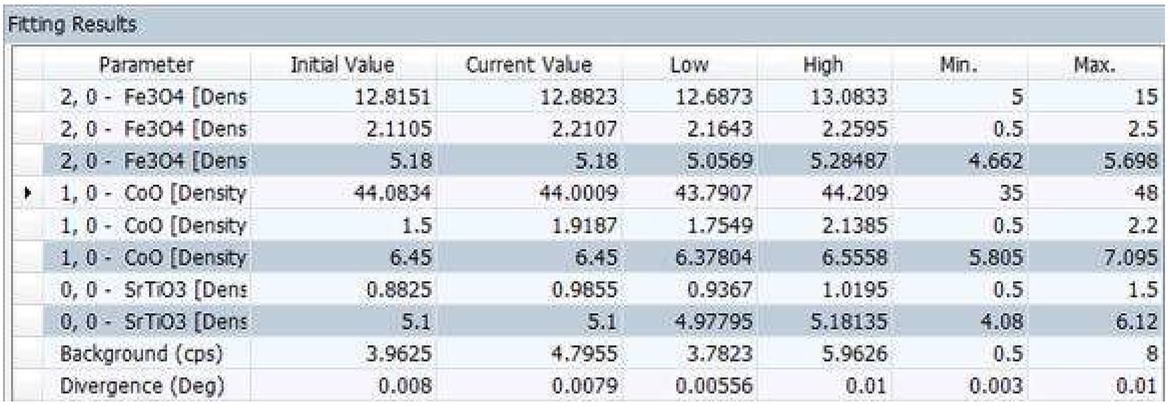


Figure 9.8 *Simulated and fitted specular reflectivity curves*

16. If you want to accept simulated and fitted curves, double-click them in the **Scan List** pane. If you do another simulation, these curves are saved. If you do not accept the curves, they are overwritten with the next simulation.
17. If the results are good, press F5 to update the sample with the refined parameters.

9.4.2 Confidence analysis

1. Press F6 to do the fitting confidence analysis.
2. Go to **Simulation and Fitting > Perform Fitting Confidence Analysis**. The results of the confidence analysis are shown in the table of the **Fitting Results** tab. It will show the columns **Low** and **High** that show the calculated confidence ranges of each parameter based on the error percentage values set.


Fitting Results

	Parameter	Initial Value	Current Value	Low	High	Min.	Max.
	2, 0 - Fe3O4 [Dens	12.8151	12.8823	12.6873	13.0833	5	15
	2, 0 - Fe3O4 [Dens	2.1105	2.2107	2.1643	2.2595	0.5	2.5
	2, 0 - Fe3O4 [Dens	5.18	5.18	5.0569	5.28487	4.662	5.698
▸	1, 0 - CoO [Density	44.0834	44.0009	43.7907	44.209	35	48
	1, 0 - CoO [Density	1.5	1.9187	1.7549	2.1385	0.5	2.2
	1, 0 - CoO [Density	6.45	6.45	6.37804	6.5558	5.805	7.095
	0, 0 - SrTiO3 [Dens	0.8825	0.9855	0.9367	1.0195	0.5	1.5
	0, 0 - SrTiO3 [Dens	5.1	5.1	4.97795	5.18135	4.08	6.12
	Background (cps)	3.9625	4.7955	3.7823	5.9626	0.5	8
	Divergence (Deg)	0.008	0.0079	0.00556	0.01	0.003	0.01

Figure 9.9 *Fitting results with confidence ranges*

3. If you want more information about a particular analysis, do as follows:
   a. Select the parameter.
   b. Go to **Simulation and Fitting > Plot Parameter's Fitting Confidence**.

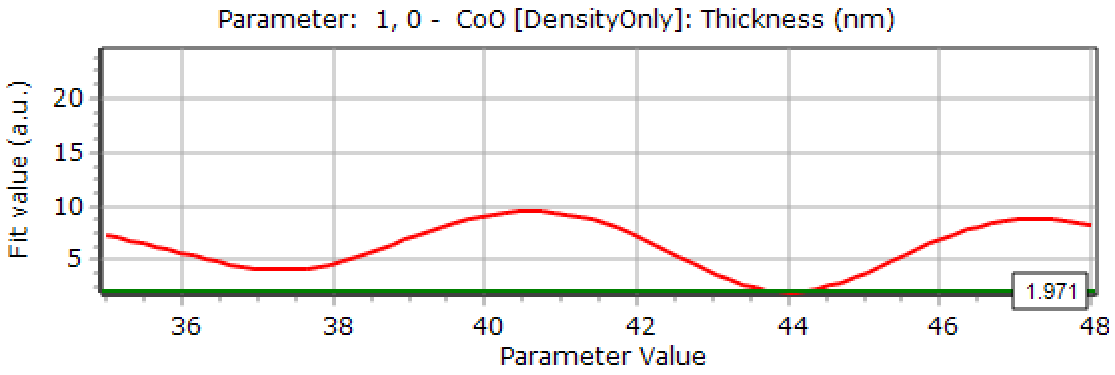


Figure 9.10 Fitting confidence plot

The green horizontal line show the predefined error percentage value. The cross sections with the red curve give the confidence range shown in the grid.

4. Save the project:
    a. Go to **File > Save Project As**.
    b. In the **File name** field, enter "XRR_Fitting.aprjxl".
    c. Click **Save**.

9.5 Set up a report

1. Go to **Report > Report Setup**.
2. In the **Available report items** field, select the item that you want to include in the report.
3. Click >.
4. Go back to step 2 until you have added all the items that you want to include in the report.
5. Click **OK**.
6. If you want to print the report, go to **Report > Print Report**.
7. If you want to save the report, go to **Report > Save Report To File As** and select the format that you want to save the report as.

CHAPTER 10 MAKE A WAFER MAP FROM A SET OF DIFFRACTION DATA

10.1 Introduction

A wafer map shows the variation in sample parameters (for example, substrate peak width or layer mismatch) as a function of position on the wafer. A minimum of 1 series of rocking curves, recorded from an array of points on the sample, is necessary as input. More than one series of different experimental data can be used. For example, to combine the analysis of rocking curves recorded at different hkl reflections and related reciprocal space maps.

There are 2 sets of example data used in these exercises. The first set is an array of rocking curves recorded on the (002) and (102) reflections from a thick gallium nitride layer on a silicon wafer. The change in position of the substrate peak is used to show the distortion of the wafer while the peak widths of the rocking curves is measured for the structural quality of the epilayer. A sample file is not necessary for this analysis. This type of wafer map can be applied to all substrate materials.

The second set is from a strained (relaxation = 0 %) gallium indium arsenide phosphide layer on an indium phosphide substrate with an indium phosphide cap. The variation in layer mismatch is calculated from the variation in the separation of the substrate and quaternary layer peaks. A sample file is necessary for this analysis.

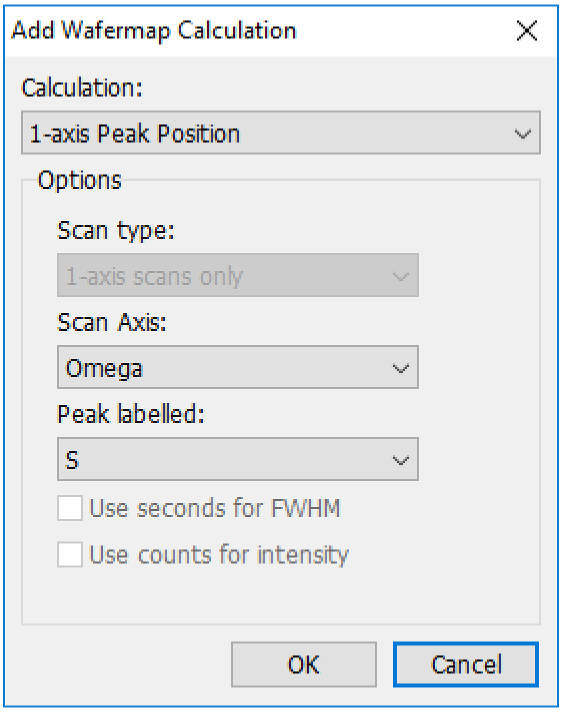
10.2 Make a wafer map to show distortion and structural quality

The measured sample was a 100 mm silicon (001) wafer with a deposited layer of gallium nitride. A regular array of rocking curves was collected on the (002) and (102) GaN reflections with a general batch program in Data Collector.

These files are supplied for this example:

- X_Y_1.xrdml: (002) rocking curve data
- X_Y_4.xrdml: (102) rocking curve data

1. Start AMASS.
2. Go to **Settings > Application Settings**.
3. Go to the **Wafer Map Defaults** tab.
4. Click **Set wafer outline**.
5. In the **Orientation (°)** field, enter "180".
6. Click **OK**.
7. In the **Calculations to perform** grid, select the default.
8. Click **Edit**.
9. Use these settings:



Add Wafermap Calculation

Calculation: 1-axis Peak Position

Scan type: 1-axis scans only

Scan Axis: Omega

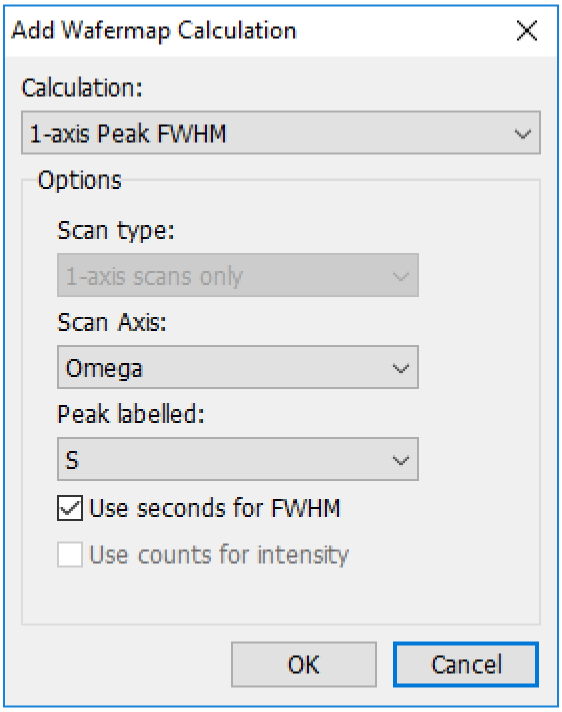
Peak labelled: S

☐ Use seconds for FWHM

☐ Use counts for intensity

Figure 10.1 1-axis peak position calculation

10. Click **OK** to close the window.
11. Click **Add**.



Add Wafermap Calculation

Calculation: 1-axis Peak FWHM

Scan type: 1-axis scans only

Scan Axis: Omega

Peak labelled: S

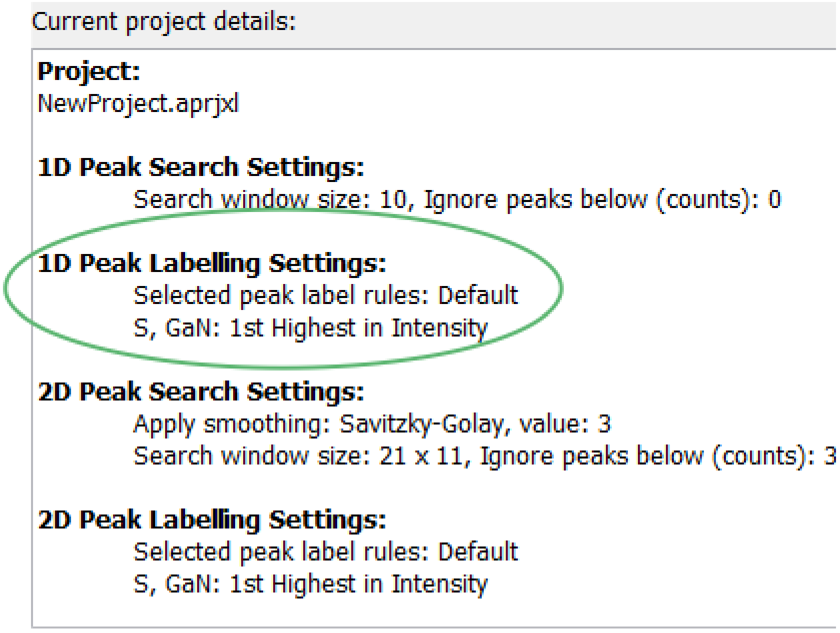
☑ Use seconds for FWHM

☐ Use counts for intensity

Figure 10.2 1-axis peak FWHM calculation

12. Click **OK** to close the window.
13. Go to the **Direct Analysis Defaults** tab.
14. Select the **Peak label** check box for measured 1-axis scan in the **Automatic peak marking on opening scans** frame.

15. Click **OK** to close the **Application Settings** window.
16. Set the 1-axis peak search details:
    a. Go to the **1-axis Peak Search Details** tab.
    b. Select the **Set window size automatically** check box.
    c. Select **Set peak to peak center**.
    d. In the **Rules** grid, select **Default**.
    e. The description must read **S, GaN: 1st Highest in Intensity**. If this is not correct, edit the rule.
17. Go to **Wafer Map > Generate Wafer Map**.
18. In the **Current project details** frame, make sure that the **1D Peak Labelling Settings** are correct.



Current project details:

Project:
NewProject.aprjxl

1D Peak Search Settings:
Search window size: 10, Ignore peaks below (counts): 0

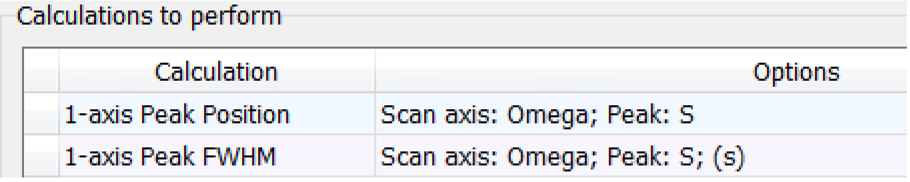
1D Peak Labelling Settings:
Selected peak label rules: Default
S, GaN: 1st Highest in Intensity

2D Peak Search Settings:
Apply smoothing: Savitzky-Golay, value: 3
Search window size: 21 x 11, Ignore peaks below (counts): 3

2D Peak Labelling Settings:
Selected peak label rules: Default
S, GaN: 1st Highest in Intensity

Figure 10.3 1D Peak Labelling Settings

19. In the **Calculations to perform** frame, make sure that the calculations are set correctly.



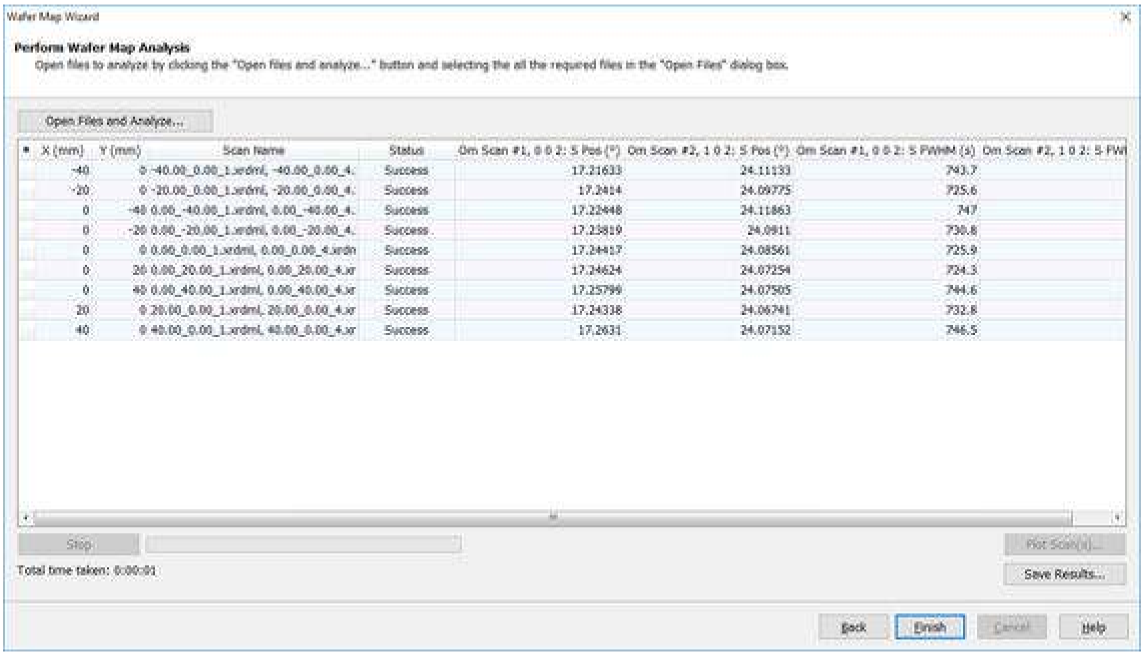
Calculations to perform

Calculation	Options
1-axis Peak Position	Scan axis: Omega; Peak: S
1-axis Peak FWHM	Scan axis: Omega; Peak: S; (s)

Figure 10.4 Calculations for Wafermap1

20. Save the project:
    a. Click **Save Project File**.
    b. In the **File name** field, enter "Wafermap1.aprjxl".
    c. Click **Save**.
21. Click **Next**.
22. Click **Open Files and Analyze**.
23. Go to **C:\Users\User.Name\Documents\PANalytical\AMASS\Examples\Wafermap1**.

24. Select all files.
25. Click **Open**. The analysis is automatically done and the results are shown.



Perform Wafer Map Analysis

Open files to analyze by clicking the "Open files and analyze..." button and selecting the all the required files in the "Open Files" dialog box.

•	X (mm)	Y (mm)	Scan Name	Status	Om Scan #1, 0 0 2: S Pos (°)	Om Scan #2, 1 0 2: S Pos (°)	Om Scan #1, 0 0 2: S FWHM (s)	Om Scan #2, 1 0 2: S FW
	-40	0	-40.00_0.00_1.xrdml, -40.00_0.00_4.	Success	17.21633	24.11133	743.7	
	-20	0	-20.00_0.00_1.xrdml, -20.00_0.00_4.	Success	17.2414	24.09775	725.6	
	0	-40	0.00_-40.00_1.xrdml, 0.00_-40.00_4.	Success	17.22448	24.11863	747	
	0	-20	0.00_-20.00_1.xrdml, 0.00_-20.00_4.	Success	17.23819	24.0911	730.8	
	0	0	0.00_0.00_1.xrdml, 0.00_0.00_4.xrdn	Success	17.24417	24.08561	725.9	
	0	20	0.00_20.00_1.xrdml, 0.00_20.00_4.xr	Success	17.24624	24.07254	724.3	
	0	40	0.00_40.00_1.xrdml, 0.00_40.00_4.xr	Success	17.25799	24.07505	744.6	
	20	0	20.00_0.00_1.xrdml, 20.00_0.00_4.xr	Success	17.24338	24.06741	732.8	
	40	0	40.00_0.00_1.xrdml, 40.00_0.00_4.xr	Success	17.2631	24.07152	746.5	

Total time taken: 0:00:01

Figure 10.5 Results of wafer map analysis

The status of the results is shown in the **Status** column. If necessary, review and correct the result for each **X** or **Y** position:

a. Select a coordinate.
b. Click **Plot Scan(s)**.
c. Move the cursor to the correct position.
d. Right-click and then go to **Define Main Cursor As > Peak** to correct the peak position.
e. Click **OK**.

26. Click **Finish** to continue with the wafer map results representation. The **Wafer Map Results** window shows the results and gives different choices to show the results.
27. Click **Wafer Plots** to see the positions of the measured rocking curves.

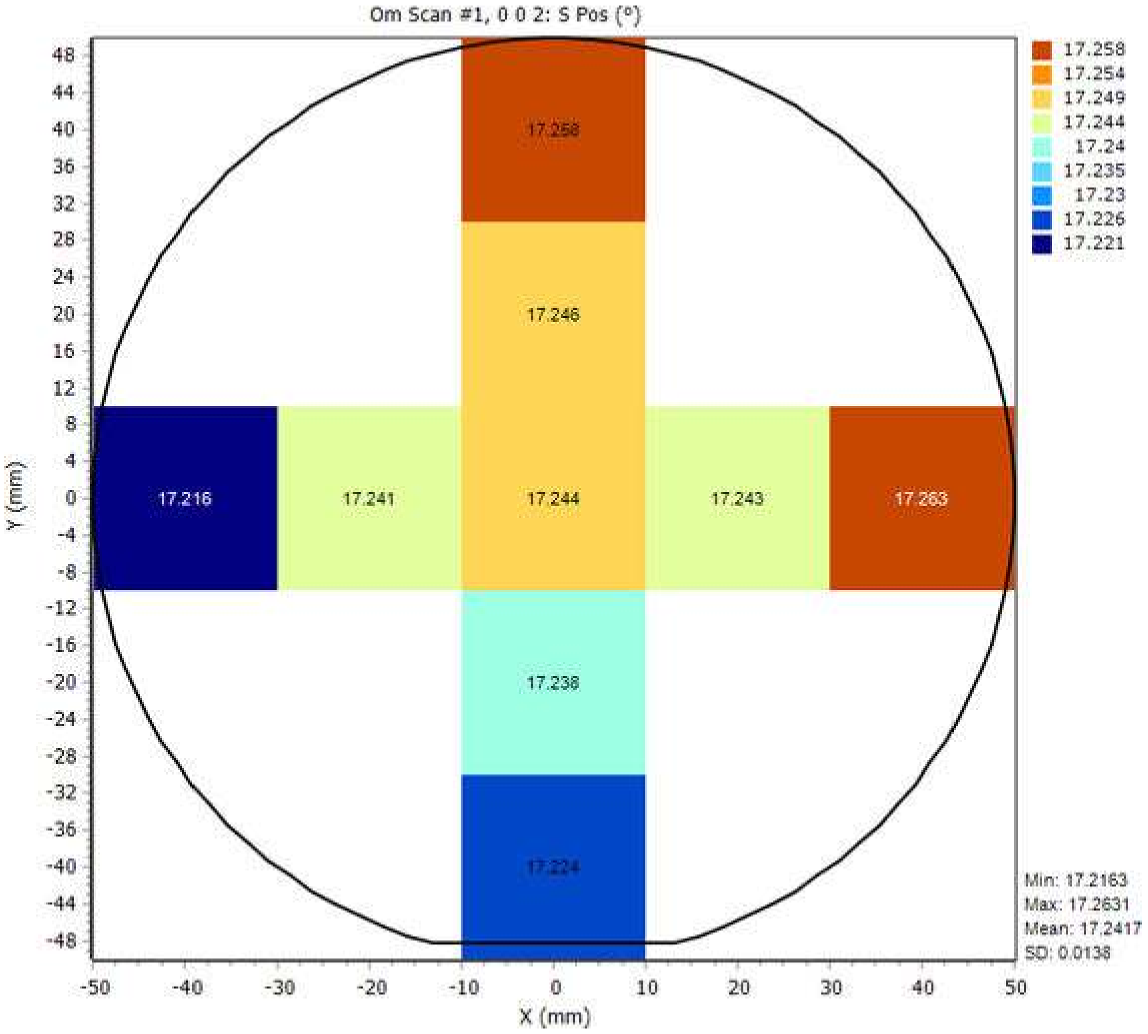


Figure 10.6 *Results of wafer map analysis as bitmap plot with values*

The mean, the minimum and maximum of the calculated data and the standard deviation are shown in the bottom right corner of the wafer map result.

28. If you want to see a different plot type, select it in the **Plot Type** frame. **Contours** is only available for data on a regular grid.
29. Save the results:
    a. Click **Save Results**.
    b. In the **File name** field, enter a file name.
    c. Click **Save**.

10.3 Make a wafer map to show mismatch variation in quaternary layer

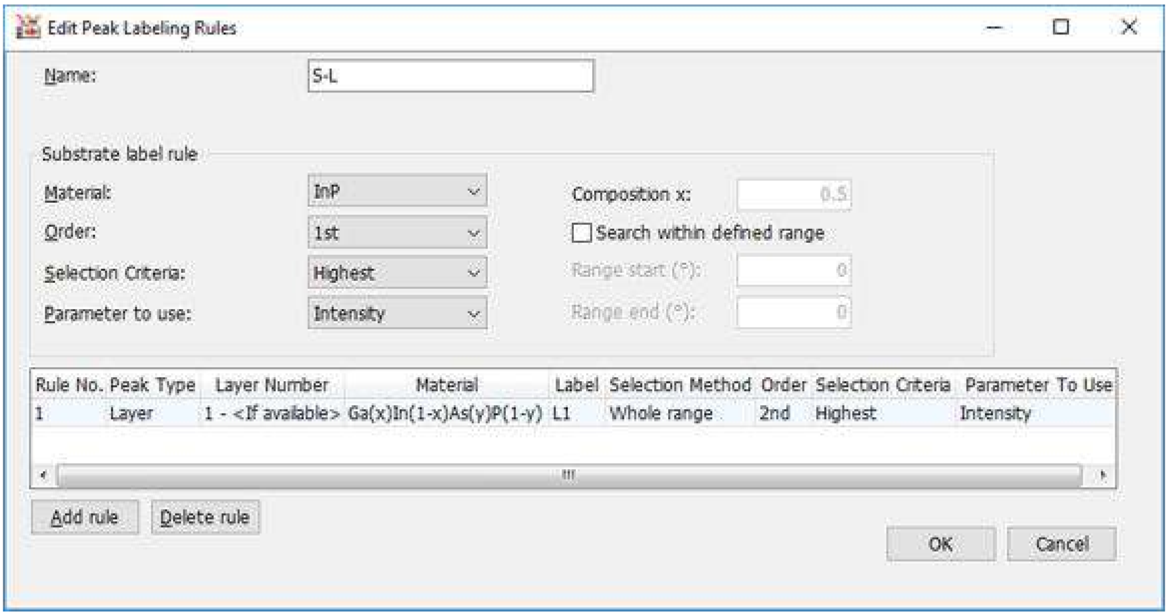
The measured sample was half of a 2-inch indium phosphide (001) wafer with a heteroepitaxial quaternary (gallium indium arsenide phosphide) layer with an indium phosphide cap. There are 36 individual 004 rocking curves scans given. These were recorded for a 9x4 rectangular array of points. The mismatch is calculated from the substrate-layer peak separation with information about the substrate and layer materials from the sample file.

The sample was installed on the MRD cradle. The coordinates were X = -1, Y = -2 for the center point of the full 2-inch wafer.

These files are supplied for this example:

- InP_Q.d00 to InP_Q.d35: 36 rocking curves in a 4x9 grid
- InP_Q.asamxl: the sample file

1. Start AMASS.
2. Go to **Sample > Open Sample**.
3. Go to **C:\Users\User.Name\Documents\PANalytical\AMASS\Examples\Wafermap2**.
4. Select "InP_Q.asamxl".
5. Click **Open**.
6. Go to the **1-axis Peak Search Details** tab.
7. Click **Add**.
8. Add a rule with these settings:



Name: S-L

Substrate label rule

Material: InP

Order: 1st

Selection Criteria: Highest

Parameter to use: Intensity

Composition x: 0.5

☐ Search within defined range

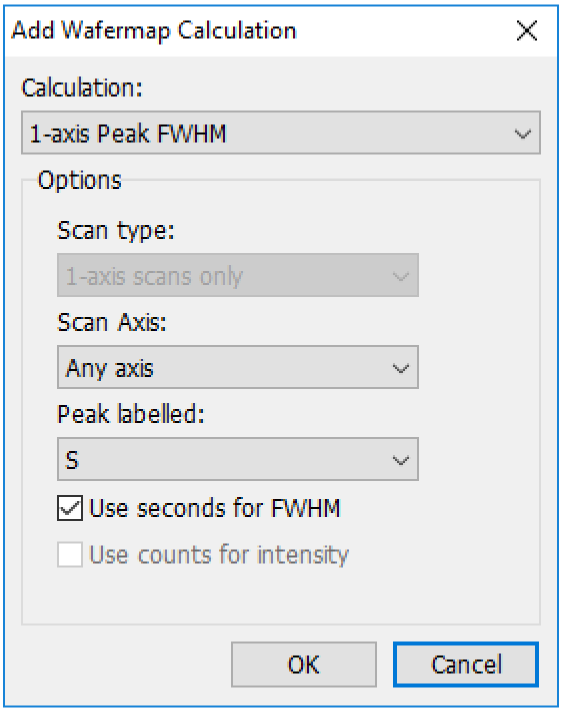
Range start (°): 0

Range end (°): 0

Rule No.	Peak Type	Layer Number	Material	Label	Selection Method	Order	Selection Criteria	Parameter To Use
1	Layer	1 - <If available>	Ga(x)In(1-x)As(y)P(1-y)	L1	Whole range	2nd	Highest	Intensity

Figure 10.7 Edit Peak Labeling Rules for Wafermap2

9. Click **OK** to close the window.
10. Go to **Wafer Map > Generate Wafer Map**.
11. Add these calculations.


Add Wafermap Calculation

Calculation: 1-axis Peak FWHM

Options

Scan type: 1-axis scans only

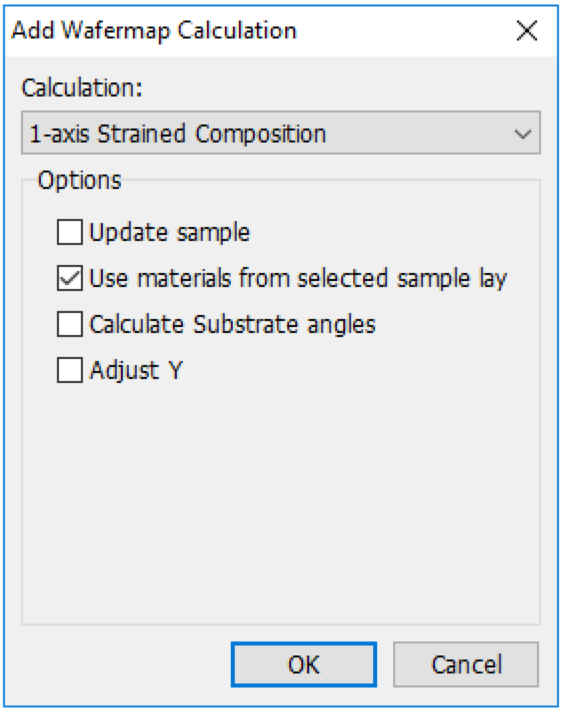
Scan Axis: Any axis

Peak labelled: S

☑ Use seconds for FWHM

☐ Use counts for intensity

Figure 10.8 1-axis peak FWHM calculation


Add Wafermap Calculation

Calculation: 1-axis Strained Composition

Options

☐ Update sample

☑ Use materials from selected sample lay

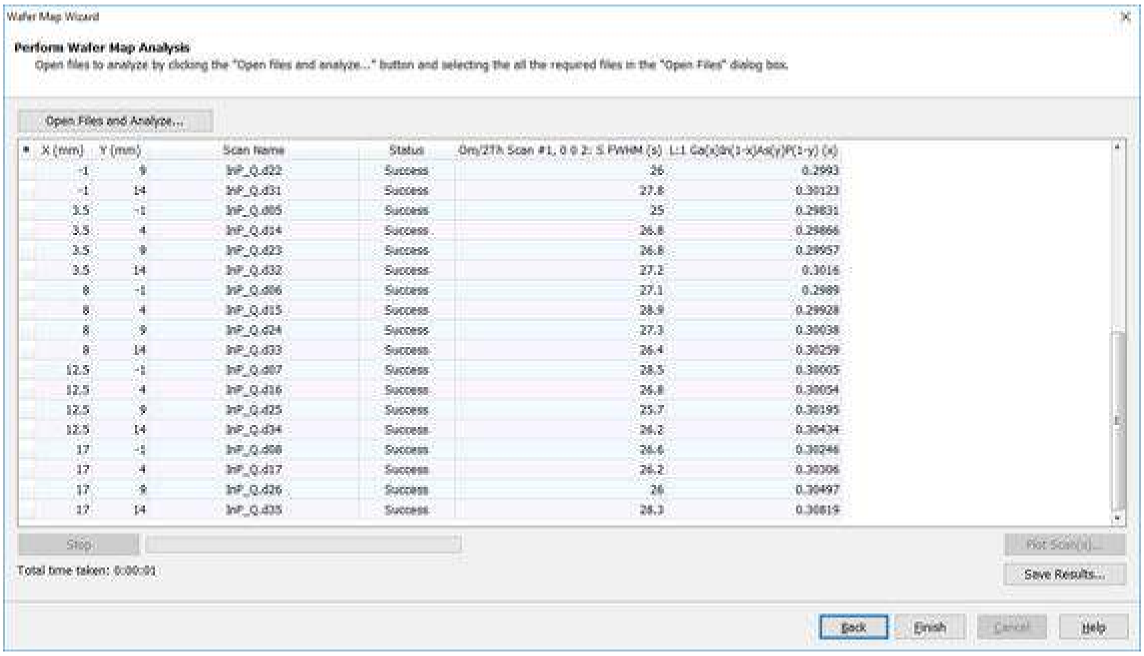
☐ Calculate Substrate angles

☐ Adjust Y

Figure 10.9 1-axis strained composition calculation

12. If there are other calculations in the list, remove them.
13. Save the project:
    a. Click **Save Project File**.
    b. In the **File name** field, enter "Wafermap2.aprjxl".
    c. Click **Save**.
14. Click **Next**.

15. Click **Open Files and Analyze** to open all files for the analysis.
16. Select the files "InP_Q.d00" to "InP_Q.d35".
17. Click **Open**. The analysis is automatically done and the results are shown.



Perform Wafer Map Analysis

Open files to analyze by clicking the "Open files and analyze..." button and selecting the all the required files in the "Open Files" dialog box.

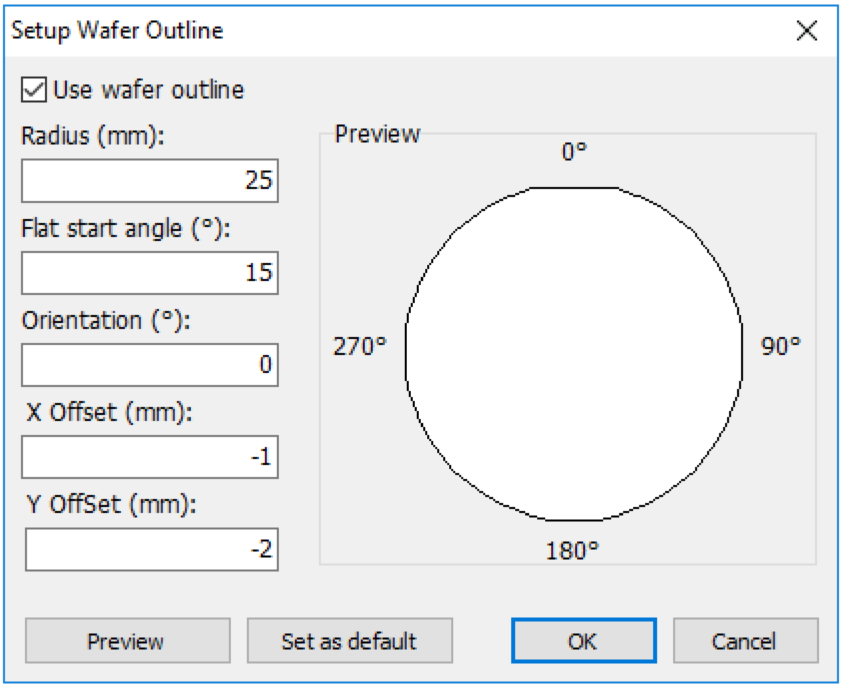
X (mm)	Y (mm)	Scan Name	Status	Om/2Th Scan #1, 0 0 2: S FWHM (s)	L:1 Ga(x)In(1-x)As(y)P(1-y) (x)
-1	9	InP_Q.d22	Success	26	0.2993
-1	14	InP_Q.d31	Success	27.8	0.30123
3.5	-1	InP_Q.d05	Success	25	0.29831
3.5	4	InP_Q.d14	Success	26.8	0.29866
3.5	9	InP_Q.d23	Success	26.8	0.29957
3.5	14	InP_Q.d32	Success	27.2	0.3016
8	-1	InP_Q.d06	Success	27.1	0.2989
8	4	InP_Q.d15	Success	28.9	0.29928
8	9	InP_Q.d24	Success	27.3	0.30038
8	14	InP_Q.d33	Success	26.4	0.30259
12.5	-1	InP_Q.d07	Success	28.5	0.30005
12.5	4	InP_Q.d16	Success	26.8	0.30054
12.5	9	InP_Q.d25	Success	25.7	0.30195
12.5	14	InP_Q.d34	Success	26.2	0.30434
17	-1	InP_Q.d08	Success	26.6	0.30246
17	4	InP_Q.d17	Success	26.2	0.30306
17	9	InP_Q.d26	Success	26	0.30497
17	14	InP_Q.d35	Success	28.3	0.30819

Total time taken: 0:00:01

Figure 10.10 Results of wafer map analysis

The table shows the x-coordinates, y-coordinates, scan names , status of the analysis, peak widths and gallium compositions.

18. Click **Finish** to continue with the wafer map results representation. The **Wafer Map Results** window shows.
19. Add information about the wafer shape:
    a. Click **Wafer Outline Details**.
    b. In the **Radius (mm)** field, enter "25".
    c. In the **X Offset (mm)** field, enter "-1".
    d. In the **Y Offset (mm)** field, enter "-2".



Setup Wafer Outline

☑ Use wafer outline

Radius (mm): 25

Flat start angle (°): 15

Orientation (°): 0

X Offset (mm): -1

Y OffSet (mm): -2

Figure 10.11 Setup Wafer Outline window

  e. Click **OK**.

20. Show and print the maps for the peak width:
    a. Click **Wafer Plots**.
    b. Click **Contours**. The layer gallium composition is shown.

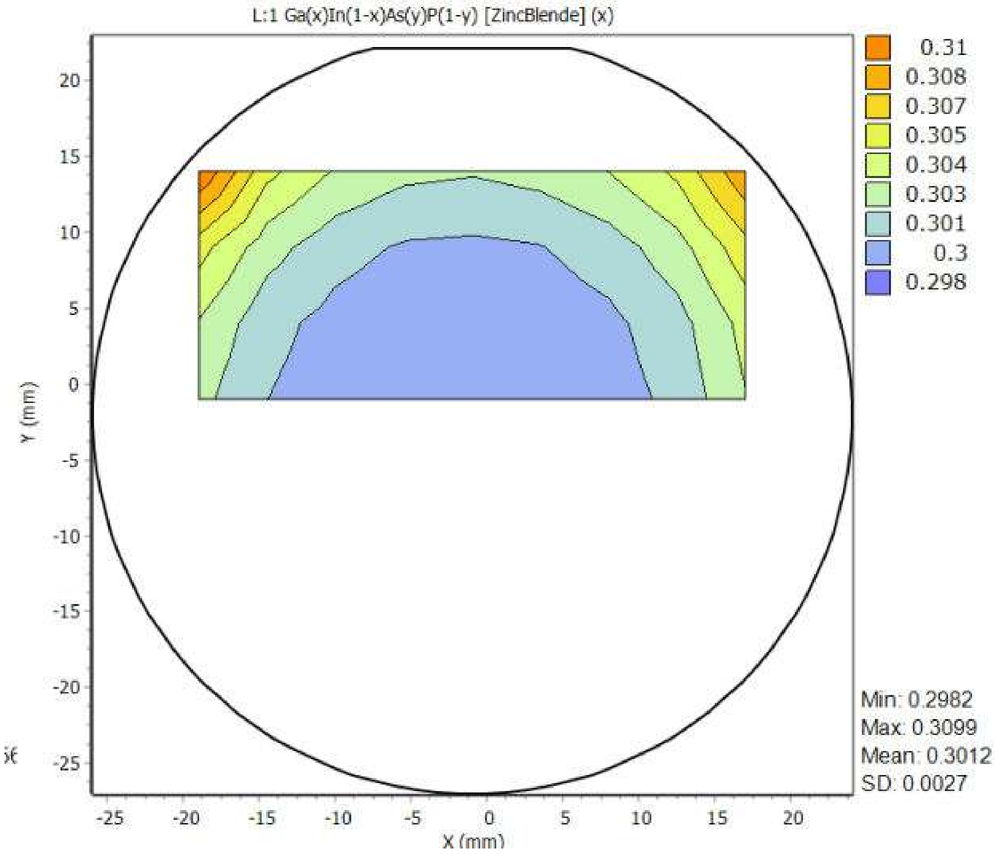


Figure 10.12 Map of gallium composition

21. Save the results:
    a. Click **Save Results**.
    b. In the **File name** field, enter a file name.
    c. Click **Save**.
22. Go to **Report > Report Setup**.
23. In the **Available report items** field, select the item that you want to include in the report.
24. Click >.
25. Go back to step 2 until you have added all the items that you want to include in the report.
26. Click **OK**.
27. If you want to print the report, go to **Report > Print Report**.
28. If you want to save the report, go to **Report > Save Report To File As** and select the format that you want to save the report as.

10.4 Wafer map analysis with AMASS Controller

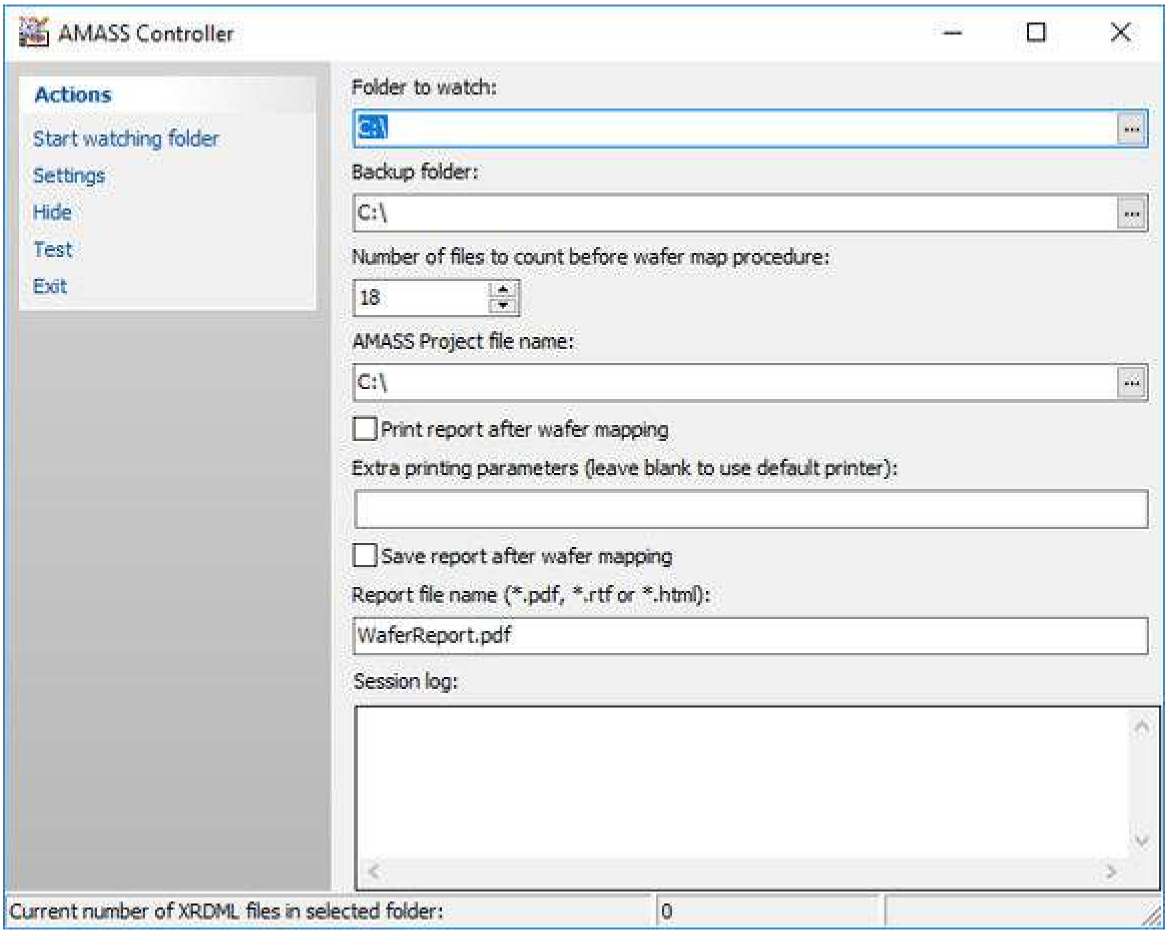
The wafer map analysis can also be done automatically with AMASS Controller. This software is installed with the AMASS installation.

The AMASS Controller monitors the number of XRDML files in a selected folder. If the number of files is the same as the specified number in the controller software, the files are moved to the backup folder. The number is specified by the measurement strategy of the wafer map in Data Collector. Then AMASS Controller reads the project file that contains all settings and parameters of the analysis followed by each measurement file. The analysis is done with the given parameters and a wafer map report is made that can be printed and saved.

If you want to use the controller software, a project file is necessary. These project files were made in the previous sections. Refer to Section 10.2., 10.3.

Set up an automatic wafer map analysis as follows:

1. On the Windows **Start** menu, go to **Start > All Programs > PANalytical AMASS > AMASS_Controller**.
2. In the **Folder to watch** field, select the folder where Data Collector saves each scan data file of a wafer map. Make sure that the folder exists.
3. In the **Backup folder** field, select the correct folder.
4. In the **Number of files to count before wafer map procedure**, enter the number of files that must be in the folder before the automatic analysis starts.
5. If you want to get a report of the analysis, fill in the necessary fields.
6. If you want to make sure that all information is filled in correctly, click **Test**.
7. Click **Start watching folder**.



Folder to watch: C:\

Backup folder: C:\

Number of files to count before wafer map procedure: 18

AMASS Project file name: C:\

☐ Print report after wafer mapping

Extra printing parameters (leave blank to use default printer):

☐ Save report after wafer mapping

Report file name (*.pdf, *.rtf or *.html): WaferReport.pdf

Session log:

Current number of XRDML files in selected folder: 0

Figure 10.13 AMASS Controller

CHAPTER 11 DIFFUSE SCATTER

11.1 Introduction

This sample used in these exercises has a superlattice structure that contains 10 periods of GaAs and AlAs with an interface roughness of 0.5 nm and a lateral correlation of 200 nm. In the first exercise, a reciprocal space map is simulated with the settings contained in a sample file. The sample file is supplied with the software. In the next exercise, the vertical correlation settings are changed to show the influence on the simulation pattern of the vertical correlation of the roughness between the layers.

11.2 Set up the simulation

1. Start AMASS.
2. Go to **Sample > Open Sample**.
3. Go to **C:\Users\User.Name\Documents\PANalytical\AMASS\Examples**.
4. Select "QSG11.asamxl".
5. Click **Open**.
6. Go to **View > View as Reflectivity**.
7. Go to the **Simulation Setup** tab.
8. From the **Scan type** drop-down list, select **Coplanar RSM** to simulate a map to see the effects of vertical radiation.
9. From the **Algorithm** drop-down list, select **DWBA** (Distorted Wave Born Approximation).
10. Press F2 to start the simulation. The progress of the simulation is shown in the status bar.

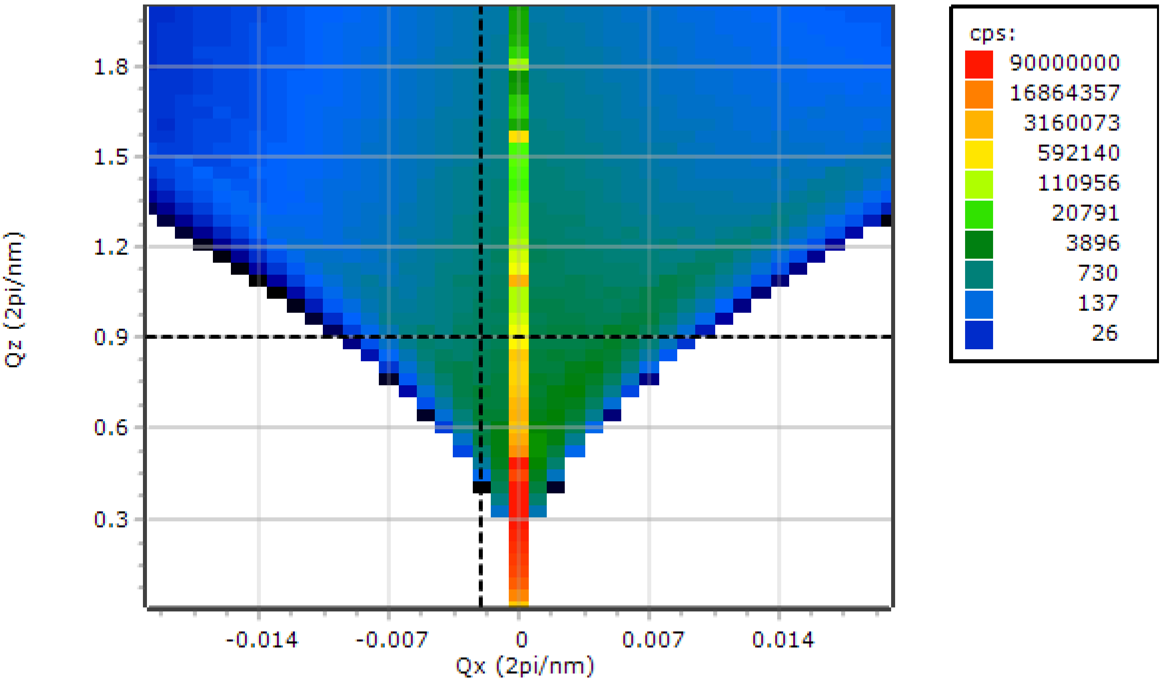


Figure 11.1 Simulation of reciprocal space map of periodic structure

11. Click 📈 to open the **Area Scan Plot Settings** window.
12. From the **Plot type** drop-down list, select **Bitmap**.
13. From the **Interpolation factor** drop-down list, select **6x**.
14. Clear the **Maintain aspect ratio** check box.
15. Click **OK**.

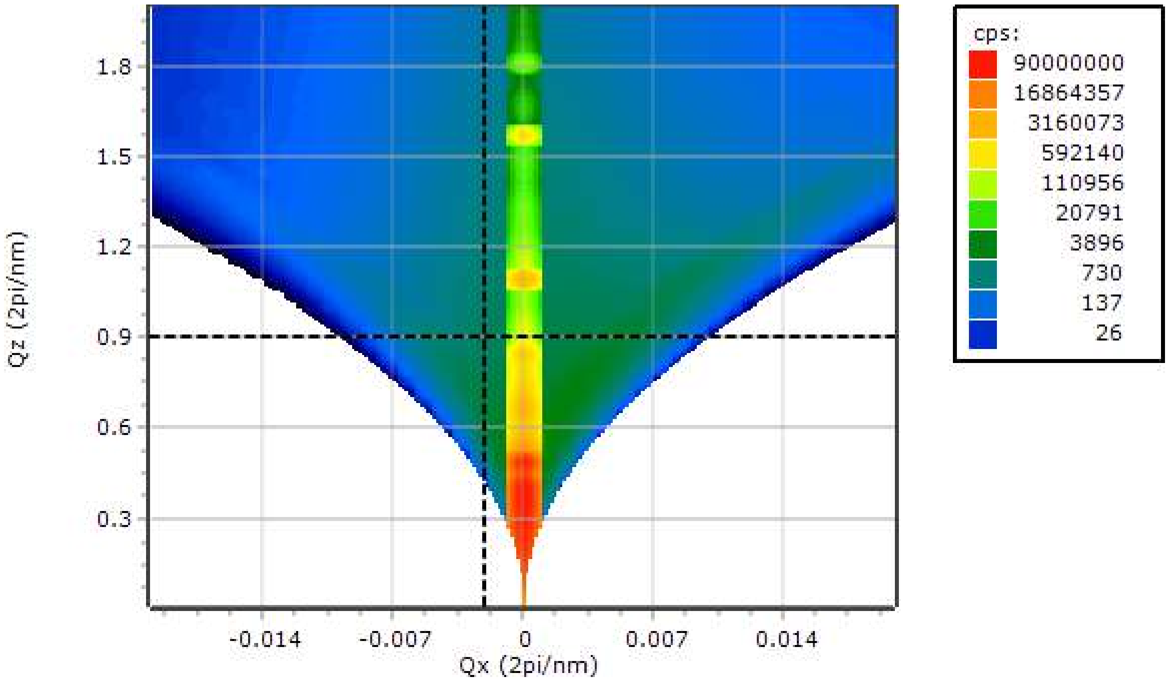


Figure 11.2 Simulation after bitmap interpolation

11.3 Examine the influence of vertical correlation

1. Go to the **Sample Details** tab.
2. Go to the **Diffuse Scattering and GISAXS Details** tab.
3. From the **Correlation type** drop-down list, select **Fully correlated**.
4. Press F2 to start the simulation. The progress of the simulation is shown in the status bar.

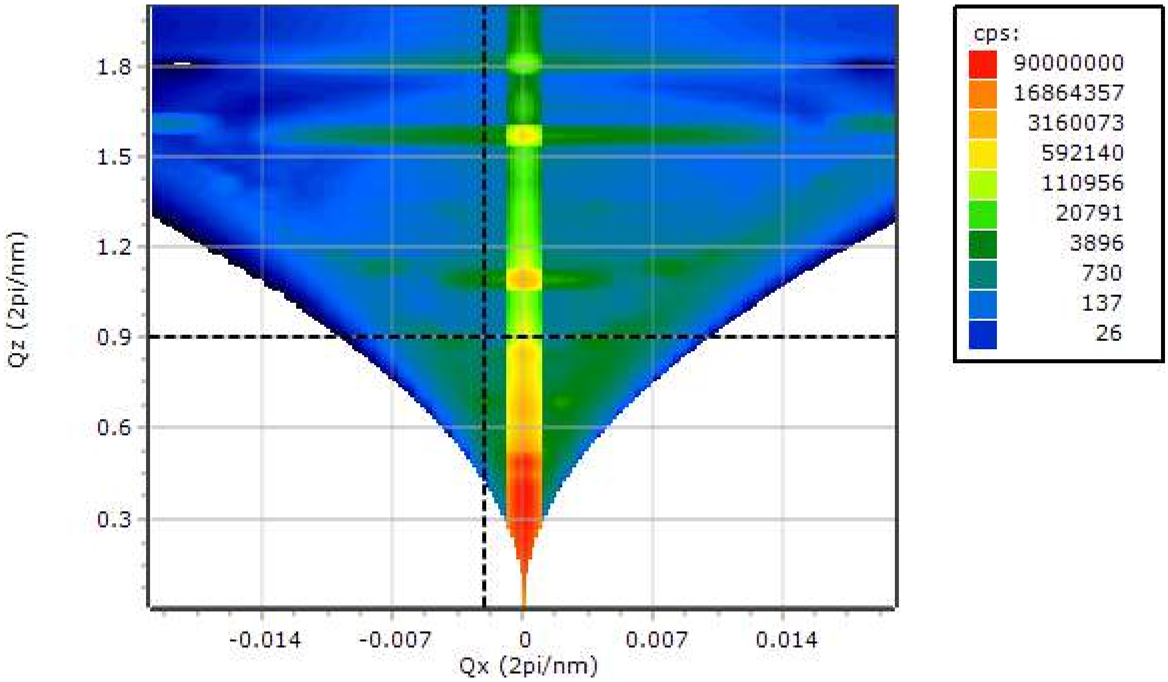


Figure 11.3 *Simulation after bitmap interpolation and fully correlated*

Because of the correlation of roughness of the interfaces, the clearest feature is the concentration of the intensity on the equidistantly placed RDS (Resonant Diffuse Scatter) sheets in the reciprocal space map. In this example, the RDS sheets are the horizontal green lines. They show that there is a vertical correlation between the roughness of the interfaces. This is a "normal" example of how you can quickly see these effects.

5. If you want to see more details, select a smaller step size:
   a. Go to the **Simulation Setup** tab.
   b. Select a smaller step size.
   c. Press **F2** to start the simulation. The simulation can take longer to complete.
   d. If the simulation takes too long, press **F4** to stop the simulation.

CHAPTER 12 AUTOMATE YOUR DIFFRACTION MEASUREMENTS AND ANALYSES

12.1 Introduction

It is possible to automate your analyses by with either Automatic Processing Program (APP) supplied as an add-on with Data Collector, or directly with AMASS from the command line. You can, for example, make a shortcut.

This chapter shows 2 simple examples with the command line. It is also possible to use scripts. For more information about scripts, refer to the Automatic Processing Program Help.

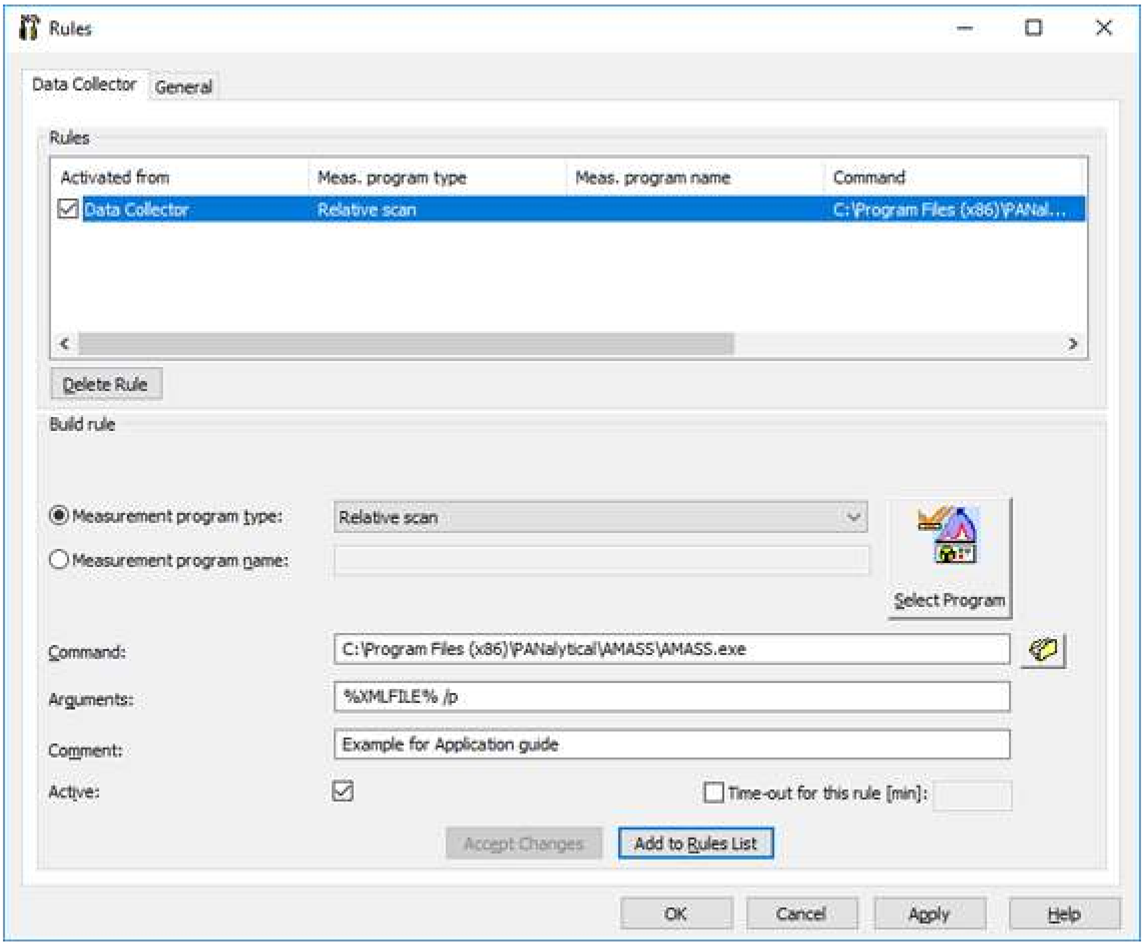
12.2 Print scan data with Automatic Processing Program

This example shows how to print out scan data immediately after it has been collected with Data Collector.

1. On the right of the taskbar, right-click the Automatic Processing Program icon and then select **Rules**.
2. In the **Measurement program type** field, select the correct program type. In this example, **Relative scan**.
3. In the **Command** field, enter the path name to run AMASS: "C:\Program Files (x86)\PANalytical\AMASS\AMASS.exe".
4. In the **Arguments** field, enter "%XMLFILE% /p".

   "%XMLFILE%" identifies the full path and file name of the measured file.

   "p" identifies that the scan must be printed.
5. Select the **Active** check box.
6. Click **Add to Rules List**.



Activated from	Meas. program type	Meas. program name	Command
☑ Data Collector	Relative scan		C:\Program Files (x86)\PANal...

● Measurement program type: Relative scan

○ Measurement program name:

Command: C:\Program Files (x86)\PANalytical\AMASS\AMASS.exe

Arguments: %XMLFILE% /p

Comment: Example for Application guide

Active: ☑

☐ Time-out for this rule [min]:

Figure 12.1 Rules for Data Collector

7. Click **OK**.

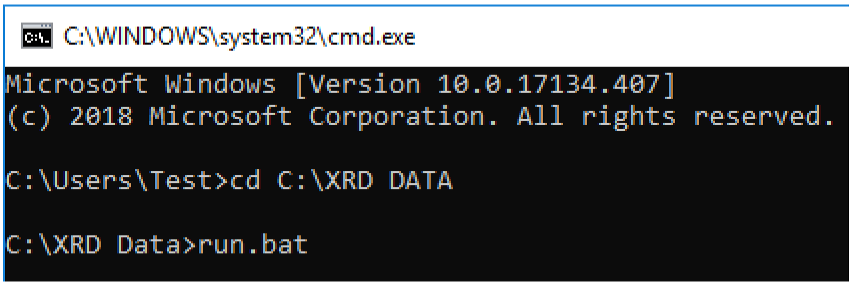
12.3 Fit scans automatically with AMASS's command line

1. Open an editing tool. For example, Notepad.
2. Enter this code:

```
"SET AppName="c:\Program Files (x86)\PANalytical\AMASS\AMASS.EXE""
"SET FolderName="C:\XRD Data"
"SET Project-File=%FolderName%\HR_Fitting_Example1.aprjxl""
"SET ScanFile=SiGe.d00"
"%AppName% %ProjectFile% %FolderName%\%ScanFile%" /fit:%FolderName
%FittedScan1.x01",%FolderName%\Fitted.aprjxl" /s:%FolderName%\FitReport.pdf""
```

3. If necessary, update the file paths or make the folder **C:\XRD Data** and then copy the files "HR_Fitting_Example1.aprjxl" and "SiGe.d00" to this folder. Refer to Chapter 8.
4. Save the batch file as "run.bat".
5. Open Command Prompt:
   a. Press **⊞ Win** + **R**.
   b. Enter "CMD".
   c. Press **Enter**.

6. Change the directory to the directory where the batch file is located. In this example, enter "cd C:\XRD Data".
7. Press **Enter**.
8. Enter the command "run.bat".



```
Microsoft Windows [Version 10.0.17134.407]
(c) 2018 Microsoft Corporation. All rights reserved.

C:\Users\Test>cd C:\XRD DATA

C:\XRD Data>run.bat
```

Figure 12.2 Change directory command line

9. Press **Enter**. The batch will run. When it is done, the report is saved to the folder **C:\XRD Data**.
10. Exit Command Prompt:
    a. Enter "Exit".
    b. Press **Enter**.

12.4 Command line specifications

The command line interface can be used to do different analyses of X-ray scattering data. Enter a command as follows:

"AMASS.exe [<files>] [<options>]"

where "<files>" is a list of filenames separated by spaces. The file type is specified by its file extension.

Parameter	Description
Scan file	One experimental scan file (.xrdml, .dnn, .xnn, .ascnxl, .asc, .znn)
Sample file	One sample file (.asamxl)
Initialization file	One initialization file (.ini)
Database file	One database file (.amatx)

Enter options as follows:

"/<option name>[:<option value>]"

Options must be separated by at least 1 space character.

Option name	Option value	Description
p	:<Printer> (optional)	Print the built-in report (**Report > Print Report**) that has been set up to a specified printer. If the printer is not specified, the default printer is used. If the printer is specified, the syntax must be as follows: <PrinterName>:[Driver]:[File] The program stops when printing is done.
nologo		Start AMASS without the splash screen.
fit	:<Files>	Start fitting of specular or high-resolution diffraction data. Fitting of diffuse scattering curves is not supported. <Files> is a comma-separated list of file names where output files will be written to 1 sample file and/or 1 simulated scan and/or 1 project file. If a file name already exists and it is not read-only, it will be overwritten. If the file is read-only, the file will not be written and the program stops with exitcode=1. A sample file, or project file and scan file is necessary. You do not have to load the sample files if you want to use default settings. The program stops automatically when fitting is done.
res	:<options>	There are 3 result options (peak grid, results summary and RSM result summary) for single scan analysis. It is possible to call multiple options. Each call starts with /res.
s	:<Files>	Report files (.pdf, .rtf, .html, .xml).
wmafolder	:<Folder>	Load all files in the folder and map wafers.
wmafiles	:<File1>,<File2>, ... <FileN>	Load the list of individual comma-separated files and map wafers. Add a filename with an .xml extension to save wafer map results to a file with that name.
wmaopen	:<File>	Open and show a wafer map results file. It must have the extension .xml.
xslt	:<File>	Generates and saves a result file (.html, txt) based on an xslt transform file.

Example 1:

"AMASS.exe xxx.xrdml xxx.aprjxl /fit:FittedScan.x00, FittedSam-ple.asamxl, FittedSettings.aprjxl / s:FitReport.pdf /p: /nologo."

Starts AMASS and opens scan data (.xrdml) and a project file (.aprjxl). Then, the scan data will be fitted with the sample model and fitting settings of the project. The fitting results are saved and a PDF report is made.

Example 2:

"AMASS.exe Scan.xrdml /p /nologo."

AMASS starts, opens the scan data file and prints a default report to the default printer.

NOTE: You can do automatic analysis of similar data in a simple way with AMASS Controller software. Refer to the AMASS Help for more information.