DIFFRAC.SUITE

Tutorial

DIFFRAC.EVALUATION PACKAGE
DIFFRAC.EVA

Original Instructions

Innovation with Integrity

XRD

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We have checked the contents of this manual for agreement with the hardware and software described. Since deviations cannot be precluded entirely, we cannot guarantee full agreement. However, the data in this manual are reviewed regularly and any necessary corrections are included in subsequent editions. Suggestions for improvement are welcome.

All configurations and specifications are subject to change without notice.

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1 Performing a Search/Match Operation

A reference database is required to perform a **Search/Match** operation.

This tutorial was prepared using **PDF 4+ 2016** as a reference database. You may have another reference database.

If you have no database, you cannot perform this part of the tutorial concerning the **Search/Match**.

The following seven-step procedure describes the basic procedure for running EVA **Search/Match**, using the default parameters.

The scan used is held as a tutorial file, **BChips.RAW**, found in the Tutorial directory.

These are boiling chips coming from the stockroom of the Department of Chemistry, North Dakota State University.

The boiling chips are crushed Dolomite/calcite marble. Quartz from the precursor limestone is a third, routinely identified phase. In the metamorphic rock, weak peaks from one or more layer Silicates are detected. They may be too weak to identify by computer routines, but important low angle d-spacings, familiar to clay mineralogists, suggest a Chlorite (e.g. Clinochlore) phase.

Steps

1. Creating a new EVA document and importing BChips.RAW.
2. Setting of the search parameters and performing the initial search.
3. Matching procedure:
   Identification of Dolomite, Calcite and Quartz
4. Preparing the residual scan.
5. Performing a subsequent search on the residual scan.
6. Matching procedure
7. Identification of Clinochlore
8. Saving the EVA document containing the scan.

1.1 Step 1: Creating a New EVA Document and Importing Bchips.RAW

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   - The EVA document is empty.

2. Click the **Import from files** data command or the **Import from files** button.
   - The **Import From Files** dialog box will be displayed.
3. Search the **Tutorials/EVA*** directory and select the **Bchips.RAW file**.
4. Click **Open**.

⇨ The scan **Bchips** will be displayed in the **Graphical view** of the EVA document.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

Figure 1.1: Importing the Bchips.Raw file

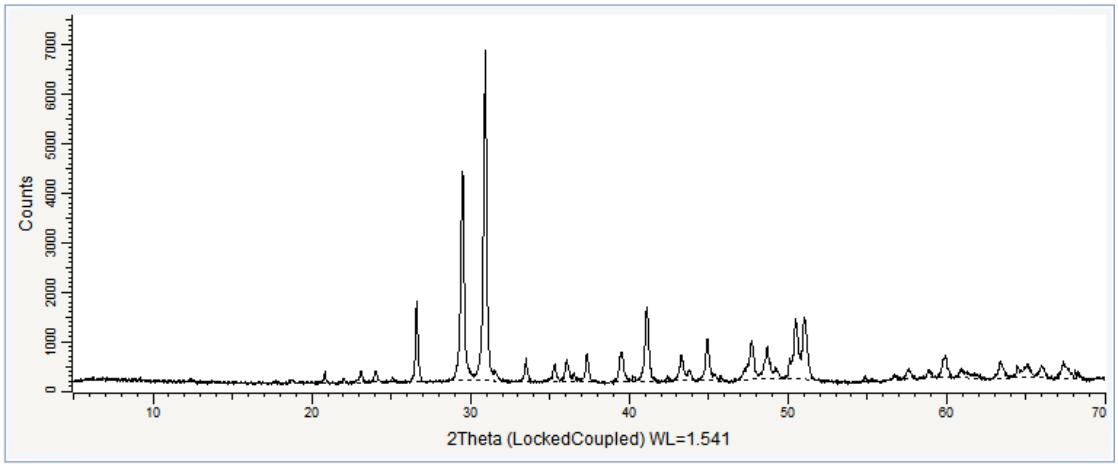


Figure 1.2: Bchips.RAW file imported in the graphical view

1.2 Step 2: Setting the Search Parameters

▷ Make certain the scan is selected; if not, select it either in the Data tree or in the graphical view.

1. Click **Search / Match** in the Data Command panel
   — or —
   click the **Search/Match** button on the Search/Match toolbar
   — or —
   right-click the scan, click **Tool** on the context menu and then **Search / Match** on the related submenu.

➨ The **Search / Match** dialog box will be displayed.

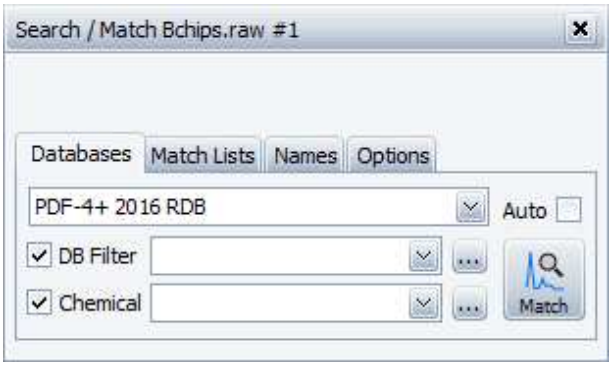


Figure 1.3: Search/match dialog box

2. Keep the default parameters as follows.
3. In the **Databases** tab:
   - No DB Filter defined
   - No Chemical filter defined
   - **Auto** check box cleared
4. In the Match Lists tab:
   - No Match List defined
5. In the **Options** tab:
   - Criterion = **2** : **Neutral** selected
   - **Whole Range** selected

Figure 1.4: Options tab

6. In the **Databases** tab, click the **Match** button.

⇨ The candidates are listed in the **Search list** tab of the Data Tree Panel.

1.3 Step 3: Matching Procedure

From the patterns listed in the Search list, the user chooses the best candidates to identify the unknown, by comparing the stick patterns with the peaks of the current scan.

▷ It is recommended to select the **Group Duplicates** check box.

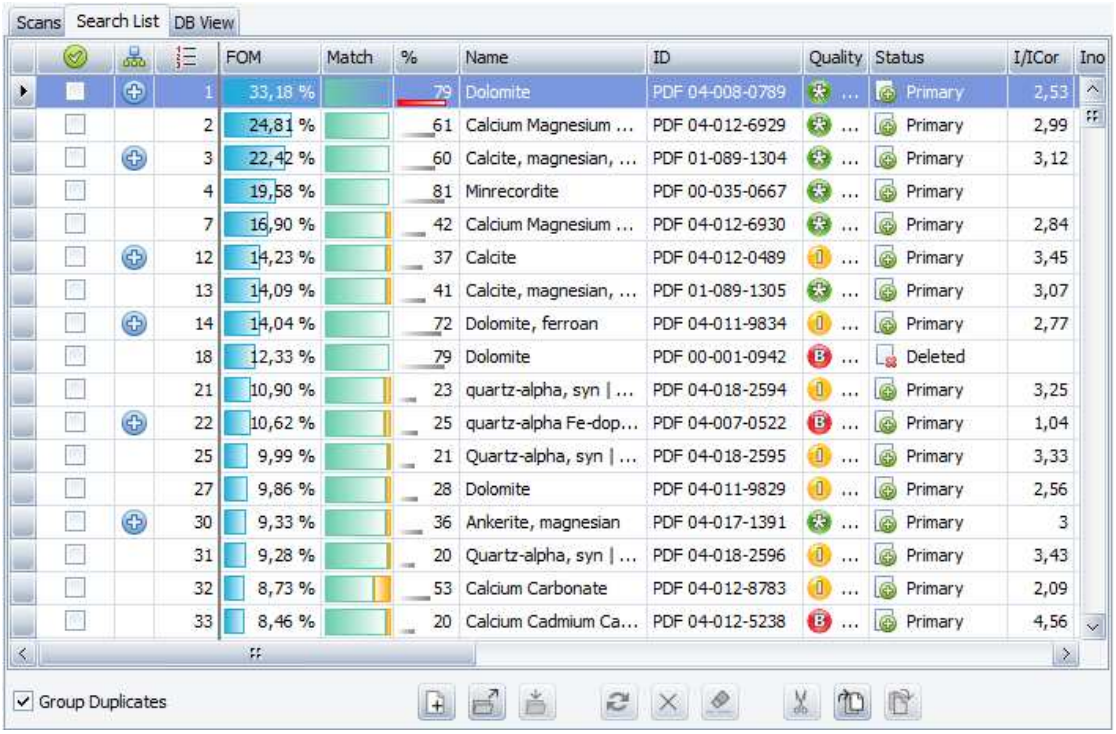
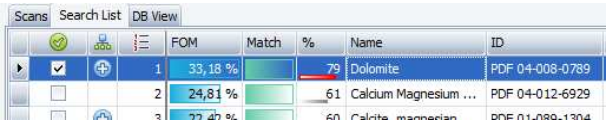


Figure 1.5: Candidate List with the first pattern selected

1. In the **Candidate List** tab, the first pattern in the list is selected (highlighted in blue): it is **Dolomite**.
   - ➨ The corresponding ghost stick pattern (sticks and dotted lines) is displayed in the **Graphical view**.
2. Compare the stick pattern with the current scan.
   - ➨ The first pattern 04-008-0789 matches a part of the peaks of the scan.
3. Mark this pattern by selecting the corresponding check box.



   - ➨ The pattern is associated to a color. The image of its stick patterns remains when it is no longer selected (highlighted) in the **Search List**. Moreover, it is added to the data tree.
4. Go down in the list. Compare the stick patterns to the scan peaks.
   - ➨ The **Calcite** and **Quartz** patterns (01-089-1304 and 00-046-1045) appear to match the scan.
5. Select the corresponding **check** boxes:
   - ➨ They are added to the data tree and the images of their stick patterns remain when they are no longer selected.
6. Leave the non-matching stick patterns unchecked.

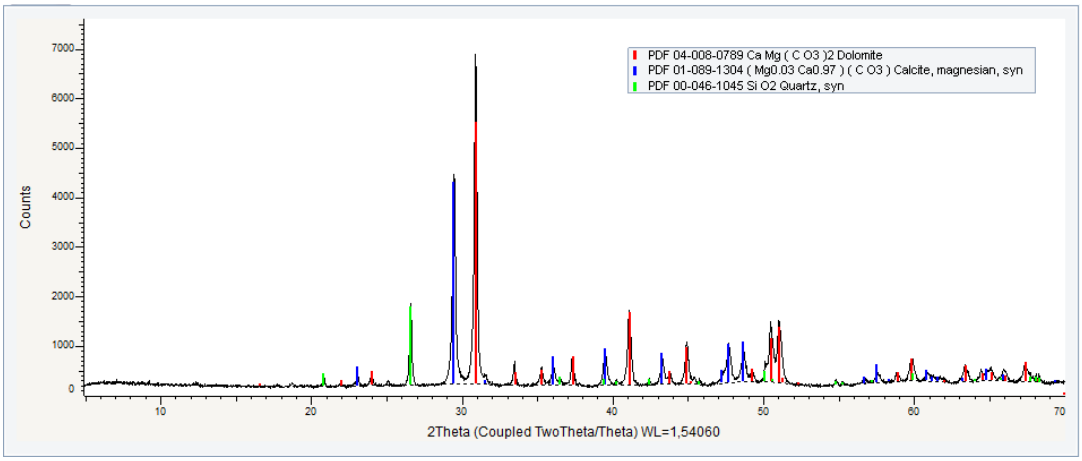


Figure 1.6: Bchips scan displayed in the graphical view with the three identified patterns

Results

The three main phases are found with the initial EVA **Search/Match** run. A residual scan must be prepared to identify the last phase.

1.4 Step 4: Preparing the Residual Scan

The **explained areas** (peaks which were found by the **Search/match**) given by the identified phases must be removed.

1. Multi-select the three identified patterns in the Data tree.
2. Click **Auto Residue** in the Tool list of the Data Command panel
   — or —
   click the **Auto Residue** button on the Pattern toolbar
   — or —
   right-click the multi-selection and then click **Tool** on the context menu. Click **Auto Residue** on the Tool submenu.
   ➨ The already explained areas are automatically removed. They are displayed with the ghost color in the **Graphical view**.

The Automatic residue is used here but you can also adjust the residue pattern by pattern using the Residue dialog box.

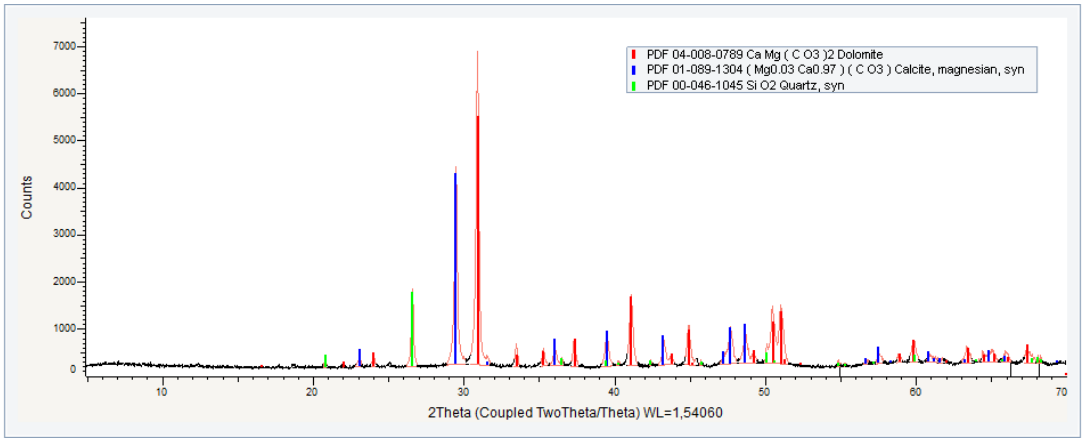


Figure 1.7: Scan with the removed zones in red (ghost color)

1.5 Step 5: Performing a Subsequent Search on the Residual Scan

1. Select the scan in the Data tree.
2. Keep the default parameters:
   - No database filter
   - No chemical filter
   - No Match list
   - **Auto** check box cleared
   - Criterion = **2**:**Neutral** selected
   - **Whole Range** selected
   - **Auto** check box cleared
3. In the **Databases** tab, click the **Match** button.

⇨ The candidates will be listed in the Search list of the Data tree panel

1.6 Step 6: Matching Procedure

1. Working only on relatively low angles for the identification of clay materials is highly recommended. Thus, zoom in on the first half of the diagram (5° to about 36° 2θ).
2. In the **Search List** tab, the first pattern in the list is selected: it is **Nickel Tin** (pattern PDF 00-004-0851).
   ➨ The corresponding ghost stick pattern is displayed in the **Graphical view**.
3. Compare the stick patterns to the current scan peaks. Identify the **Clinochlore** which ranks 5. It ranks 1 selecting the **Mineral** database only.
4. Mark this pattern by selecting the corresponding check box.

Scans | Search List | DB View

		FOM	Match	%	Name	ID
☐	1	116,13 %		8	Nickel Tin	PDF 00-004-0851
☐	2	102,21 %		4	Erbium Titanium Oxide	PDF 04-001-9755
☐	3	101,63 %		4	Hafnium Silicate	PDF 04-002-0611
☐	4	100,85 %		4	Gadolinium Lutetium Titanium ...	PDF 04-001-9758
☑	5	98,49 %		2	Clinochlore-2MIIb	PDF 00-029-0854
☐	6	93,55 %		1	Clinochlore, ferroan, oriented	PDF 00-060-0325

   ➨ The pattern is associated to a color. It is added to the Data tree and the image of its stick patterns remains when it is no longer selected (highlighted) in the **Search List**.
5. Leave the non-matched stick patterns unchecked.

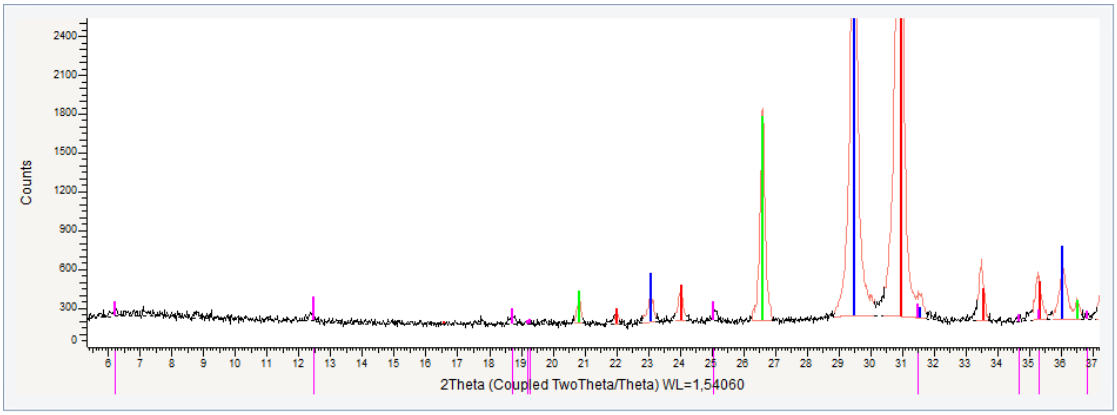


Figure 1.8: Zoom on the first half of the diagram with the Clinochlore phase identified

1.7 Step 7: Saving

1. Click **Save As** on the **File** menu.
   ➨ The **Save EVA File As** dialog box will be displayed.
2. Select the appropriate disc drive and directory.
3. Type in the file name. (To overwrite an **.EVA** file, use the same name).
4. Click **Save**.

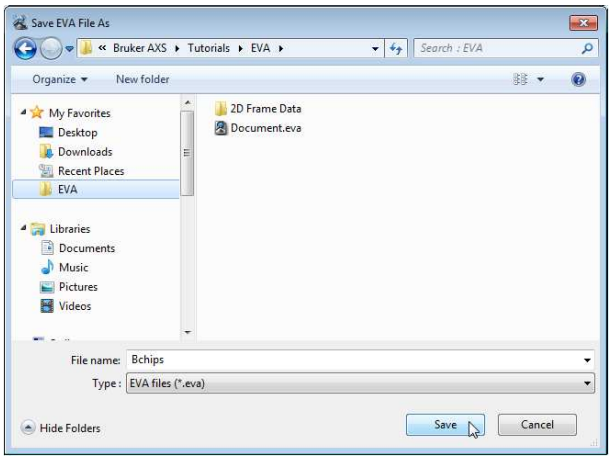


Figure 1.9: Bchips.EVA document

2 Performing an Automatic Search/ Match Operation

A reference database is required to perform a **Search/Match** operation.

This tutorial was prepared using **PDF 4+ 2016** as a reference database. You may have another reference database.

If you have no database, you cannot perform this part of the tutorial concerning the **Search/ Match**.

The following 4-step procedure describes the basic procedure for running EVA Search/Match using the automatic mode.

The automatic search/match algorithm has been rewritten in EVA V6 to provide good results for real-life applications. Many internal improvements have been applied, which make the automatic search applicable for routine use. The algorithm is very fast on modern multi-core computers because it uses parallelized, multithreaded code.

An Automatic Search is likely to deliver accurate results if the three following conditions are fulfilled:

- low overlap between phases
- every phase in the unknown shall have relative intensities matching the ones of its reference pattern in the database
- no phase showing a significant line broadening

The user must interpret the automatic search results carefully. Their accuracy cannot be known beforehand. In practice, it may be necessary to continue the search with the interactive Search/Match after initially employing the a**utomatic search**.

To support the visual phase identification with the automatic search, a setting “Auto-Search Results as Candidates” has been introduced with V6. This setting is turned off by default and the tutorial examples are created with this default. If this setting is checked, the search results will be displayed unchecked as in the interactive Search/Match.

A dialog with information about a computed displacement may be shown at the end of the automatic search (license level 6). The given displacement has to be judged carefully and applied. The calculated displacement can indicate either a real displacment or radiation penetration or it can be a sign for an inaccurate automatic analysis.

The scans used are held as tutorial files, m1.RAW and CPD-2.RAW found in the Tutorials directory.

Steps

1. Creating a new EVA document and importing the scan
2. Setting of the search parameters and performing the initial search
3. Automatic matching procedure:
   - Identification of the compounds
   - Checking with a “normal” matching procedure (for the m1 scan)
4. Saving the EVA document containing the scan.

2.1 Case #1: m1.RAW

M1 is a mixture of **Calcite**, **Aragonite** and **Brucite**.

2.1.1 Step 1: Creating a New EVA Document and Importing m1.RAW

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   - ➨ The EVA document is empty.

2. Click the **Import from files** data command or the **Import from files** button.
   - ➨ The **Import From Files** dialog box will be displayed.
3. Search the **Tutorials/EVA*** directory and select the **m1.RAW file**.
4. Click **Open**.
   - ➨ The scan **m1** will be displayed in the graphical view of the EVA document.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

Figure 2.1: Importing the m1.RAW file

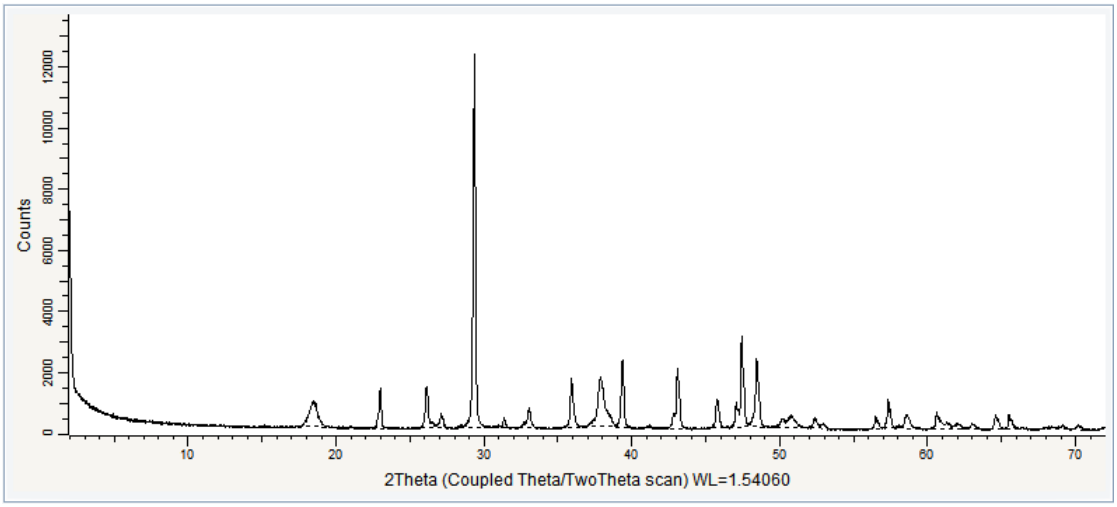


Figure 2.2: m1.RAW file imported in the Graphical view

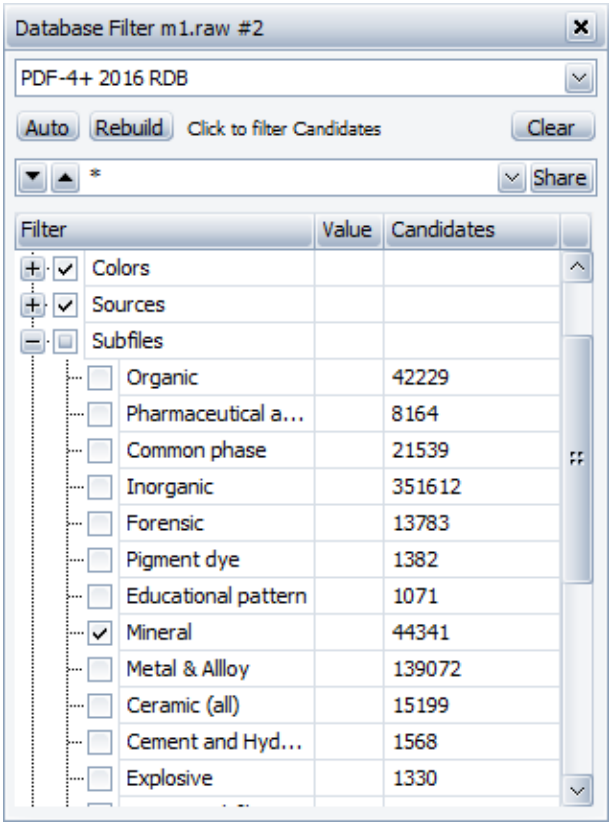
2.1.2 Step 2: Setting the Search Parameters

▷ Make certain the scan is selected; if not, select it either in the **Data tree** or in the **Graphicalview**.

1. Click **Search / Match** in the Data Command panel
   — or —
   click the **Search/Match** button on the Search/Match toolbar
   — or —
   right-click the scan, click **Tool** on the context menuand then **Search / Match** on the related submenu.
   ➨ The **Search / Match** dialog box will be displayed.

*Figure 2.3: **Search/Match** dialog box*

2. Set the parameters to use for the **Search/Match**.
3. In the **Databases** tab:
   - Database filer: **Mineral** subfile selected
   - No chemical filter defined



4. Select the **Auto** check box.
5. In the **Match Lists** tab:
   - No Match list defined
6. In the **Options** tab:
   - Criterion = **2**:**Neutral** selected
   - **Whole Range** selected.

7. In the **Databases** tab, click the **Match** button.

⇨ The candidates are listed in the **Search list** tab of the Data tree panel.

2.1.3 Step 3: Automatic Matching Procedure

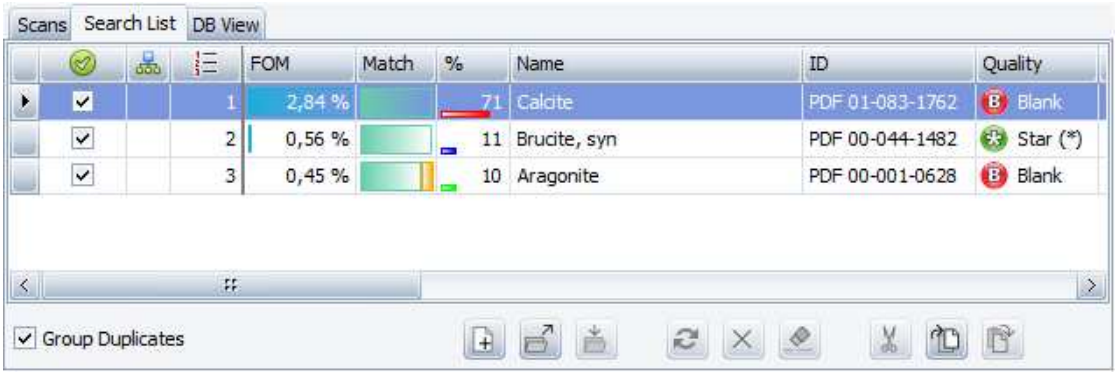


Figure 2.4: Candidate List with the identified patterns marked

The results of the **Automatic Search/Match** are displayed in the **Search List** tab of the Data Tree Panel. The three patterns identified : Calcite, Brucite and Aragonite, are automatically checked and therefore added to the **Data tree** and to the **Graphical view**.

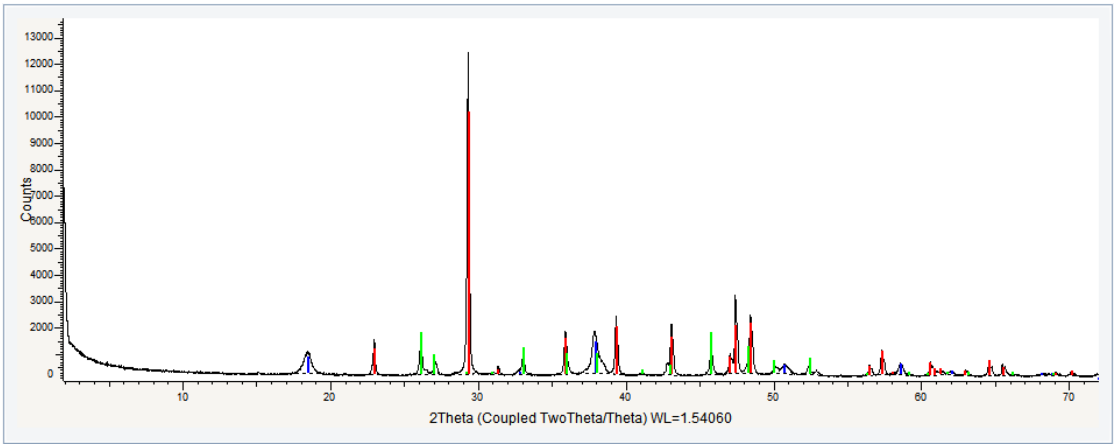


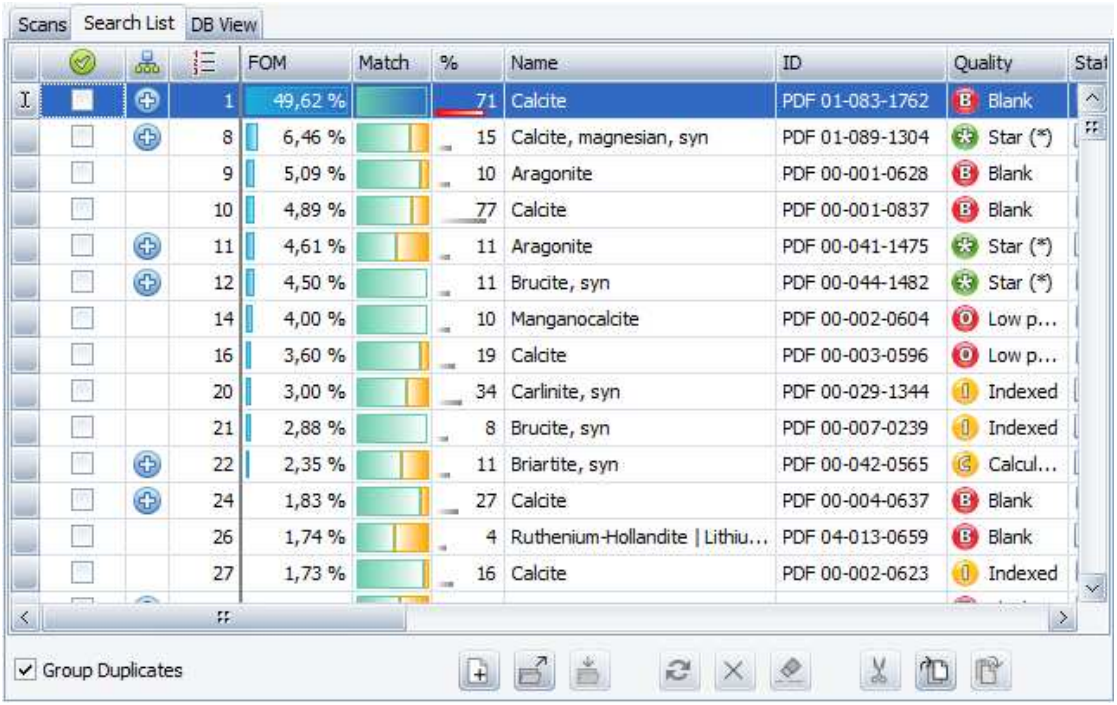
Figure 2.5: m1 scan displayed in the Graphical view with the three identified patterns (Calcite, Brucite and Aragonite)

Results

The three phases found with the automatic EVA **Search/Match** run match well the scan and correspond to the expected results. Nevertheless it can be interesting to check with a **"non-automatic" Search/Match**.

"Normal" matching procedure

1. Set the same parameters then for the automatic search but clear the **Auto** check box before running the search.



2. From the patterns listed in the dialog box, the user chooses the best candidates to identify the unknown, by comparing the stick patterns with the peaks of the current scan.
3. In the **Search List** tab, the first pattern in the list is highlighted: it is **Calcite**.
   - ➨ The corresponding ghost stick pattern (sticks and dotted lines) is displayed in the **Graphical view**.
4. Compare the stick pattern with the current scan.

➨ The first pattern 01-083-1762 matches a part of the peaks of the scan.

5. Mark this pattern by selecting the corresponding check box.

➨ The pattern is associated to a color. The image of its stick patterns remains when it is no longer selected (highlighted) in the **Candidate List**.

6. Go down in the list. Compare the stick patterns to the scan peaks.

➨ The **Aragonite** and **Brucite** patterns (00-001-0628 and 00-044-1482) appear to match the scan.

7. Select the corresponding **check** boxes:

➨ The images of their stick patterns remain when they are no longer selected.

8. Leave the non-matching stick patterns unchecked.

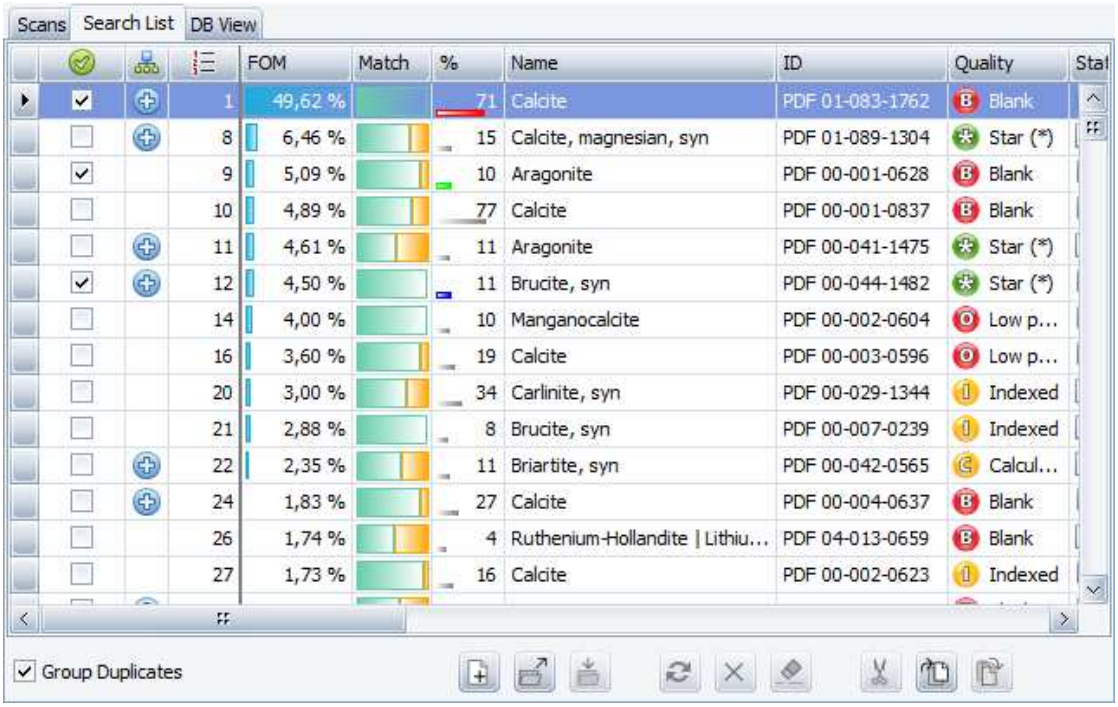


Figure 2.6: Search List with the three patterns identified

Results

The three phases found with the **Automatic Search/Match** are the same than those identified with the “normal” **Search/Match**.

2.2 Case #2: CPD-2.RAW

CPD-2 is a mixture of Zincite, Fluorite, Al_20_3 and Brucite from the Rietveld quant round-robin.

2.2.1 Step 1: Creating a New EVA Document and Importing CPD-2.RAW

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.

➨ The EVA document is empty.

2. Click the **Import from files** data command or the **Import from files** button.

➨ The **Import From Files** dialog box will be displayed.

3. Search the **Tutorials/EVA*** directory and select the **CPD-2.RAW file**.
4. Click **Open**.

⇨ The scan **CPD-2** will be displayed in the **Graphical view** of the EVA document.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

Figure 2.7: Importing the CPD-2.RAW file

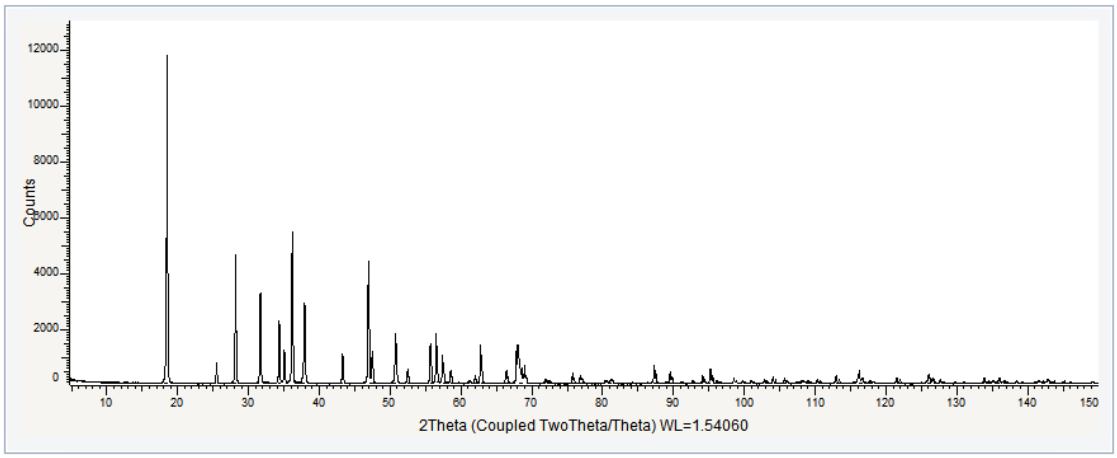


Figure 2.8: CPD-2.RAW file imported in the graphical view

2.2.2 Step 2: Setting the Search Parameters

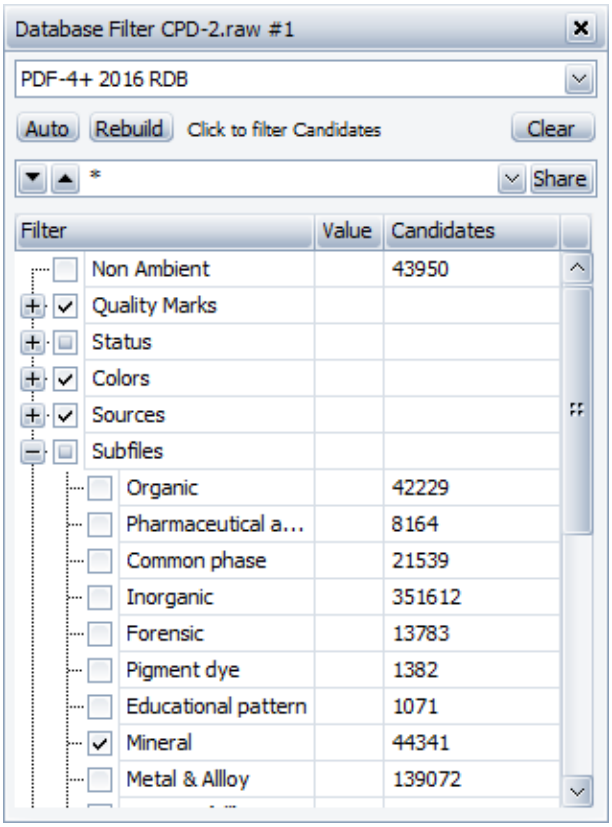
▷ Make certain the scan is selected; if not, select it either in the **Data tree** or in the **Graphicalview**.

1. Click **Search / Match** in the Data Command panel
   — or —
   click the **Search/Match** button on the Search/Match toolbar
   — or —
   right-click the scan, click **Tool** on the context menuand then **Search / Match** on the related submenu.

   ➨ The **Search / Match** dialog box will be displayed.

Figure 2.9: ***Search/Match*** *dialog box*

2. Set the parameters to use for the **Search/Match**.
3. In the **Databases** tab:
   - Database filer: **Mineral** subfile selected
   - No chemical filter defined



4. Select the **Auto** check box.
5. In the **Match Lists** tab:
   - No Match list defined
6. In the **Options** tab:
   - Criterion = **2**:**Neutral** selected
   - **Whole Range** selected.
7. In the **Databases** tab, click the **Match** button.

⇨ The candidates are listed in the **Search list** tab of the Data tree panel.

2.2.3 Step 3: Automatic Matching Procedure

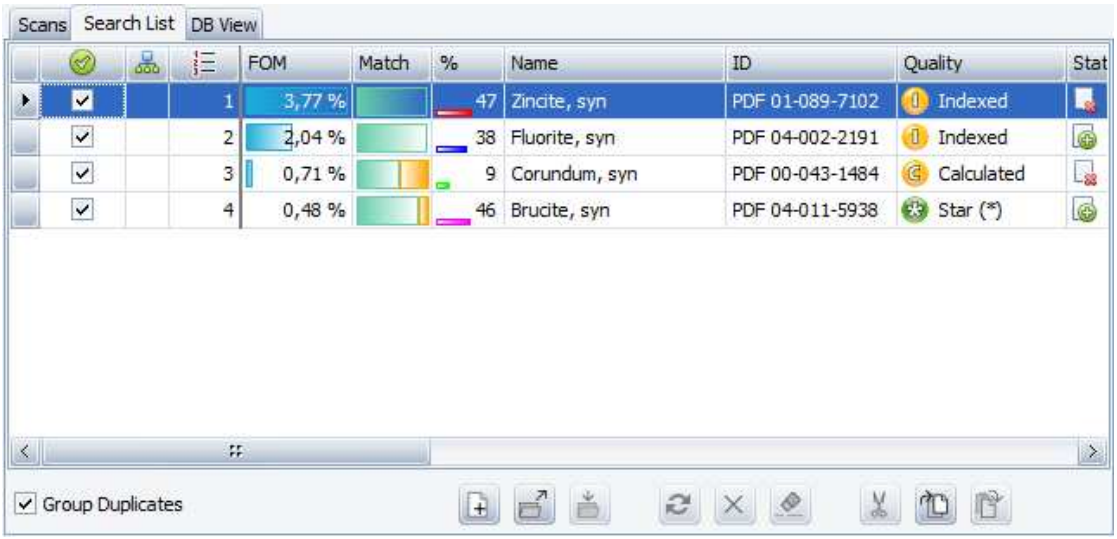


*Figure 2.10: **Search List** with the identified patterns marked*

The results of the **Automatic Search/Match** are displayed in the Search list. The four patterns identified are automatically checked and therefore added to the **Data tree** and to the **Graphical view.**

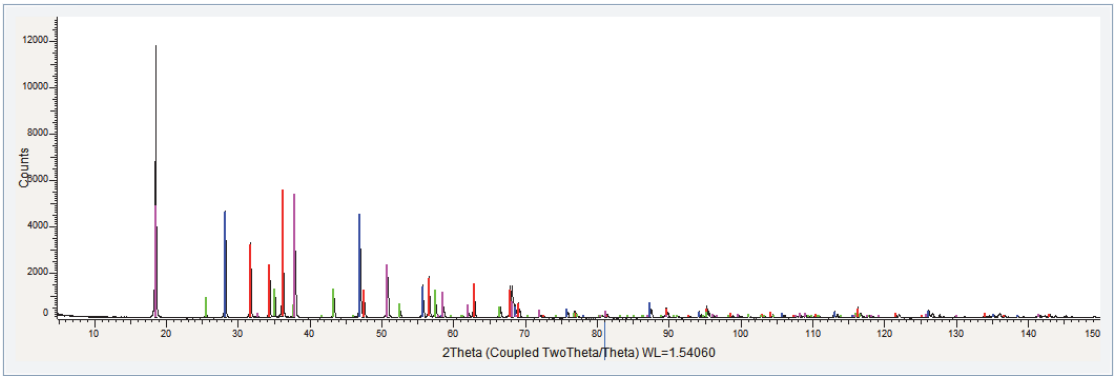


*Figure 2.11: CPD-2 scan displayed in the **Graphical view** with the four identified phases: Zincite, Fluorite, Corundum and Brucite*

Results

The four phases found with the automatic EVA **Search/Match** run match well the scan and correspond to the expected results.

3 Using a Match Peak

A reference database is required to perform a **Search/Match** operation.

This tutorial was prepared using **PDF 4+ 2016** as a reference database. You may have another reference database.

If you have no database, you cannot perform this part of the tutorial concerning the **Search/Match**.

The following five-step procedure describes the basic procedure for using a Match peak in a Search/Match procedure.

The scan used is held as a tutorial file, **BX100.RAW**, found in the Tutorial directory.

Steps

1. Creating a new EVA document and importing BX100.RAW.
2. Setting of the search parameters and performing the initial search.
3. Matching procedure:
   Identification of Boehmite and Hematite
4. Defining a Match peak and performing a subsequent search.
5. Saving the EVA document containing the scan.

3.1 Step 1: Creating a New EVA Document and Importing BX100.RAW

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   - ➡ The EVA document is empty.
2. Click the **Import from files** data command or the **Import from files** button.
   - ➡ The **Import From Files** dialog box will be displayed.
3. Search the Tutorials/EVA* directory and select the BX100.RAW file.
4. Click **Open**.
   - ➡ The scan BX100 will be added to the Data tree and displayed in the graphical view of the EVA document.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

Figure 3.1: Importing BX100.raw

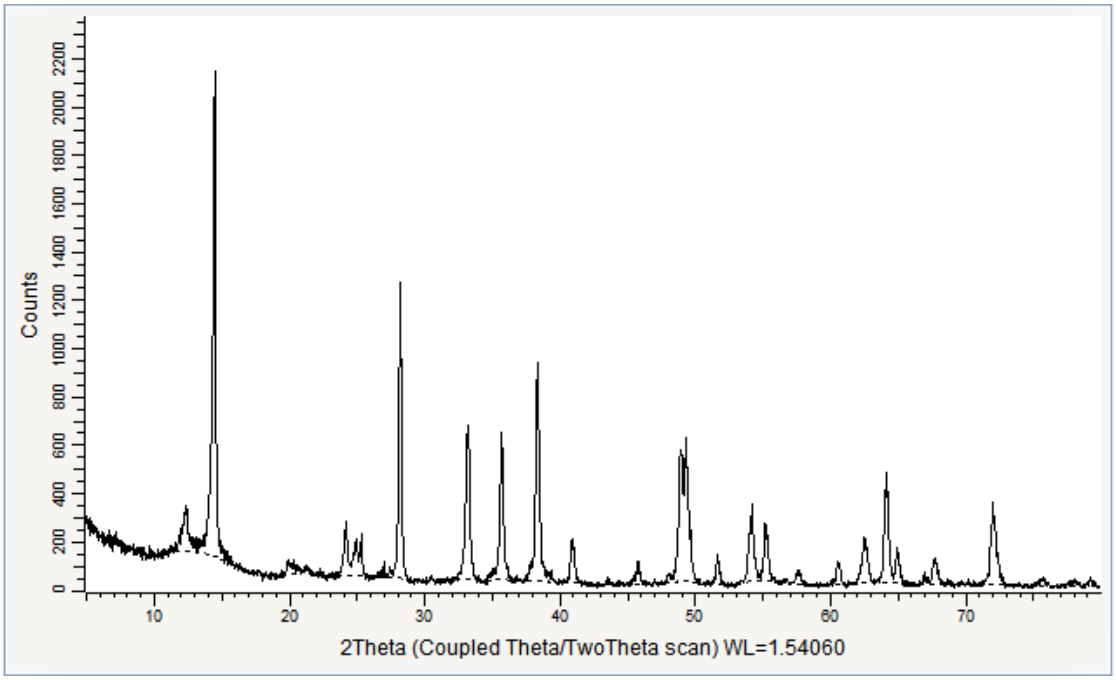


Figure 3.2: BX100.RAW imported in the graphical view

3.2 Step 2: Setting the Search Parameters

▷ Make certain the scan is selected; if not, select it either in the Data tree or in the graphical view.

1. Click **Search / Match** in the Data Command panel
   — or —
   click the **Search/Match** button on the Search/Match toolbar
   — or —
   right-click the scan, click **Tool** on the context menu and then **Search / Match** on the related submenu.
   ➨ The **Search / Match** dialog box will be displayed.

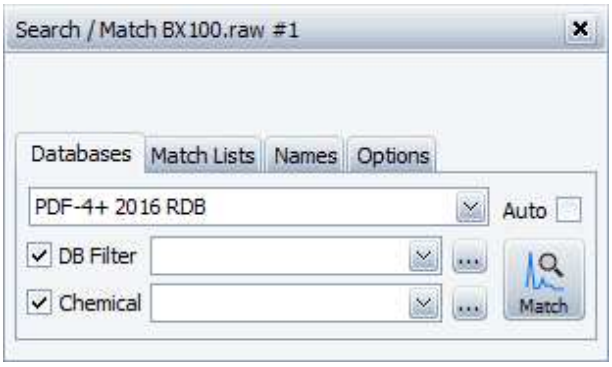
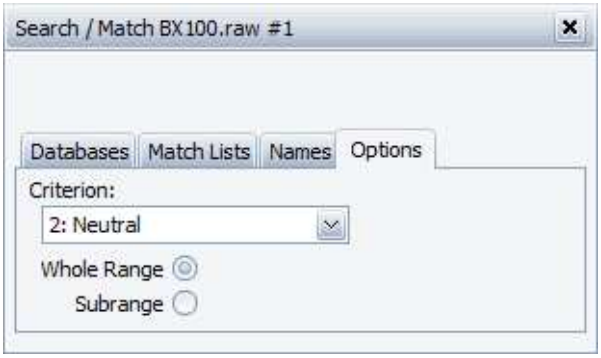


Figure 3.3: Search/match dialog box

2. Keep the default parameters as follows.
3. In the **Databases** tab:
   - No DB Filter defined
   - No Chemical filter defined
   - **Auto** check box cleared
4. In the Match Lists tab:
   - No Match List defined
5. In the **Options** tab:
   - Criterion = **2** : **Neutral** selected
   - **Whole Range** selected



6. In the **Databases** tab, click the **Match** button.

⇨ The candidates are listed in the **Search list** tab of the Data Tree Panel.

3.3 Step 3: Matching Procedure

From the patterns listed in the Search list, the user chooses the best candidates to identify the unknown, by comparing the stick patterns with the peaks of the current scan.

▷ It is recommended to select the **Group Duplicates** check box.

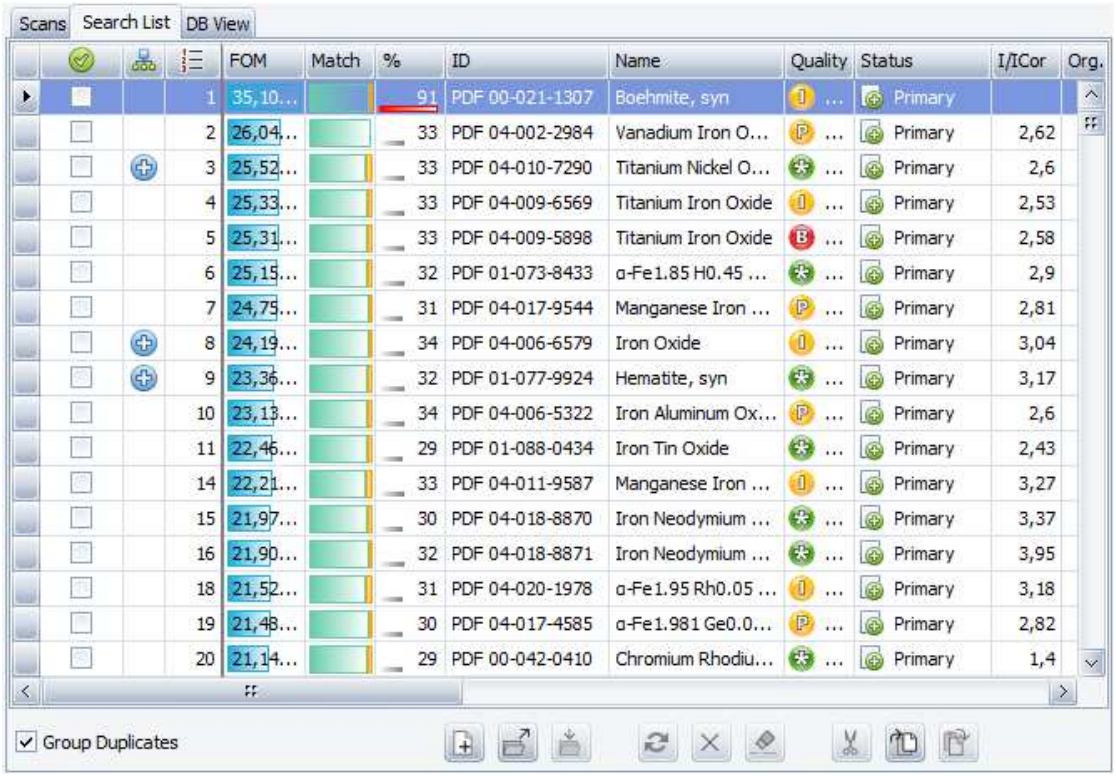
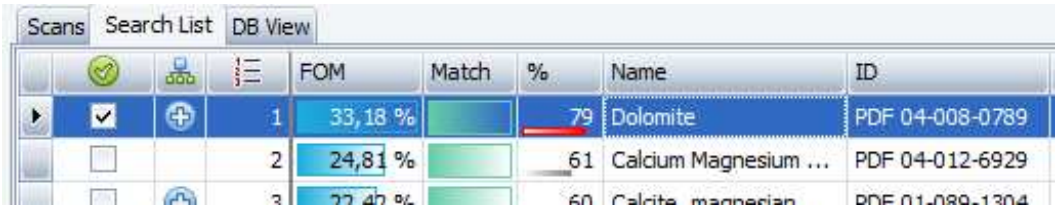


Figure 3.4: Candidate List with the first pattern highlighted

1. In the **Candidate List** tab, the first pattern in the list is selected (highlighted in blue): it is **Boehmite**.
   - ➨ The corresponding ghost stick pattern (sticks and dotted lines) is displayed in the **Graphical view**.
2. Compare the stick pattern with the current scan.
   - ➨ The first pattern 00-021-1307 matches a part of the peaks of the scan. It is an obvious good answer.
3. Mark this pattern by selecting the corresponding check box.



   - ➨ The pattern is associated to a color. The image of its stick patterns remains when it is no longer selected (highlighted) in the **Search List**. Moreover, it is added to the data tree.
4. Afterwards, we get a series of almost similar patterns and almost similar unit cells which appear to match the scan. It makes sense to select a Fe2O3 called Hematite in preference of, say, VFeO3, even if it ranks less well within a group of duplicates. We can select, for instance, pattern 01-087-1165 (star quality).
5. Select the corresponding **check** boxes:

➨ They are added to the data tree and the images of their stick patterns remain when they are no longer selected.

6. Leave the non-matching stick patterns unchecked.

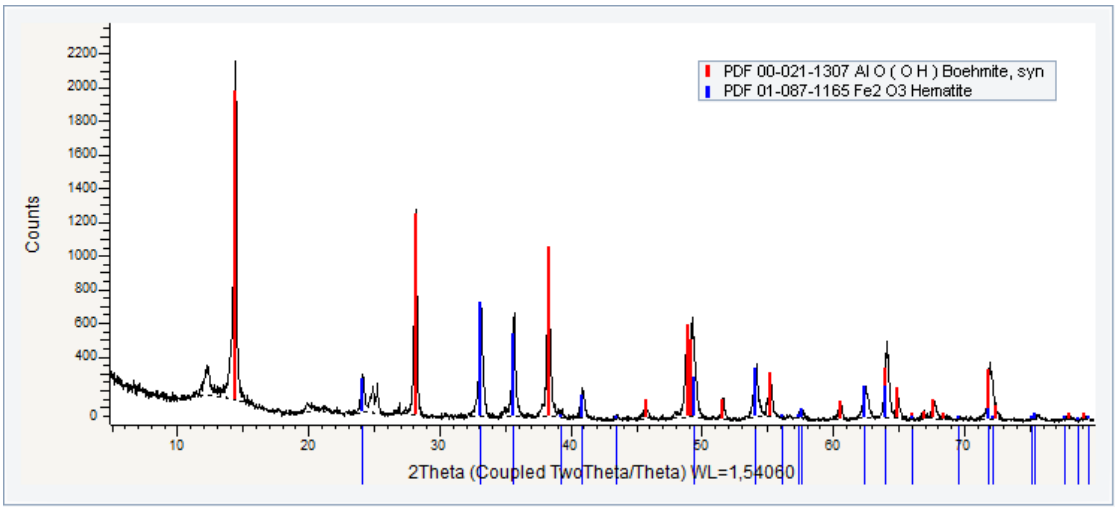


Figure 3.5: BX100 scan displayed in the graphical view with the two identified patterns

3.4 Step 4: Defining a Match Peak

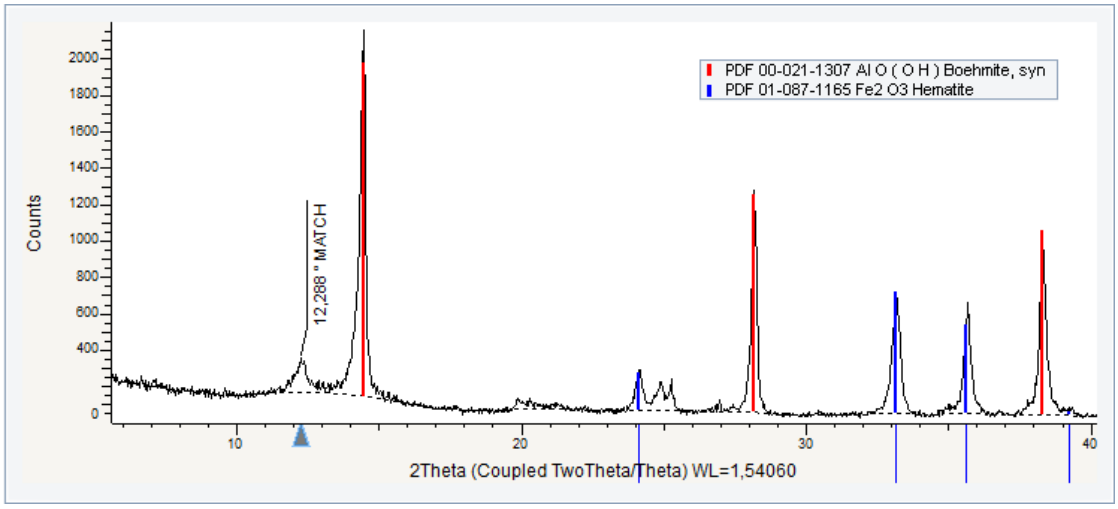
At this step, the most logical scheme is the residue one because these two phases have relatively simple patterns with strong and relatively well separated peaks. In such cases, the residue scheme is highly beneficial with almost no drawback.

Despite that, we will try here the “Match peak” scheme instead of the residue one.

▷ The Search/Match dialog box must be opened.

1. Point and right-click the peak at about 12.29°, one of the strongest residual peaks.
2. On the contextual menu that appears, click the **Create Match Peak at 2Th=… Cnt=…** command to make it a Match peak.

   ➨ The Match peak is highlighted by a large blue triangle pointing to it in the bottom ruler and the string MATCH which is added to its caption.



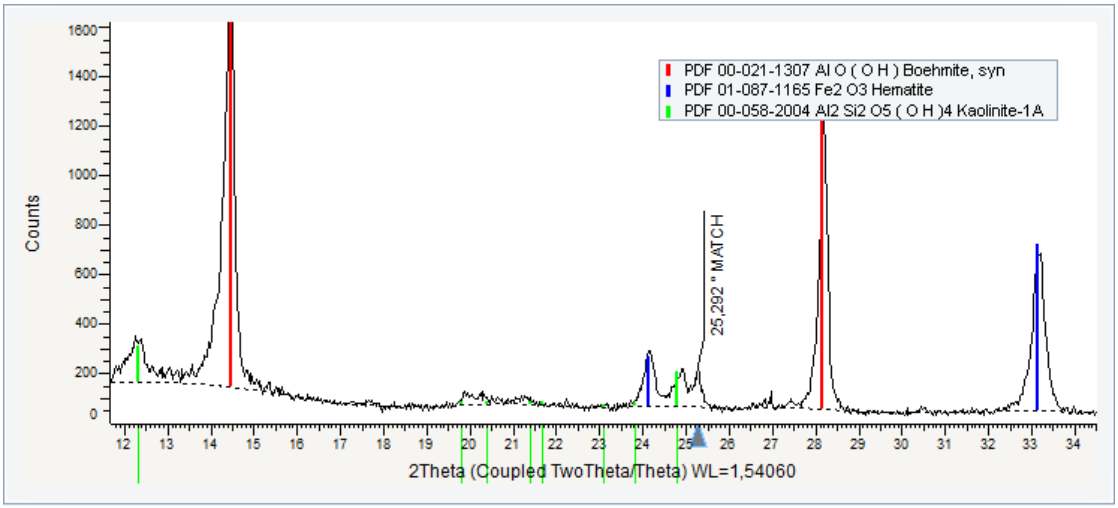
3. Run another search.

   ➨ Kaolinite will rank 3rd.

4. Select the corresponding check box.

Kaolinite is a low symmetry phase with lot of peaks which makes it unsuitable for the residue scheme, at least not for the auto residue. We will define here another Match peak.

1. First, delete the previous Match peak.
2. Point and right-click the peak at about 25.29° and set it as Match peak.



3. Run another search.
4. It makes it possible to identify Anatase ranking 8th.
5. We select a pattern with the simple TiO2 formula and of star quality, e.g. 00-021-1272, despite it is not the first Anatase in the result list.
6. Select the corresponding check box.

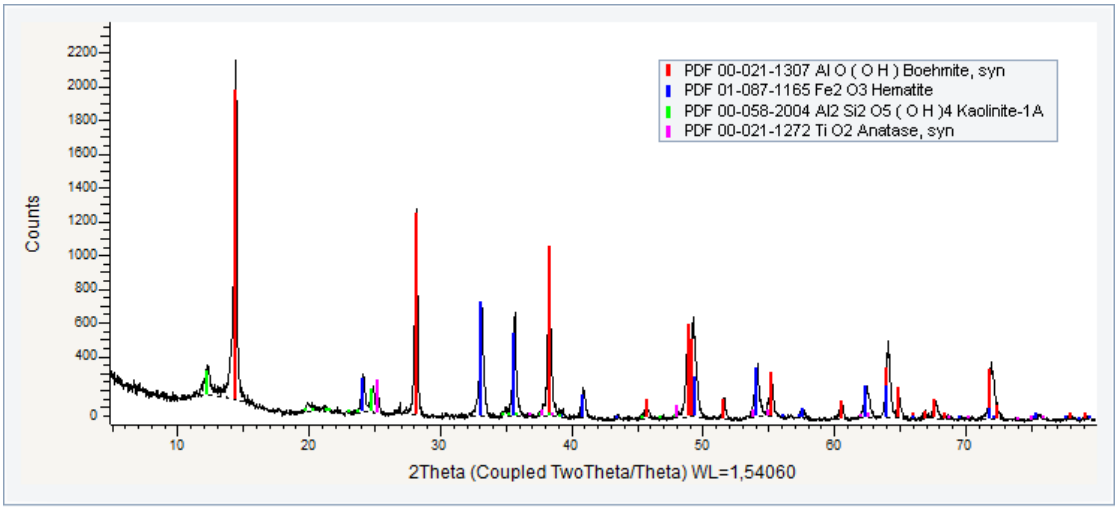


Figure 3.6: BX100 scan with the 4 phases identified

3.5 Step 5: Saving

1. Click **Save As** on the **File** menu.
   ➨ The **Save EVA File As** dialog box will be displayed.
2. Select the appropriate disc drive and directory.
3. Type in the file name. (To overwrite an **.EVA** file, use the same name).
4. Click **Save**.

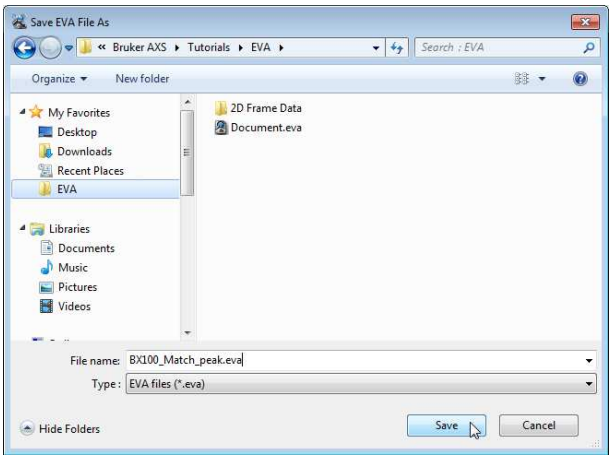


Figure 3.7: Saving BX100_Match_peak.EVA document

4 Creating and Using Filter Lists

A reference database is required to perform a **Search/Match** operation.

This tutorial was prepared using **PDF 4+ 2016** as a reference database. You may have another reference database.

If you have no database, you cannot perform this part of the tutorial concerning the **Search/Match**.

The following procedure describes how to create and use filter lists.

The document used is held as a tutorial file, m1.RAW, found in the Tutorial directory.

Steps:

1. Creating a new EVA document and importing m1.RAW.
2. Creating a filter list.
3. Using a filter list.

4.1 Step 1: Creating a New EVA Document and Importing m1.RAW

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   - ➨ The EVA document is empty.
2. Click the **Import from files** data command or the **Import from files** button.
   - ➨ The **Import From Files** dialog box will be displayed.
3. Search the **Tutorials/EVA*** directory and select the **m1.RAW file**.
4. Click **Open**.
   - ➨ The scan **m1** will be displayed in the graphical view of the EVA document.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

Figure 4.1: Importing the m1.RAW file

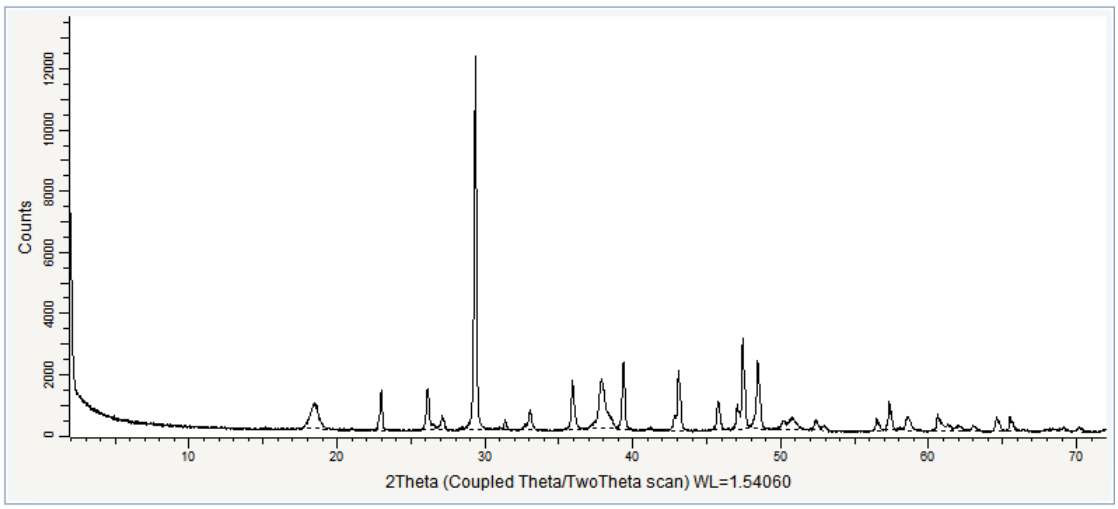
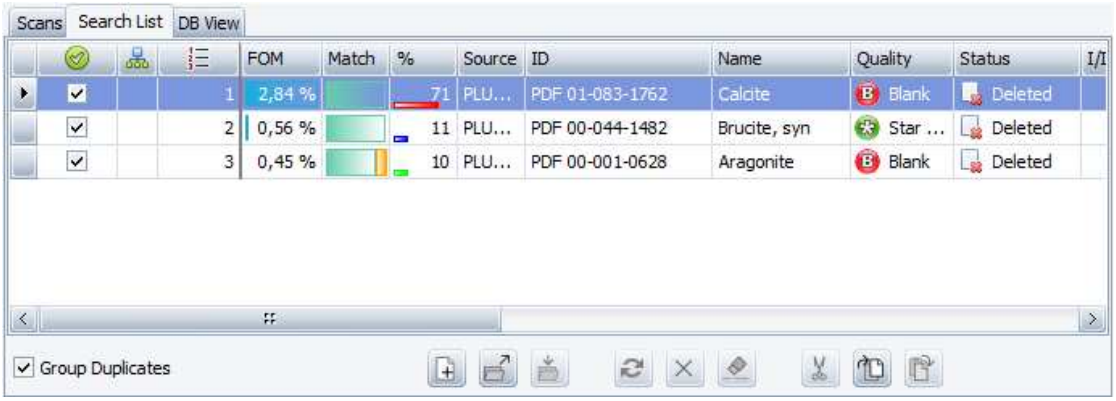


Figure 4.2: m1.RAW file imported in the Graphical view

4.2 Step 2: Creating a Filter List

Patterns can be added to a Filter List from the results of a Search by name or Search/match.

1. Perform an automatic Search/Match as described in the tutorial chapter *Case #1: m1.RAW [▶ 12]*.

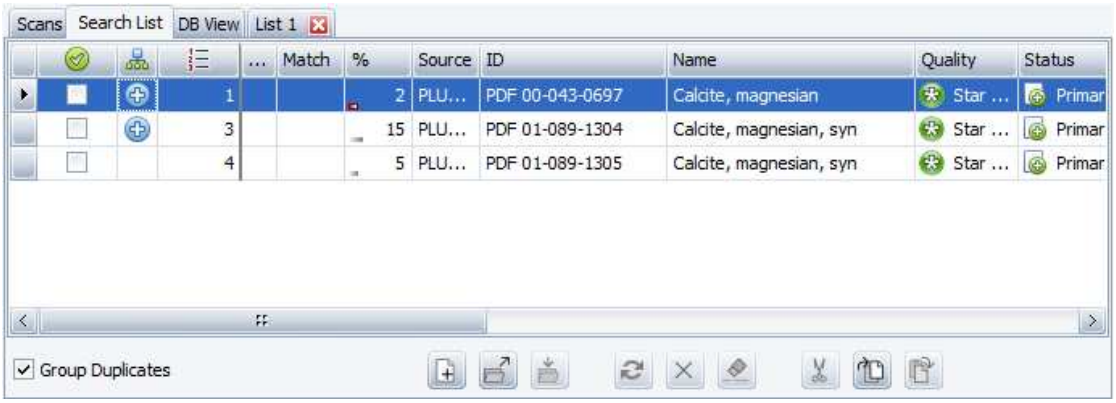


2. Below the Search list, click the **New list** button to create a new filter list.
   - ➡ A new tab containing an empty list will be added.

3. In the **Search list** tab, select the three identified patterns and click the **Copy Section to Clipboard** button.

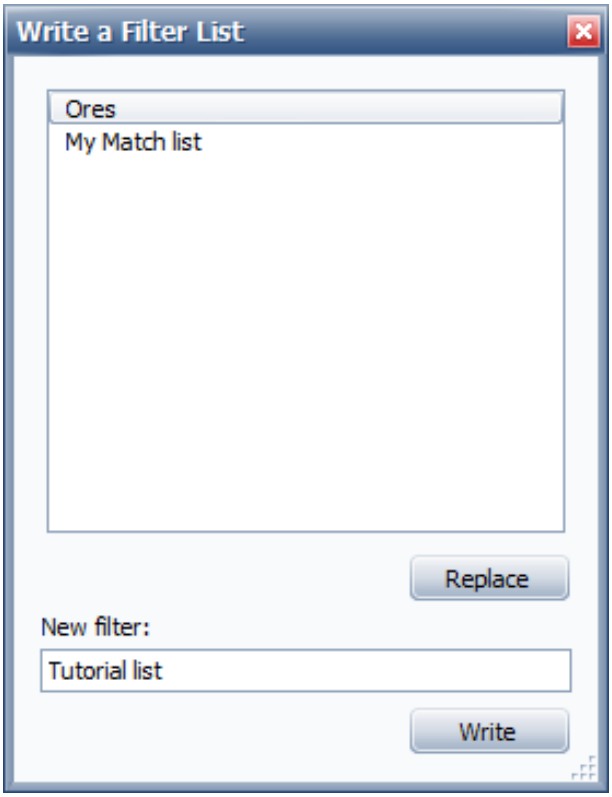
4. Go back to the new **List** tab and click the **Paste Selection to Clipboard**.
   - ➡ The patterns will be added to the list.
5. Perform a Search by Name:
6. In the **Names** tab of the Search/Match dialog box, type *Magnesian Calcite* and click the **Search by Name** button.

   - ➡ Candidates will be listed in the Search list.



7. Copy pattern PDF 01-089-1304 and paste it to the new list using the **Copy** and **Paste** buttons.

8. Click the **Save File** button.
9. In the Write a Filter List dialog box, enter a name for the list and click the **Write** button.

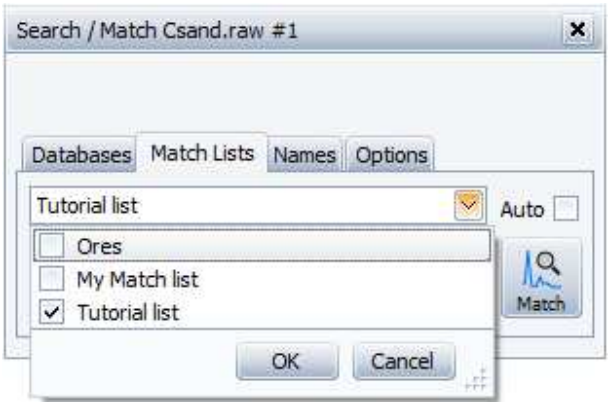


10. Close the document.

4.3 Step 3: Using a Filter List

You will be given here an example of **Search/Match** procedure using a filter list.

1. Import the **Csand.RAW** scan file and open the Search/Match dialog.
2. In the **Match list** tab, select the created filter list by selecting the corresponding check box in the drop-down list.



3. Click **OK.**
4. Click the **Match** button.
   ➨ Search results will be reduced to the patterns contained in the Match list.

5 Creating a User Database

A reference database is required to perform a **Search/Match** operation.

This tutorial was prepared using **PDF 4+ 2016** as a reference database. You may have another reference database.

If you have no database, you cannot perform this part of the tutorial concerning the **Search/Match**.

It is possible to create and maintain a separate database containing the user own patterns. This database is called a user database.
This chapter describes the basic procedure to create a user database and to use it when performing a search.

The used scans are m1.RAW and LaB6.BRML, stored in the Tutorials directory.

Steps:

1. Creating a new EVA document and importing m1.RAW.
2. Search by Name and grouping by Quality:
   Insertion of Calcite
3. Performing the Tune cell operation on the Calcite pattern.
4. Creating the user database.
5. Adding the Calcite pattern to the database.
6. Importing LaB6.BRML.
7. Adding the LaB6 DIF to the user database.
8. Using the User database during a Search/Match operation.

5.1 Step 1: Creating a New EVA Document and Importing m1.RAW

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   ➨ The EVA document is empty.

2. Click the **Import from files** data command or the **Import from files** button.
   ➨ The **Import From Files** dialog box will be displayed.
3. Search the **Tutorials/EVA*** directory and select the **m1.RAW file**.
4. Click **Open**.
   ➨ The scan **m1** will be displayed in the graphical view of the EVA document.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

Figure 5.1: Importing the m1.RAW file

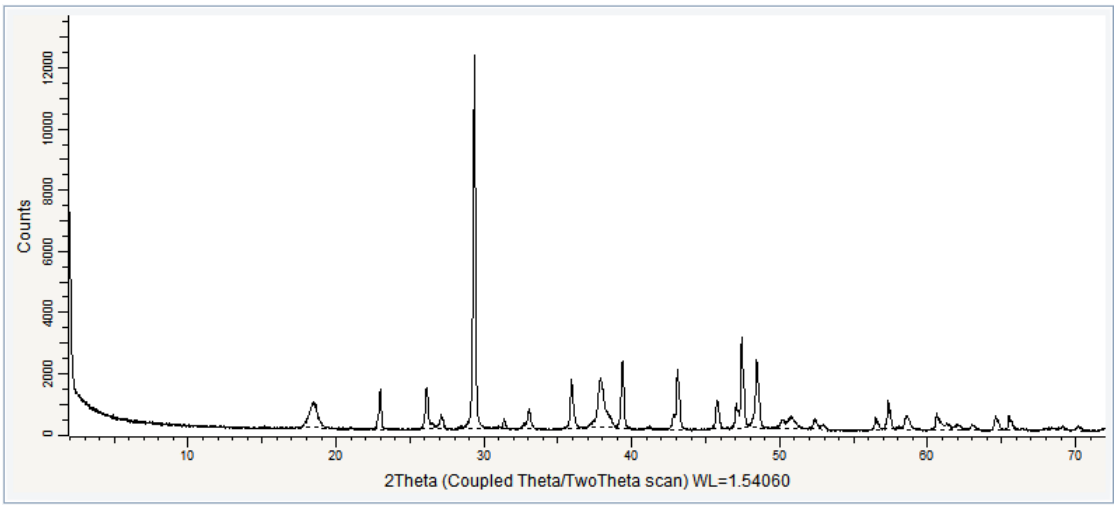


Figure 5.2: m1.RAW file imported in the Graphical view

5.2 Step 2: Performing the Search by Name

▷ Make certain the scan is selected; if not, select it either in the **Data tree** or in the **Graphical view**.

1. Click **Search by Name** in the Data Command panel
   — or —
   click the **Search by Name** button on the Search/Match toolbar
   — or —
   right-click the scan, click **Tool** on the context menu and then **Search by Name** on the related submenu.

   ➨ The **Search / Match** dialog box will open on the **Names** tab.

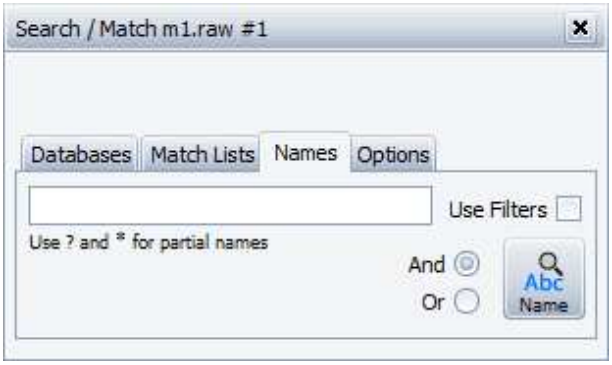
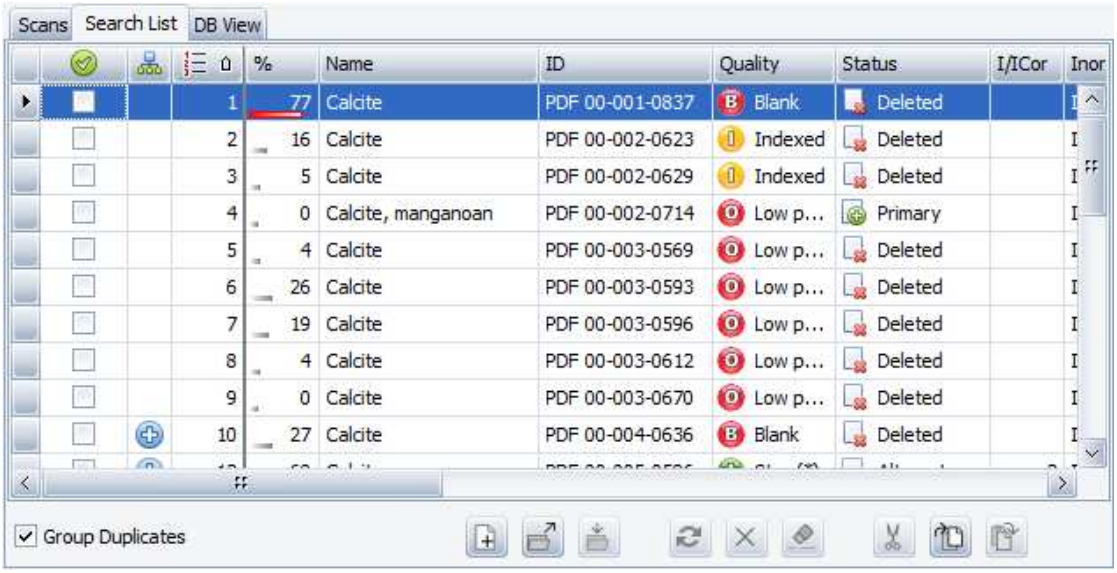


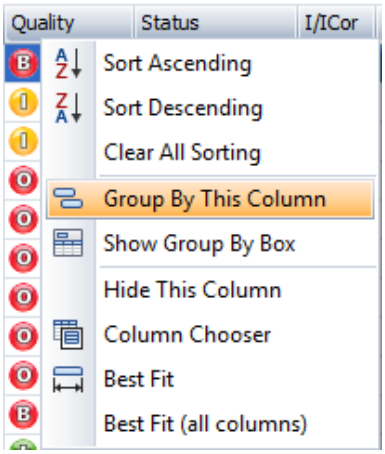
Figure 5.3: Names tab of the Search / Match dialog

2. Type **Calcite** in the Name field.
3. Let the **Use Filters** check box cleared.
4. Launch the search by clicking the **Search by Name** button.
   ➨ The candidates are listed in the **Search list** tab of the Data tree panel.

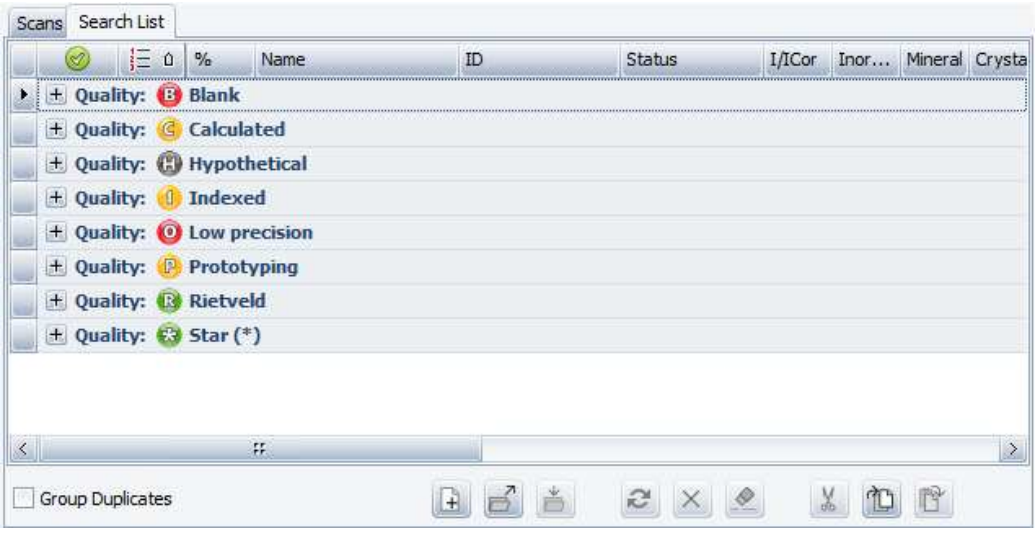


Here, we will group patterns by quality.

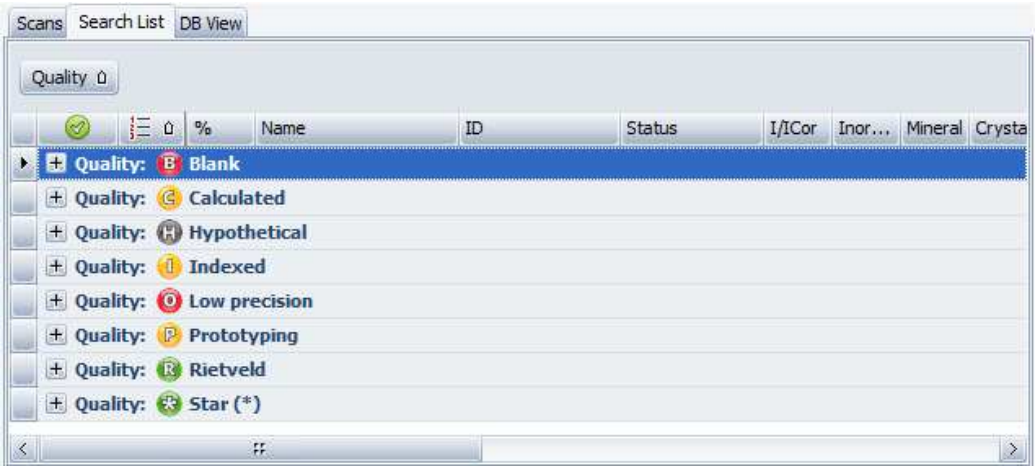
1. Right-click the **Quality** column to display the related contextual menu.



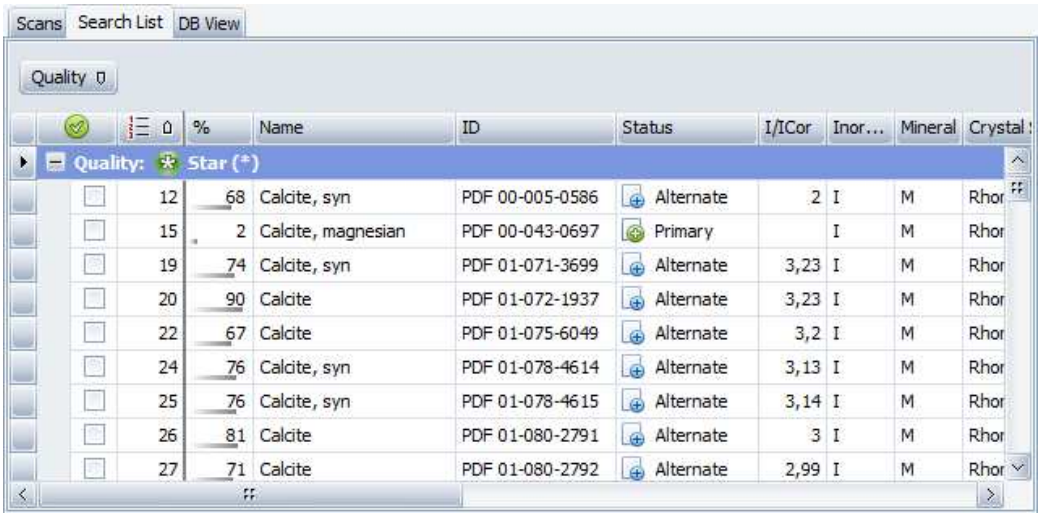
2. Click the **Group By This Column** command to group the candidates by *Quality*.



3. Right-click one of the column header and on the contextual menu that appears, click the **Show Group by Box** column.
   - The column header used for the grouping, that is to say **Quality**, will be displayed above the table.

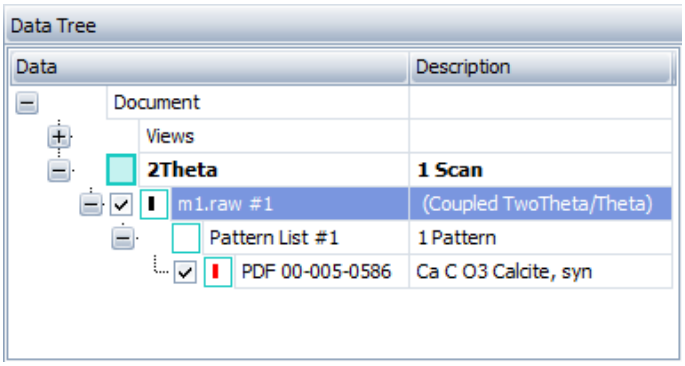


4. Click it to sort the quality groups in descending order.
5. Click the **+** sign before **Quality: Star (*)** to display all Star quality candidates.



6. Mark the first pattern PDF 00-005-0586 by selecting the corresponding check box.

⇨ The pattern will be added to the Data tree and displayed in the graphical view.

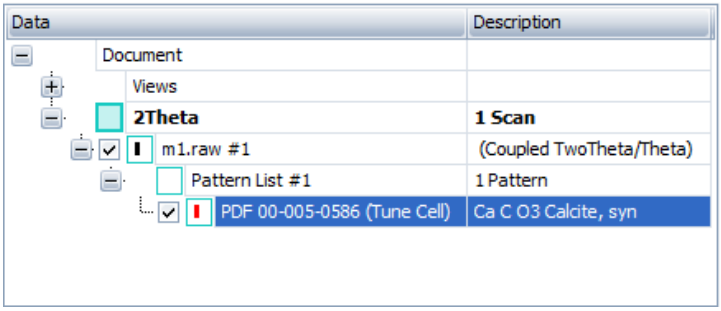


5.3 Step 3: Performing the Tune Cell Operation

It is not allowed to use genuine ICDD patterns in a user database. That is why we use the Tune cell tool. Computed d(hkl) will be used without alteration of the cell parameters.

1. Select the **Calcite** pattern in the **Data tree**.
2. Click **Tune Cell** in the **Data Command** panel
   — or —
   click the Tune Cell button of the **Pattern** toolbar
   — or —
   right-click the pattern, then click **Tune Cell** on the context menu.
   ➨ The **Tune cell** dialog box will be displayed.

3. Do not modify anything and click the **Replace** button.
   ➨ The **Calcite** pattern PDF 00-005-0586 will be replaced by the pattern PDF 00-005-0586 (Tune Cell) in the **Graphical view** as well as in the **Data Tree**.



5.4 Step 4: Creating the User Database

1. Click **User Database** in the **Data Command** panel
   — or —
   click the **User Database** button on the **Pattern** toolbar
   — or —
   right-click the tuned pattern and click **User Database** on the context menu.
   ➨ The **User Database** dialog box will be displayed.

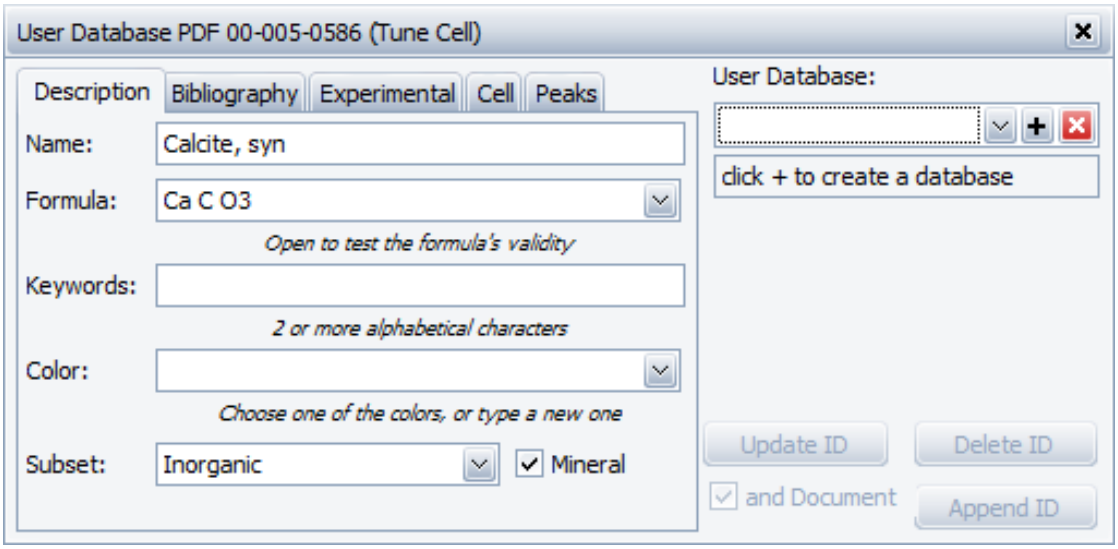


*Figure 5.4: **User Database** dialog box*

2. Click the button next to the **User database** field.
   ➨ The **User Database Creation** dialog box will be displayed.

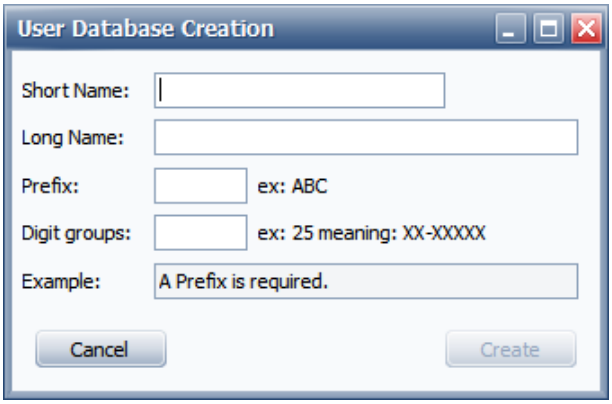
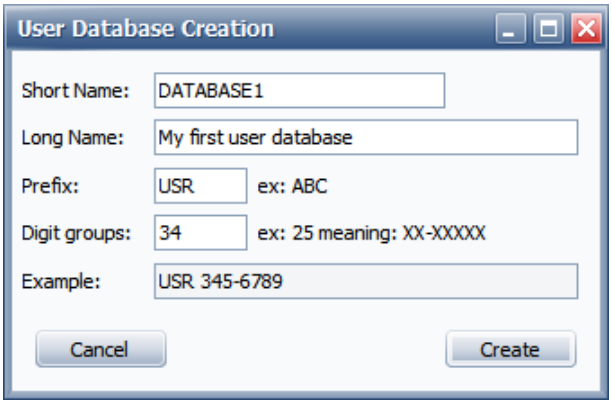


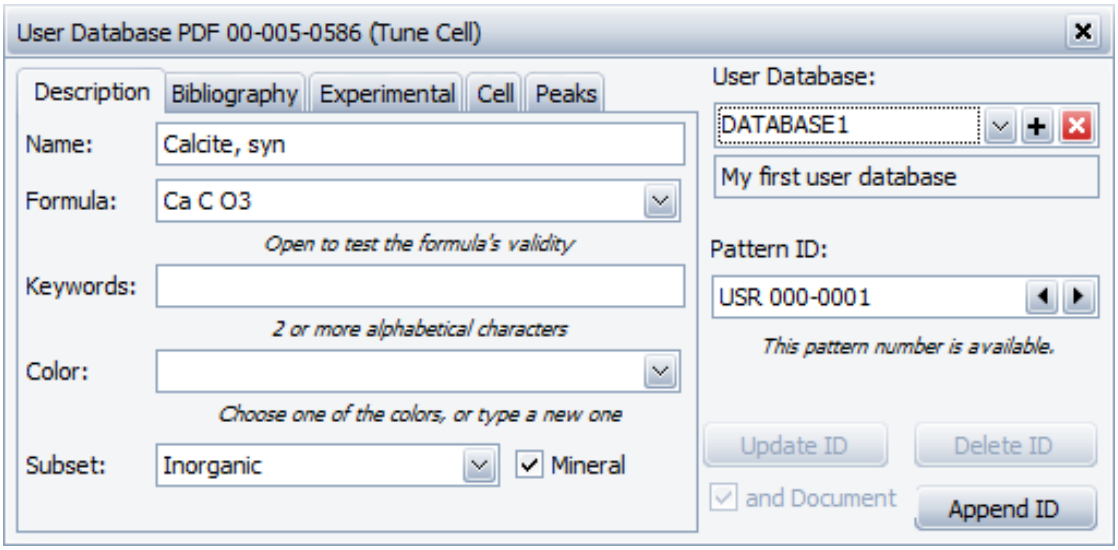
Figure 5.5: User database creation dialog box

3. Enter a **Short Name** and a **Long Name**: for example, *DATABASE1* and *My first user database*. The Long name is the name which will be used in DIFFRAC.EVA (e. g. in the **Database** tab of the **Settings** dialog box and in the **Database filter** tab of the **Search/ Match** dialog box). Please choose the name carefully. It cannot be changed after the user database has been created.
4. Enter a **Prefix** for the user patterns' name: for example, *USR*.
5. Enter the **Digit** groups to define the way the user database patterns are numbered. Enter two digits: the first digit gives the number of digits in the first digits group. The second digit gives the number of digits in the second digits group. Enter 34. The name given to the patterns will have the form XXX-XXXX.

➨ The example field will give an example of a pattern name with a prefix and a digits group chosen.



6. Finally, click the **Create** button.
   ➨ The user database will be displayed in the **User Database** dialog box and it will be then possible to add patterns.



5.5 Step 5: Adding the Calcite pattern to the database

Once the user database has been created, it is possible to create user patterns.

1. In the User database dialog box, as shown at the previous step, the tuned PDF calcite pattern is given by default the first pattern number available: USR 000-0001 (**Pattern ID** field).
2. Click the **Append ID** button to add the pattern to the user database.
   ➨ The User Database dialog box will be closed.
3. Close the document.

⇨ All the data will be removed from the screen.

5.6 Step 6: Creating a New Document and Importing LaB6.BRML

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   - ➨ The EVA document is empty.

2. Click the **Import from files** data command or the **Import from files** button.
   - ➨ The **Import From Files** dialog box will be displayed.
1. Search the Tutorials/EVA* directory and select the LaB6.BRML file.
2. Click **Open**.
   - ➨ The scan LaB6 will be added to the Data tree and displayed in the graphical view of the EVA document.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

Figure 5.6: Importing LaB6.brml

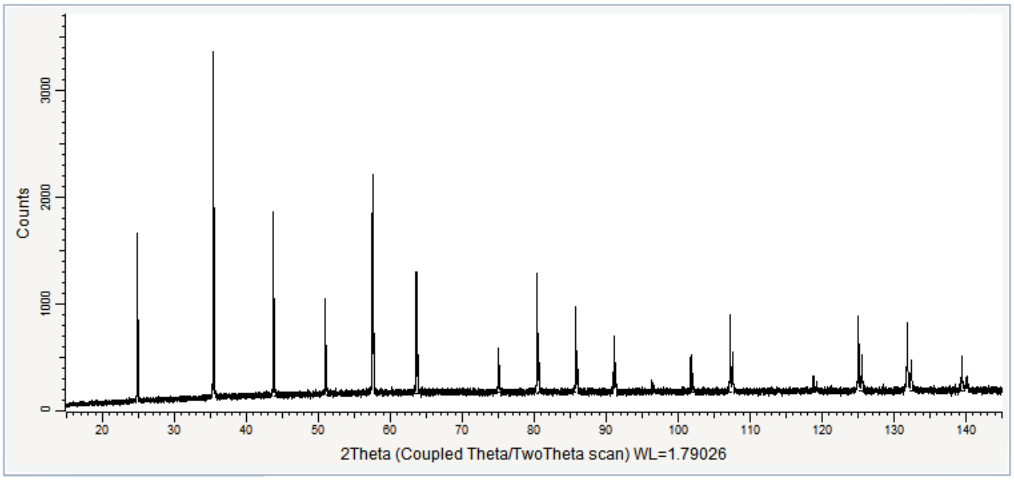


Figure 5.7: LaB6 file imported in the graphical view

5.7 Step 7: Adding the LaB6 DIF to the User Database

1. Make sure the scan has been selected. If not, select it either in the data tree or in the 1D view.

2. Click **Peak Search** in the Tool list of the Data Command panel
   — or —
   click the **Peak Search** button on the Peak/Area toolbar
   — or —
   right-click the scan, and then click **Tool** on the context menu. Click **Peak Search** on the Tool submenu.
   ➨ The **Peak Search** dialog box will be displayed.

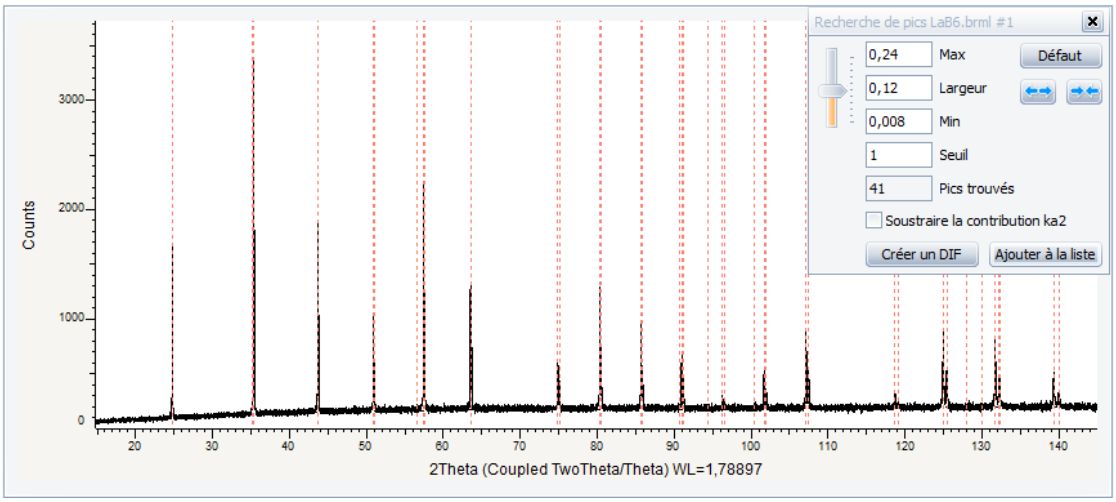


Figure 5.8: Peak Search dialog box and graphical view showing the ghost peaks

3. The default parameters are set in the Peak Search dialog box and the ghost peaks are displayed in the graphical view. The ghost peaks will be modified if the slider is moved.
4. Select the **Remove Ka2 contribution** check box and move the slider to adjust the peaks.

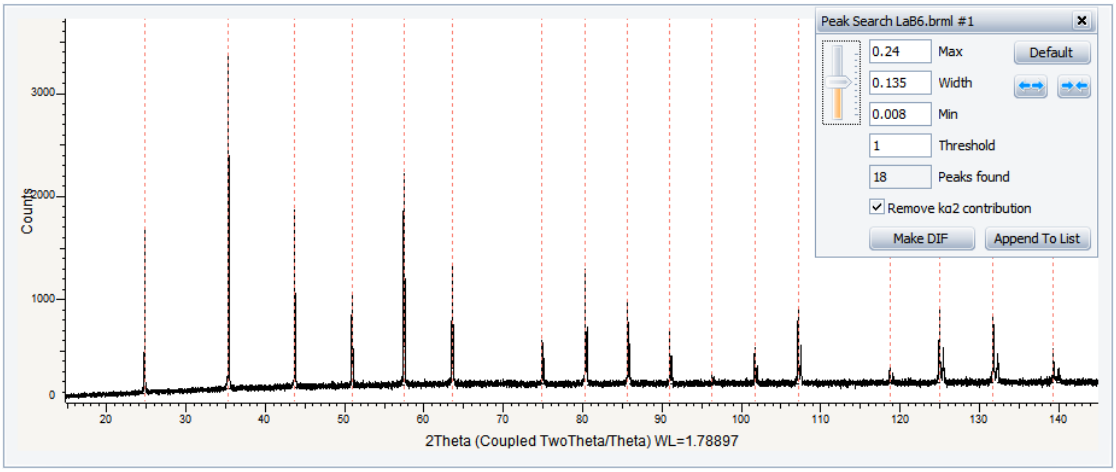
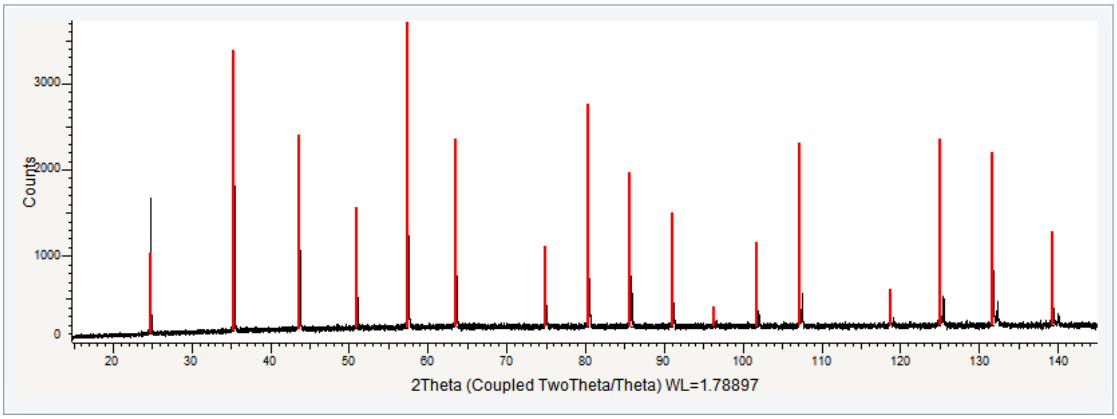
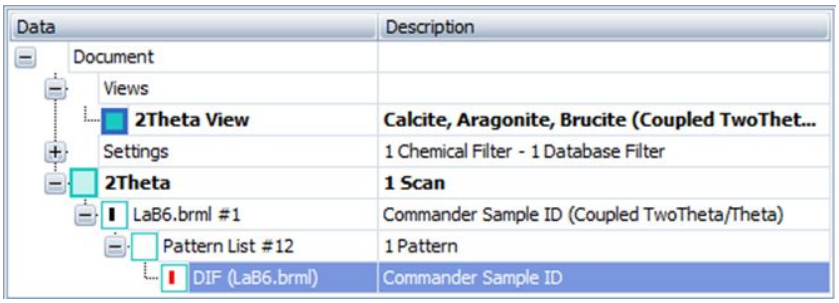


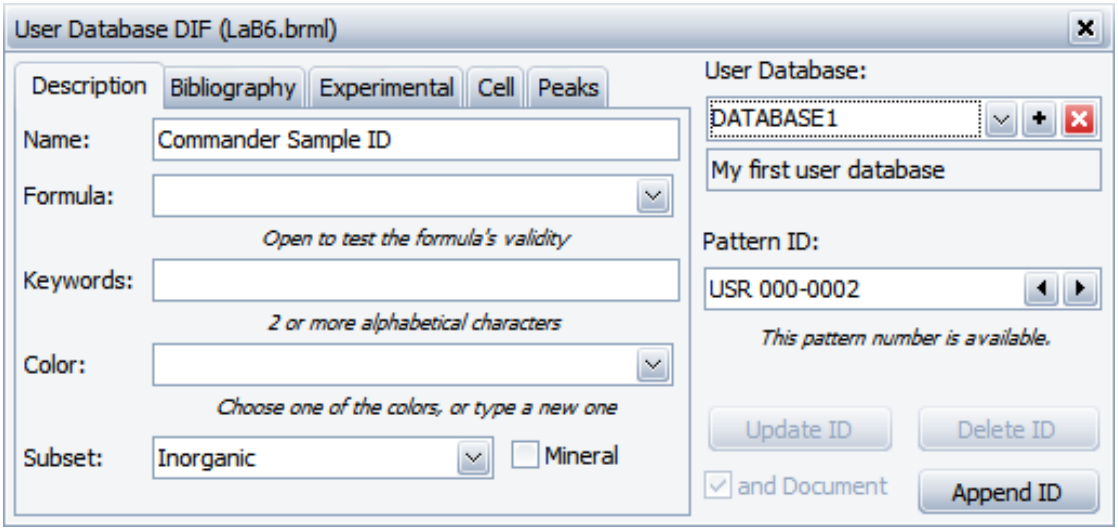
Figure 5.9: Performing a peak search on the LaB6 scan

5. Click the **Make DIF** button: the corresponding DIF is added to the data tree and to the graphical view.

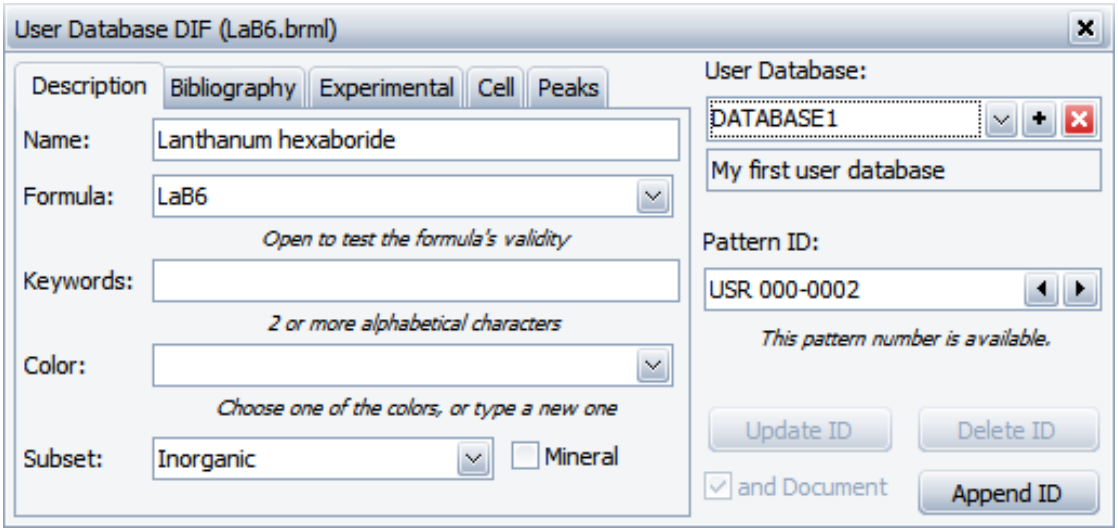




6. Click **User Database** in the Data Command panel
   — or —
   right-click the DIF and click **User Database** on the context menu.
   - The User Database dialog box will be displayed with the user database and the first pattern number available for the pattern ID (USR 000-0002).



7. Modify the **Name** and **Formula** in the Description tab on the left. Enter respectively *Lanthanum hexaboride* and *LaB6*.

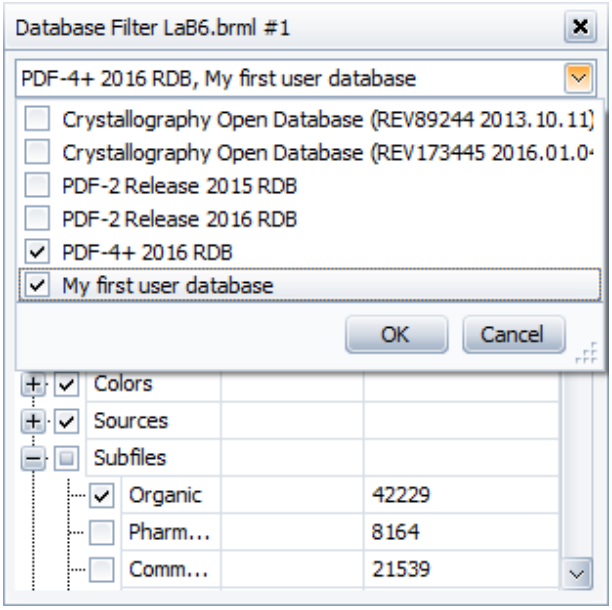


8. Click the **Append ID** button to add the new pattern to the selected user database.
   ➨ The User Database dialog box will be closed.
9. Delete the DIF from the data tree. It will also be removed from the graphical view.

5.8 Step 8: Using the User Database during a Search/Match operation

A user database can be used the same way as another pattern database. The procedure below will demonstrate how to use the user database when performing a search/match.

1. Select the LaB6.BRML scan.
2. Click **Search / Match** in the Data Command panel
   — or —
   click the **Search / Match** button on the Search/Match toolbar
   — or —
   right-click the current scan, click **Tool** on the menu which appears and then **Search / Match** on the related submenu.
3. In the **Databases** tab, select *My first user database* in addition to the PDF database (here the PDF-4+ 2016) drop-down list. Let the **DB filter** and **Chemical** fields empty.



4. Click the **Search/Match** button.

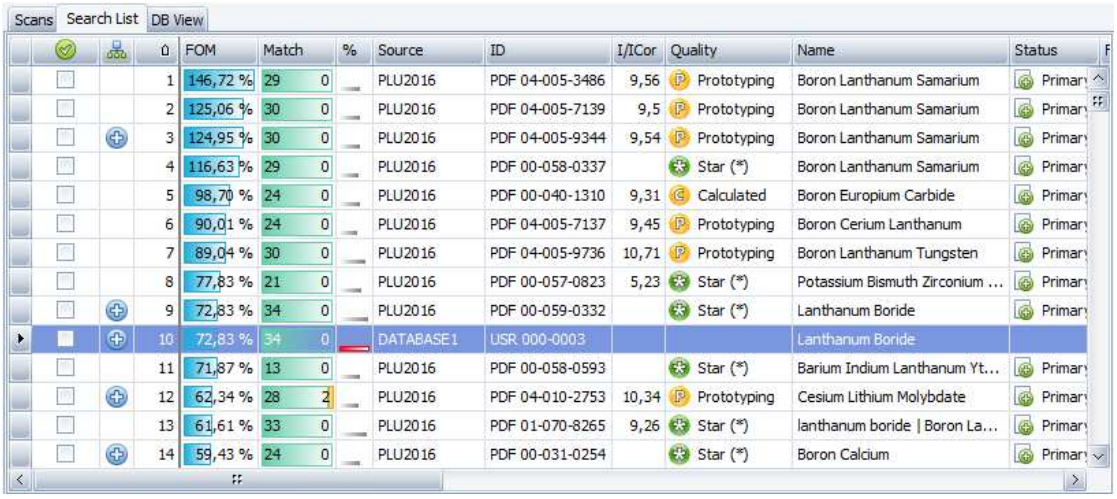


Figure 5.10: Search Results including the user pattern

⇨ The LaB6 user pattern appears in the result list like a PDF pattern and is used in the same way in the data tree and the graphical view.

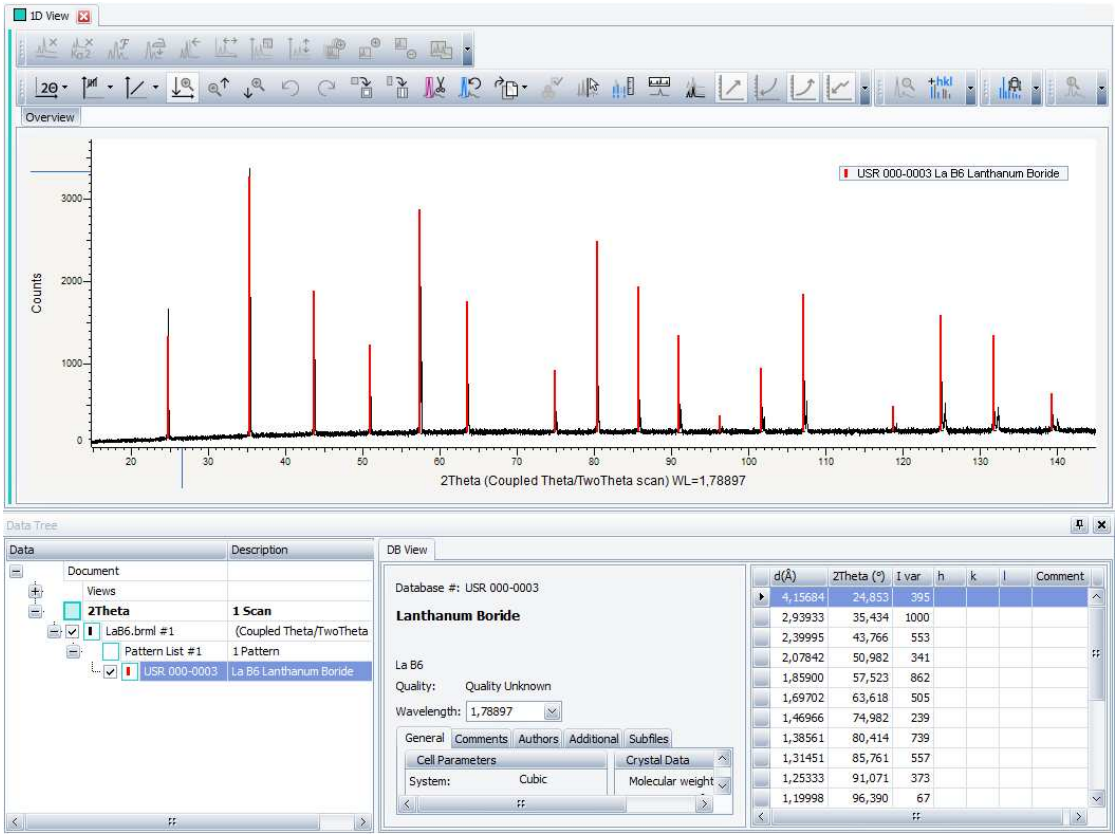


Figure 5.11: User pattern added to the data tree and the graphical view

6 Performing a Peak Search

The following chapter describes the basic procedure for running a peak search.

The scan used is held as a tutorial file, Csand.RAW, found in the Tutorial directory. Csand is white coral sand from a beach in Hawaii. It consists of three types of Carbonates, Aragonite, Calcite and Magnesian calcite.

Steps

1. Creating a new EVA document and importing Csand.RAW.
2. Setting of the setting the peak search parameters.
3. Appending the peaks.
4. Saving the EVA document containing the scan.

6.1 Step 1: Creating a New EVA Document and Importing Csand.RAW

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   ➨ The EVA document is empty.

2. Click the **Import from files** data command or the **Import from files** button.
   ➨ The **Import From Files** dialog box will be displayed.
3. Search the Tutorials/EVA* directory and select the Csand.RAW file.
4. Click **Open**. The scan Csand.RAW will be added to the Data tree and displayed in the graphical view of the EVA document.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

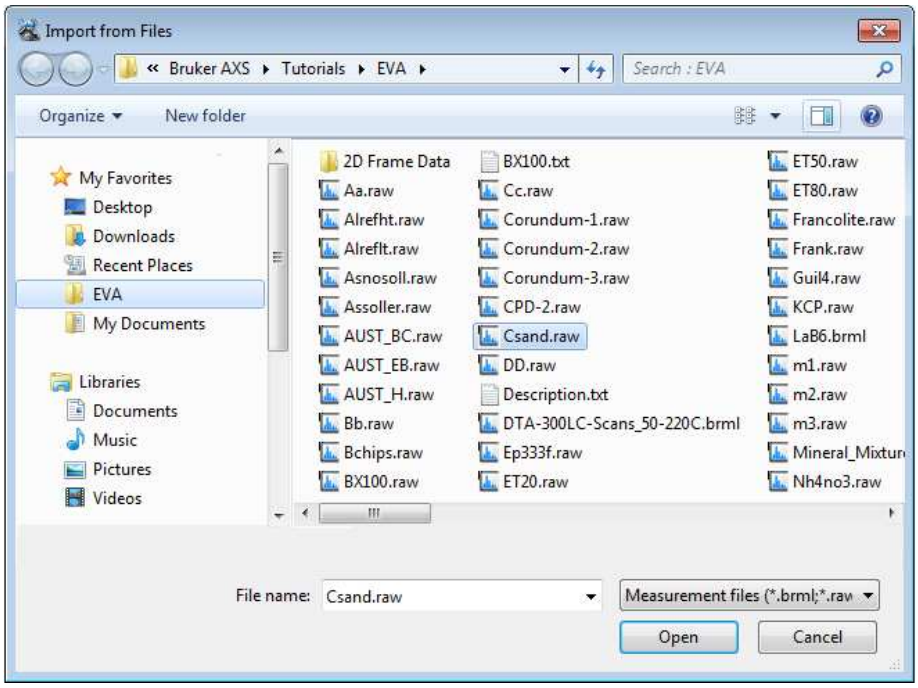


Figure 6.1: Importing Csand.raw

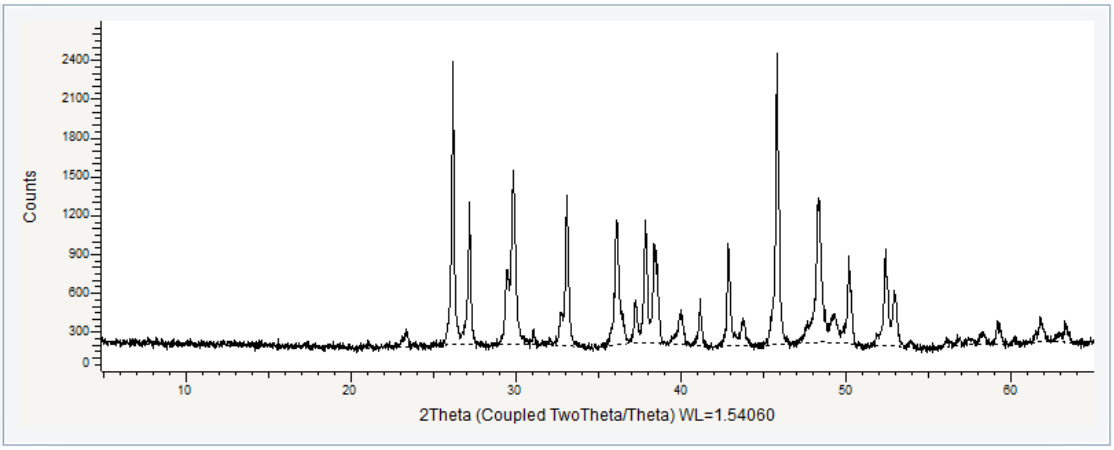


Figure 6.2: Csand scan imported in the graphical view

6.2 Step 2: Setting the Peak Search Parameters

▷ Make certain the scan is selected; if not, select it either in the data tree or in the 1D view.

1. Click **Peak Search** in the Tool list of the Data Command panel
   — or —
   click the **Peak Search** button on the Peak / Area toolbar
   — or —
   right-click the scan, and then click **Tool** on the context menu. Click **Peak Search** on the Tool submenu.

   ➨ The **Peak Search** dialog box will be displayed.

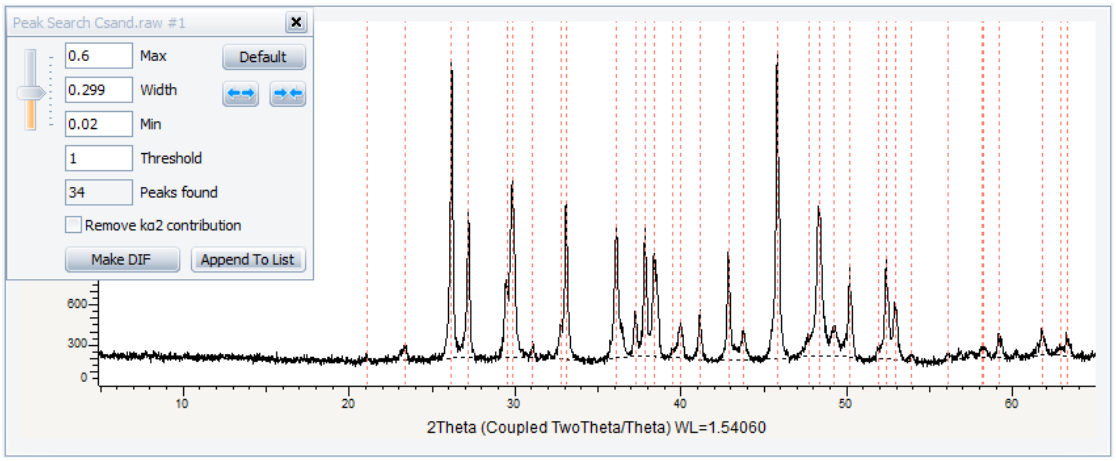


Figure 6.3: Peak Search dialog box and graphical view showing the ghost peaks

2. The default parameters are set in the Peak Search dialog box and the ghost peaks are displayed in the graphical view. If you move the slider the ghost peaks are modified. The Ka2 contribution can be removed by selecting the corresponding check box but it is not necessary here.
3. If the default parameters are satisfactory: click the **Default** button to return to the default parameters.

6.3 Step 3: Appending the Peaks

To validate the peaks and add them to the graphical view as well as to the data tree:

1. Click the **Append to List** button.

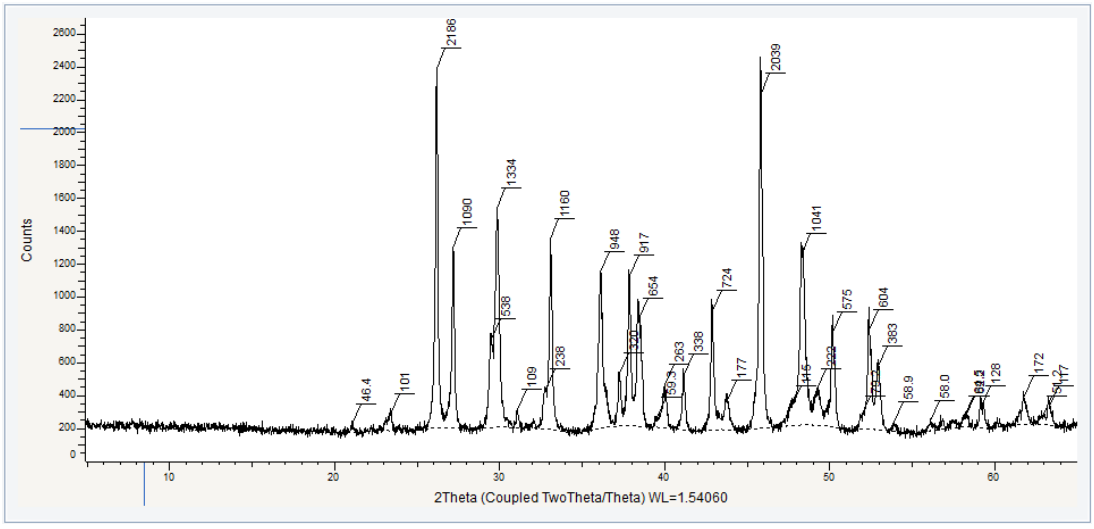


Figure 6.4: Peak Search dialog box and graphical view showing the ghost peaks

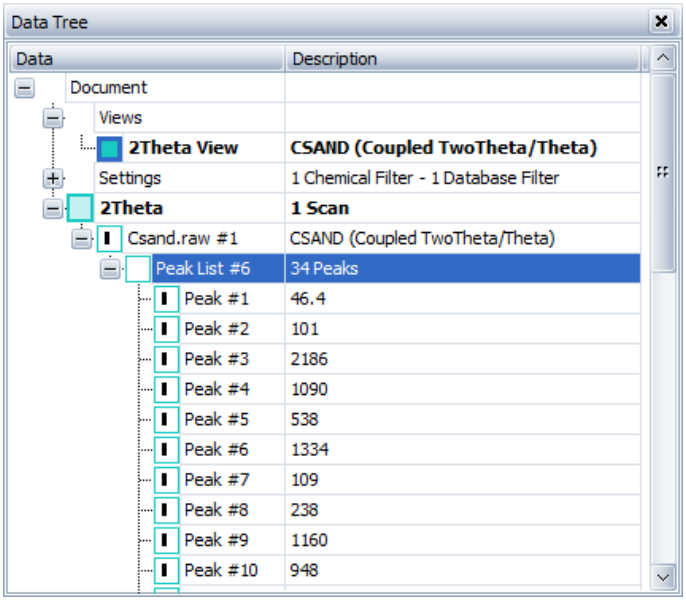


Figure 6.5: Peak List added in the Data Tree

2. You can edit each peak in the Peak Property table. For example you can modify their position or change the layout.

You can also create a DIF pattern by clicking the **Make DIF** button.

6.4 Step 4: Saving

1. Click **Save As** on the **File** menu.
   - ➨ The **Save EVA File As** dialog box will be displayed.
2. Select the appropriate disc drive and directory.
3. Type in the file name. (To overwrite an **.EVA** file, use the same name).
4. Click **Save**.

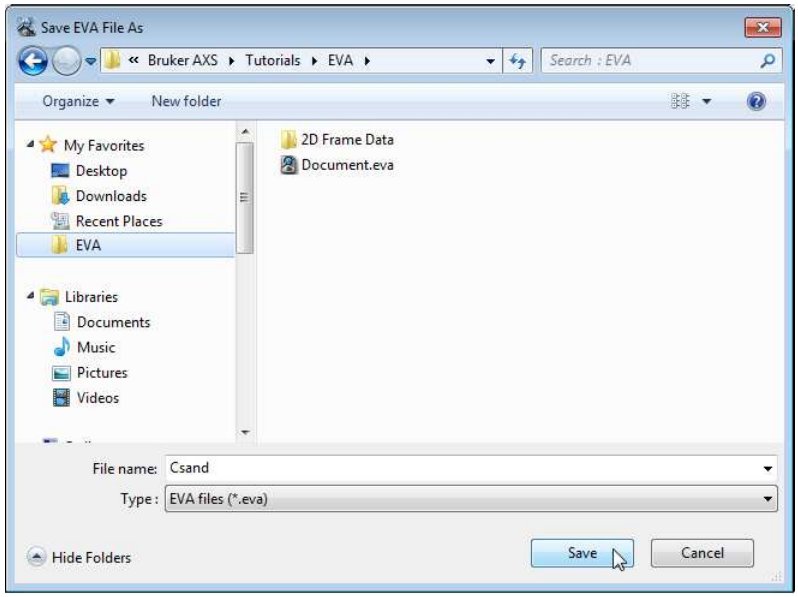


Figure 6.6: Saving Csand.EVA document

7 Computing Kα2 Stripping

The following procedure describes the basic procedure for computing Kα2 Stripping.
The scan used is held as a tutorial file, Quartz.RAW, found in the Tutorial directory.

Steps

1. Creating a new EVA document and importing Quartz.RAW.
2. Computing the Kα2 stripping.
3. Saving the EVA document containing the scan.

7.1 Step 1: Creating a New EVA Document and Importing Quartz.RAW

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   ➨ The EVA document is empty.

2. Click the **Import from files** data command or the **Import from files** button.
   ➨ The **Import From Files** dialog box will be displayed.
3. Search the Tutorials/EVA* directory and select the Quartz.RAW file.
4. Click **Open**. The scan Quartz.RAW will be added to the Data tree and displayed in the graphical view of the EVA document.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

Figure 7.1: Importing Quartz.raw

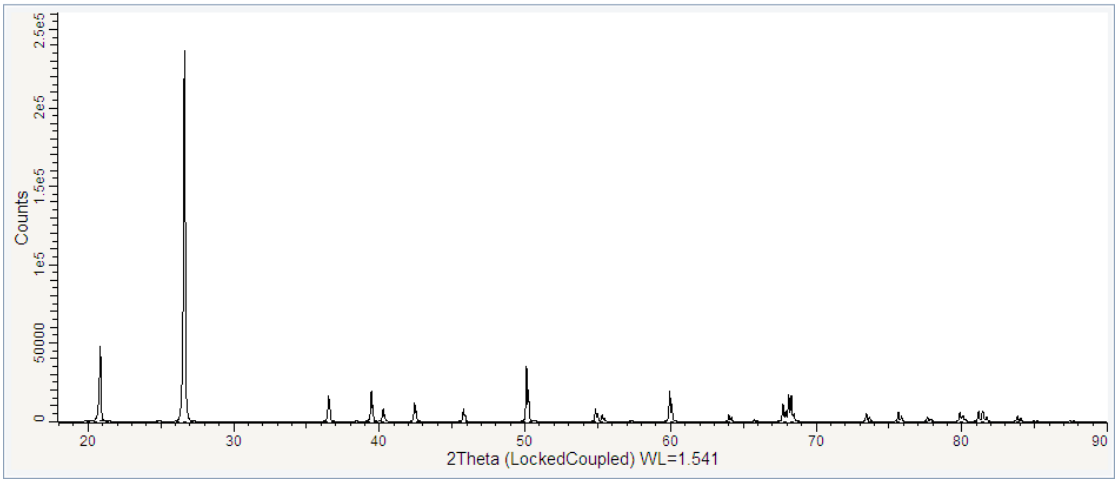


Figure 7.2: Quartz scan imported in the graphical view

7.2 Step 2: Computing the Kα2 Stripping

▷ Make certain the scan is selected; if not, select it either in the data tree or in the 1D view.

1. Right-click the scan, and then click **Tool** on the context menu. Click **Strip Kα2** on the related submenu.
   ➨ The **Strip Kα2** dialog box will be displayed.

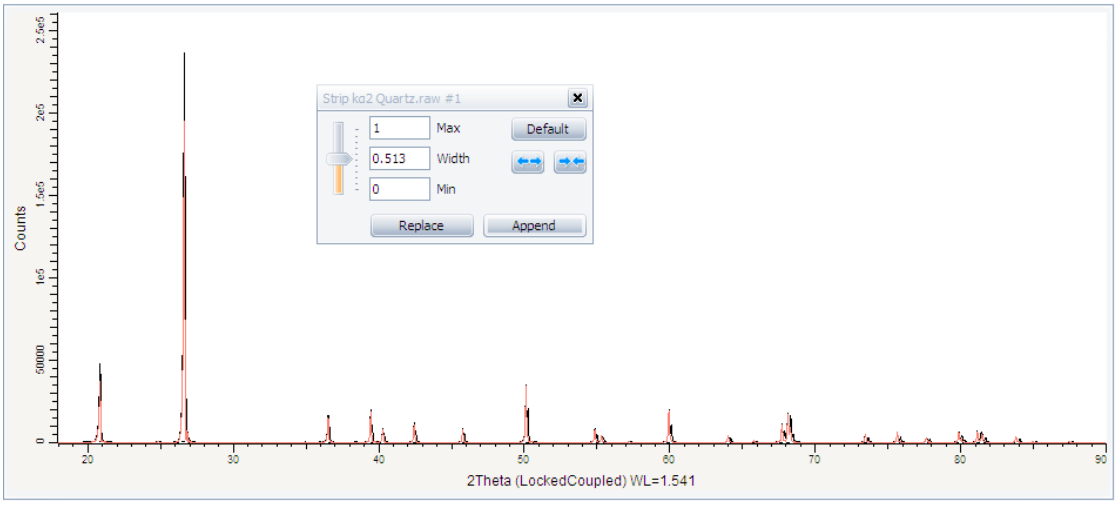


Figure 7.3: Strip Kα2 dialog box and in the graphical view: ghost Kα2-stripped line

2. The default parameters are set in the Strip Kα2 dialog box and the ghost line shows the Kα2-stripped line in the graphical view. If you move the slider the ghost line is modified.
3. Zoom in on the peaks to see the result clearly.

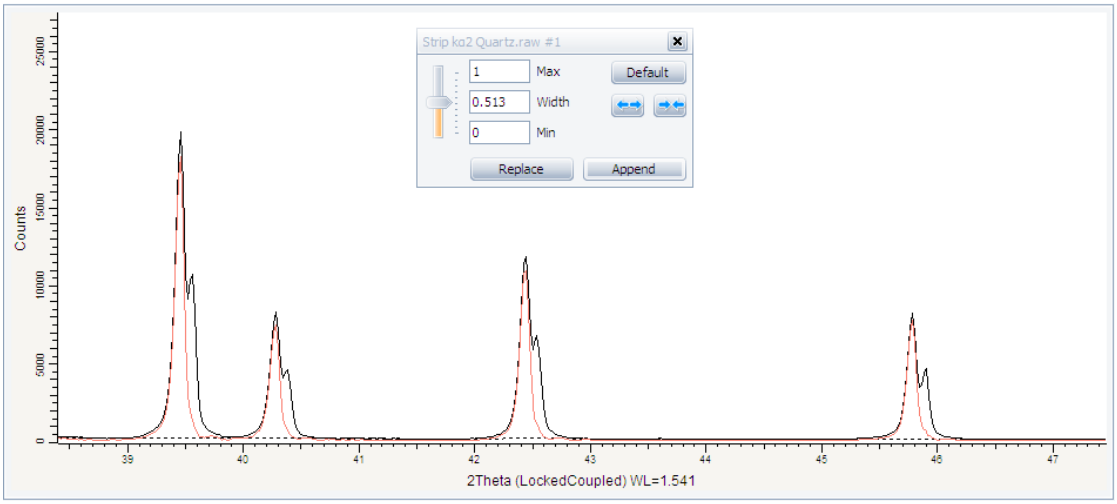


Figure 7.4: Zoom on the peaks (2θ=38° to 48°)

4. Here the default parameters are satisfactory: click the **Default** button to return to the default parameters if necessary.
5. Then, you can:
   - Click **Append** to append the Kα2 subtracted scan to the document. The scan is added to the scan list and its properties can be edited in the property table.
   - Click **Replace** to replace the original scan with the Kα2 subtracted scan.

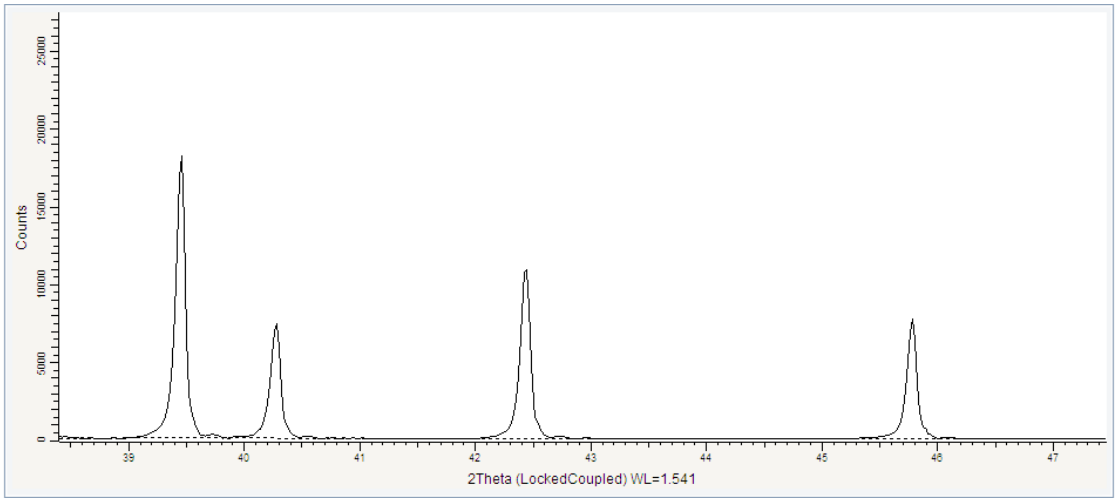


Figure 7.5: Original scan replaced with the Kα2 subtracted scan - Zoom on the peaks (2θ=38° to 48°)

7.3 Step 3: Saving

1. Click **Save As** on the **File** menu.
   ➨ The **Save EVA File As** dialog box will be displayed.
2. Select the appropriate disc drive and directory.
3. Type in the file name. (To overwrite an **.EVA** file, use the same name).
4. Click **Save**.

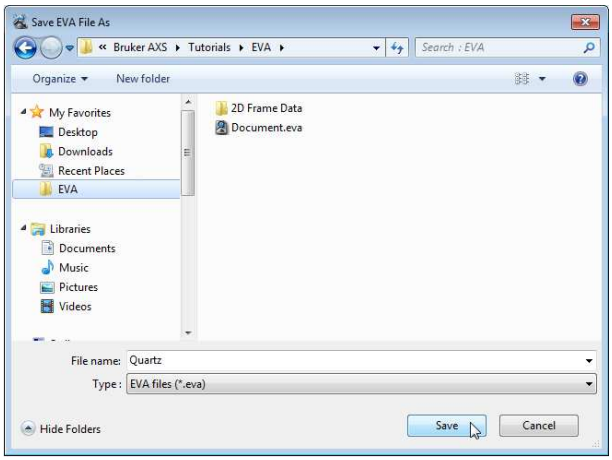


Figure 7.6: Saving the Quartz.EVA document

8 Smoothing Scans

The following procedure describes the basic procedure for smoothing scans.
The scan used is held as a tutorial file, Quartz.RAW, found in the Tutorial directory.

Steps

1. Creating a new EVA document and importing Quartz.RAW.
2. Smoothing the scan.
3. Saving the EVA document containing the scan.

8.1 Step 1: Creating a New EVA Document and Importing Quartz.RAW

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   ➨ The EVA document is empty.

2. Click the **Import from files** data command or the **Import from files** button.
   ➨ The **Import From Files** dialog box will be displayed.
3. Search the Tutorials/EVA* directory and select the Quartz.RAW file.
4. Click **Open**. The scan Quartz.RAW will be added to the Data tree and displayed in the graphical view of the EVA document.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

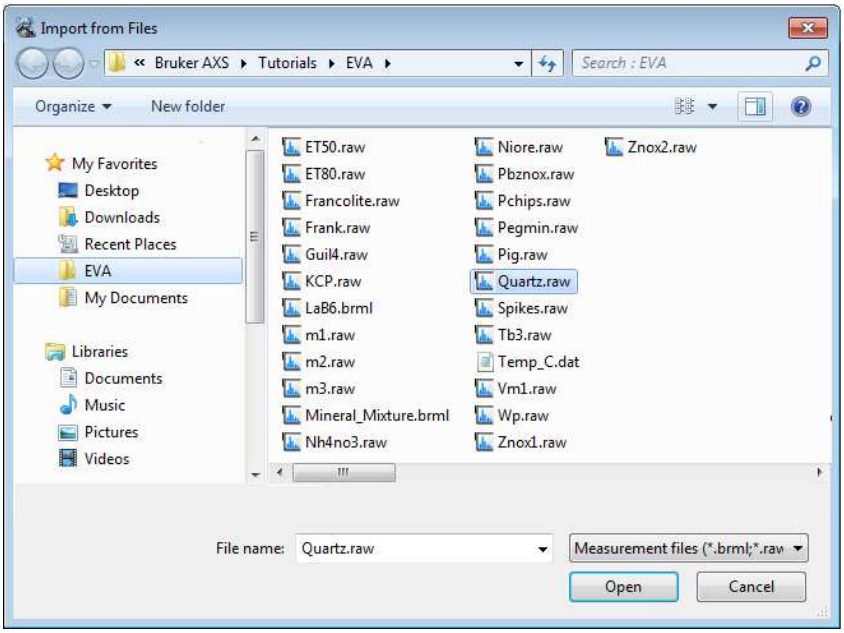


Figure 8.1: Importing Quartz.raw

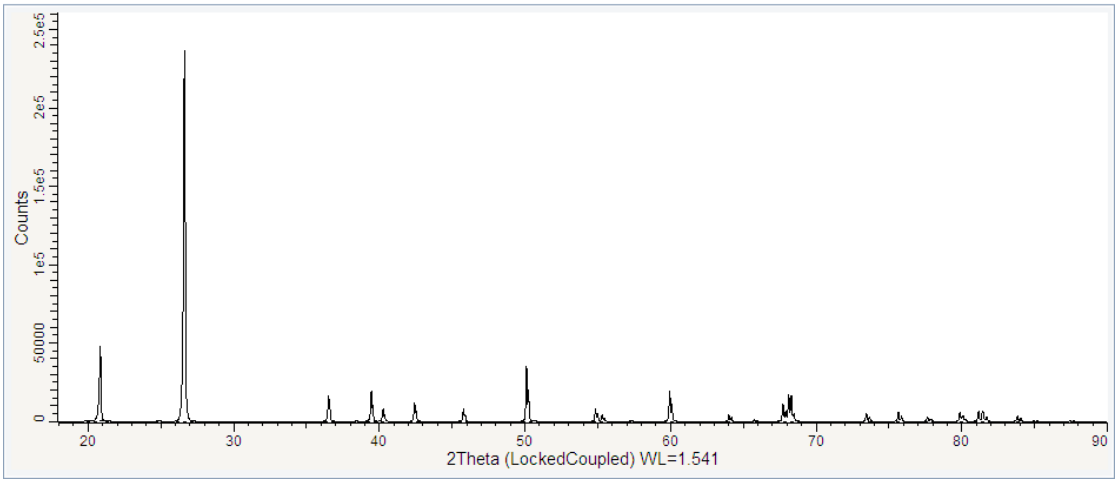


Figure 8.2: Quartz scan imported in the graphical view

8.2 Step 2: Smoothing the Scan

Case #1: Smoothing

▷ Make certain the scan is selected; if not, select it either in the data tree or in the 1D view.

1. Right-click the scan, and then click **Tool** on the context menu. Click **Smooth** on the related submenu:
   ➨ the **Smooth** dialog box will be displayed.

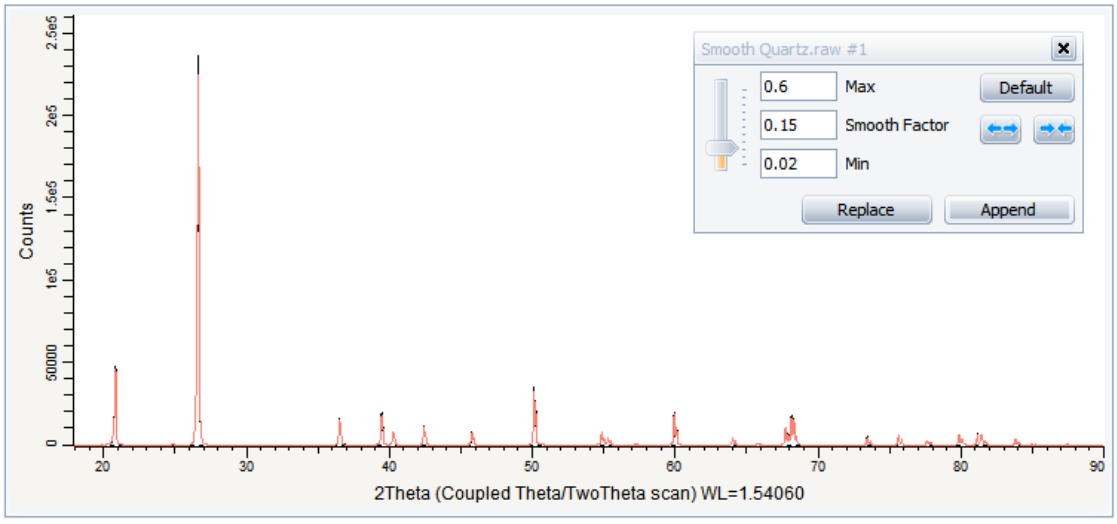


Figure 8.3: Smooth dialog box and in the graphical view: ghost smoothed line

2. The default parameters are set in the Smooth dialog box and the ghost line shows the smoothed line in the graphical view. If you move the slider the ghost line is modified.
3. Zoom on the peaks to clearly see the result.

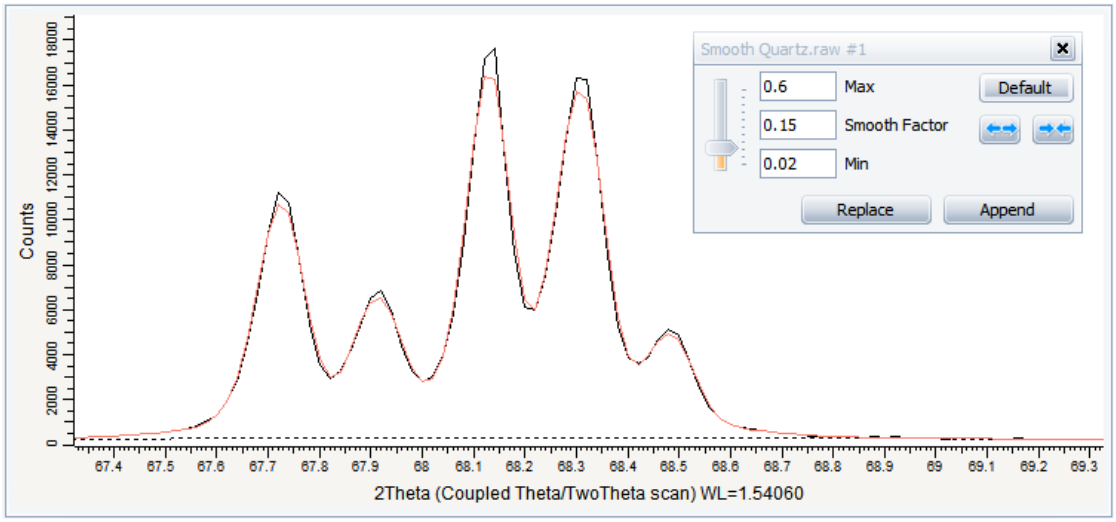


Figure 8.4: Zoom on peaks (2θ=67° to 69°)

4. Here the default parameters are satisfactory: click the **Default** button to return to the default parameters if necessary.
5. Then, you can:
   - Click **Append** to append the smoothed scan to the document. The scan is added to the scan list and its properties can be edited in the property table.
   - Click **Replace** to replace the original scan with the smoothed scan.

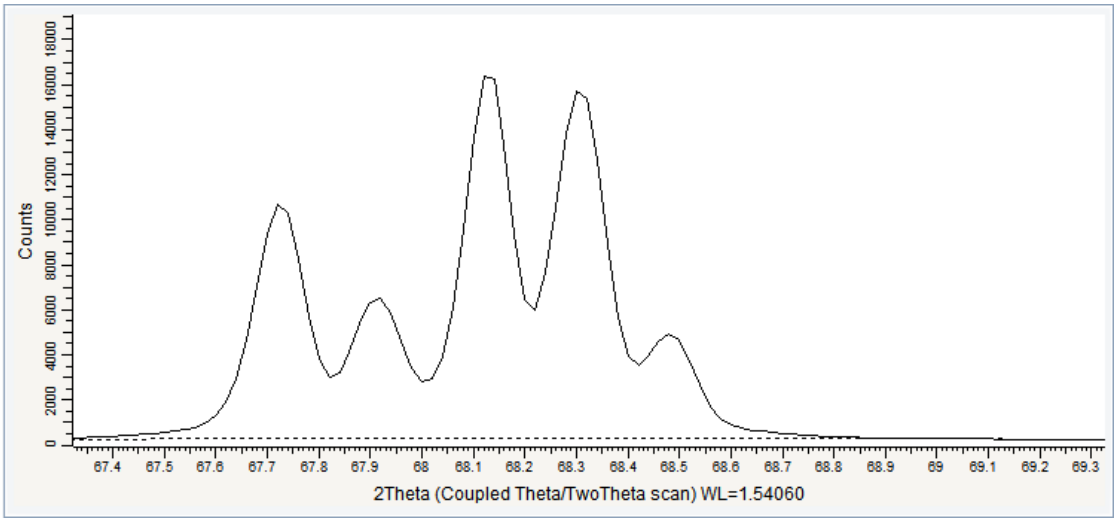


Figure 8.5: Original scan replaced with the smoothed scan - Zoom on peaks (2θ=67° to 69°)

Case #2: Fourier Smoothing

▷ Make certain the scan is selected; if not, select it either in the data tree or in the 1D view.

1. Right-click the scan, and then click **Tool** on the context menu. Click **Fourier Smooth** on the related submenu.
   ➨ The **Fourier Smooth** dialog box will be displayed.

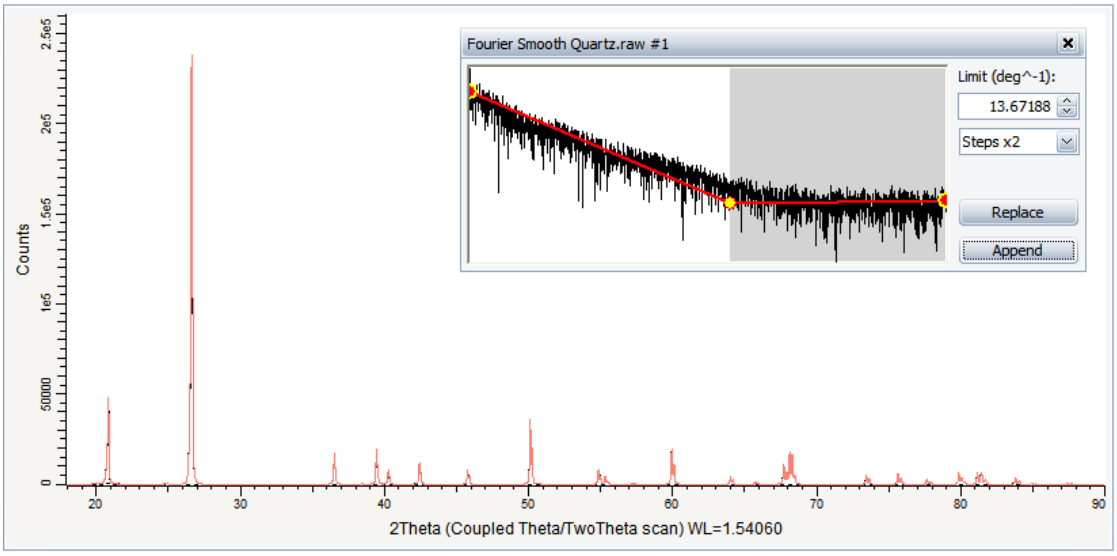


Figure 8.6: Smooth dialog box and in the graphical view: ghost smoothed line

2. Automatic adjustments are done. The ghost line shows the smoothed line in the graphical view.
3. You can modify the cutoff graphically or by changing the limit value. You can modify the expansion by selecting another **Steps multiplied by** value.
4. Zoom in on the peaks to see the result clearly.

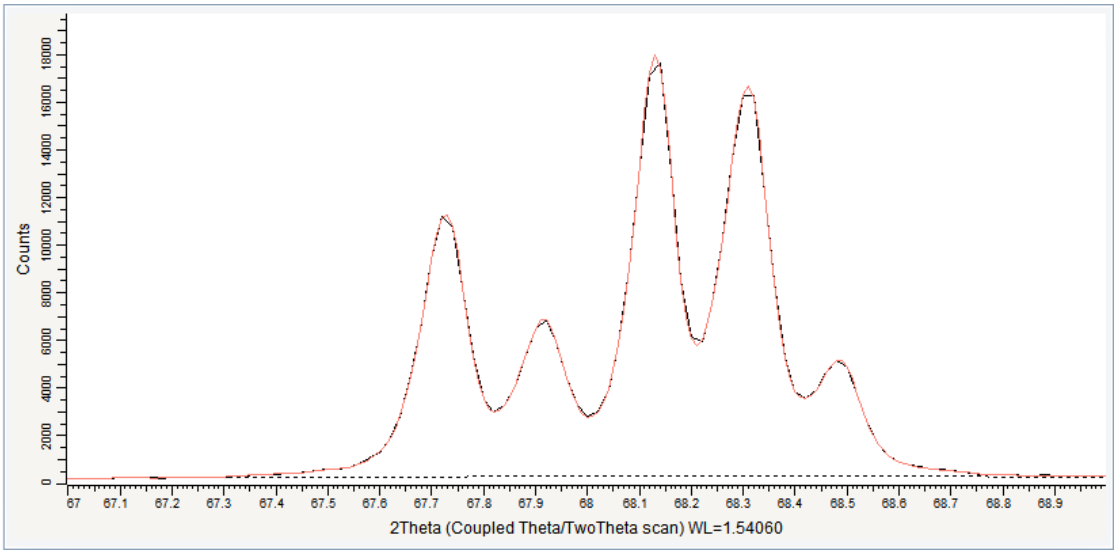


Figure 8.7: Zoom on peaks (2θ=67° to 69°)

5. Then, you can:
   - Click **Append** to append the smoothed scan to the document. The scan is added to the scan list and its properties can be edited in the property table.
   - Click **Replace** to replace the original scan with the smoothed scan.

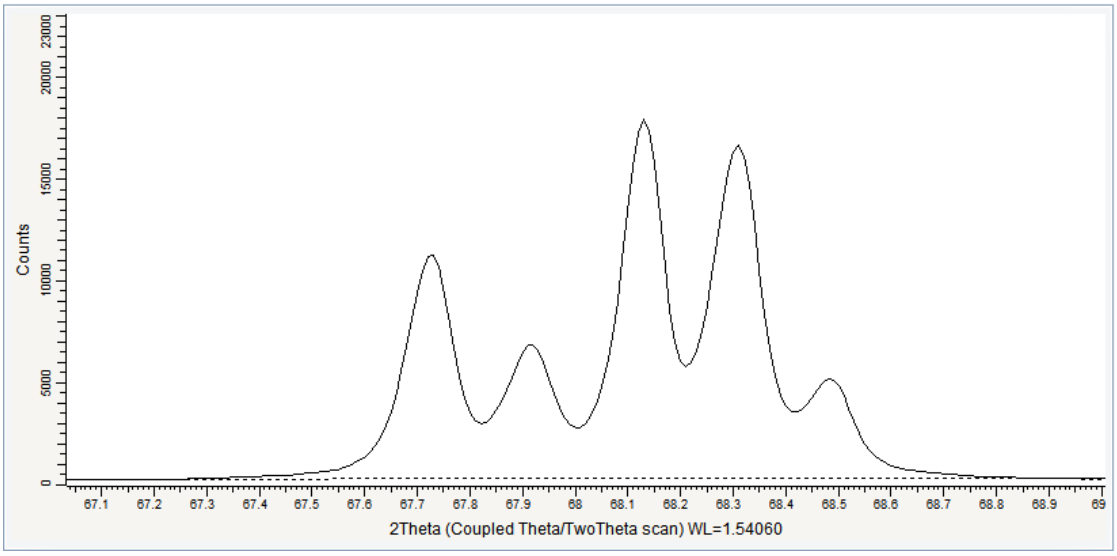


Figure 8.8: Original scan replaced with the smoothed scan - Zoom on peaks (2θ=67° to 69°)

8.3 Step 3: Saving

1. Click **Save As** on the **File** menu.
   ➨ The **Save EVA File As** dialog box will be displayed.
2. Select the appropriate disc drive and directory.
3. Type in the file name. (To overwrite an **.EVA** file, use the same name).
4. Click **Save**.

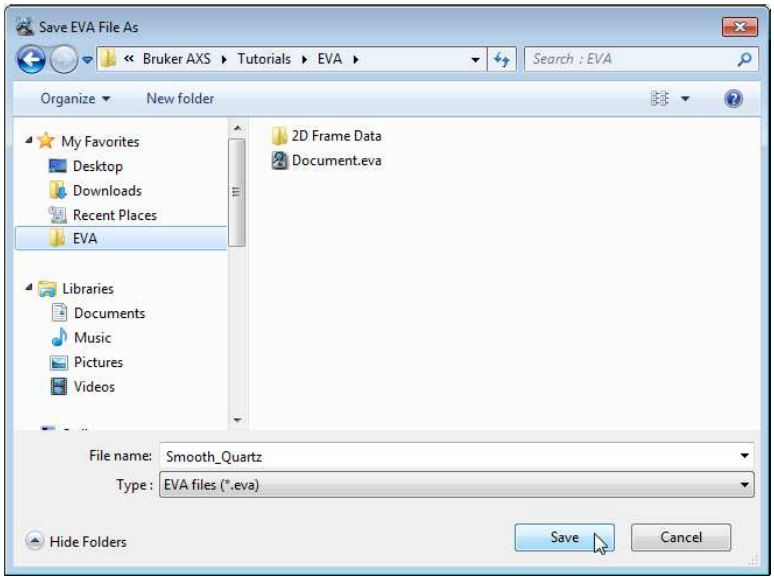


Figure 8.9: Saving the Smooth_Quartz.EVA document

9 Removing Aberrant Points

The following procedure describes the basic procedure for removing aberrant points from a scan.

The scan used is held as a tutorial file, Spikes.RAW, found in the Tutorial directory.

Steps

1. Creating a new EVA document and importing Spikes.RAW.
2. Removing the aberrant points.
3. Saving the EVA document containing the scan.

9.1 Step 1: Creating a New EVA Document and Importing Spikes.RAW

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   ➨ The EVA document is empty.

2. Click the **Import from files** data command or the **Import from files** button.
   ➨ The **Import From Files** dialog box will be displayed.
1. Search the Tutorials/EVA* directory and select the Spikes.RAW file.
2. Click **Open**. The scan Spikes.RAW will be added to the Data tree displayed in the graphical view of the EVA document.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

Figure 9.1: Importing Spikes.raw

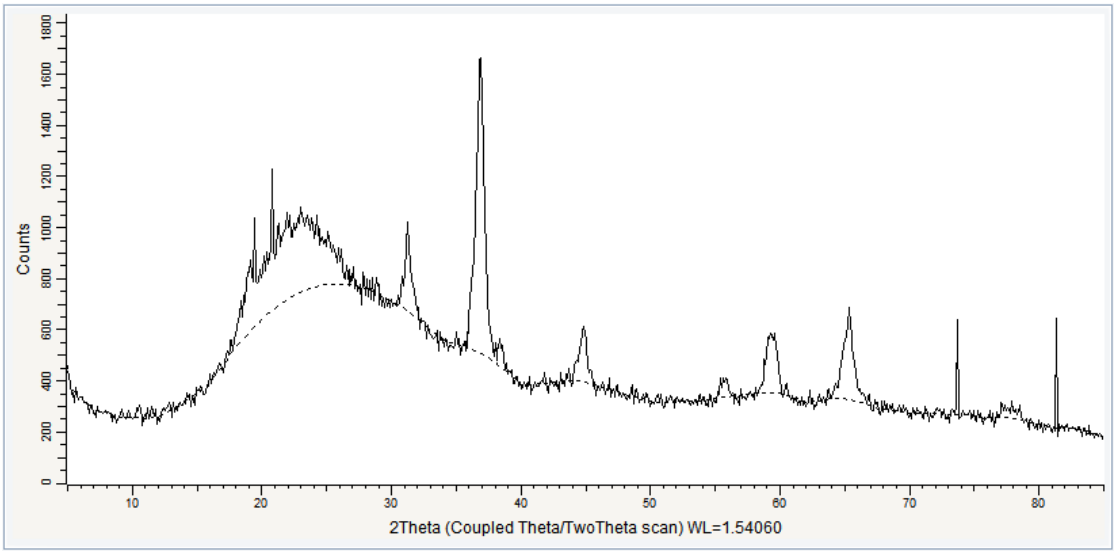


Figure 9.2: Spikes scan imported in the graphical view

9.2 Step 2: Removing Aberrant Points

▷ Make certain the scan is selected; if not, select it either in the data tree or in the 1D view.

1. Right-click the scan, and then click **Tool** on the context menu. Click **Aberrant** on the related submenu: the **Aberrant** dialog box will be displayed.

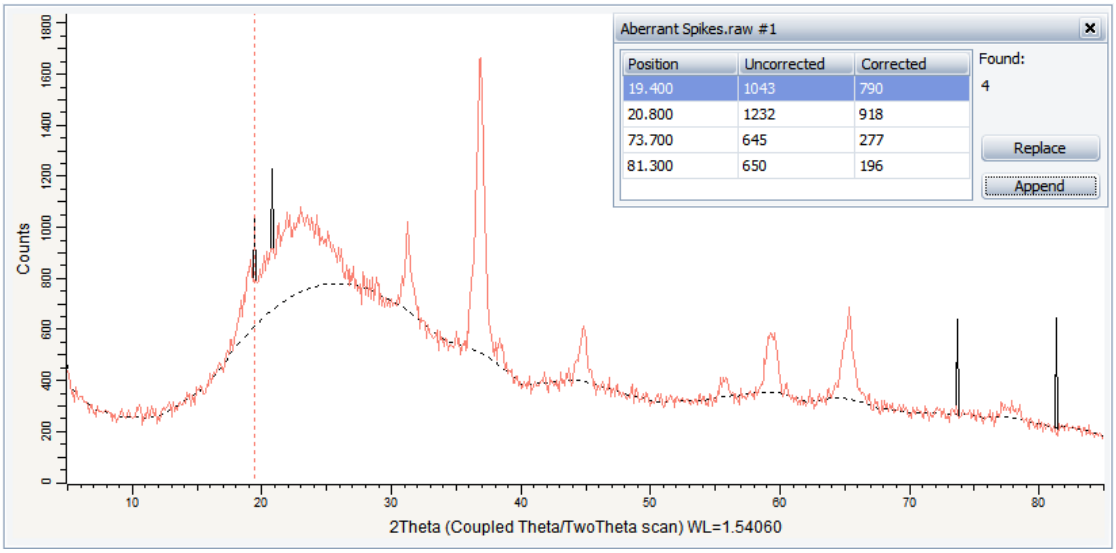


Figure 9.3: Aberrant dialog box and graphical view displaying a ghost line with the aberrant points removed

2. The Aberrant dialog box gives the positions of the aberrant points and the corresponding uncorrected and corrected intensities. A ghost line shows the corrected scan.
3. Then, you can:
   – Click **Append** to append the corrected scan to the document. The scan is added to the scan list and its properties can be edited in the property table.
   – Click **Replace** to replace the original scan with the corrected scan.

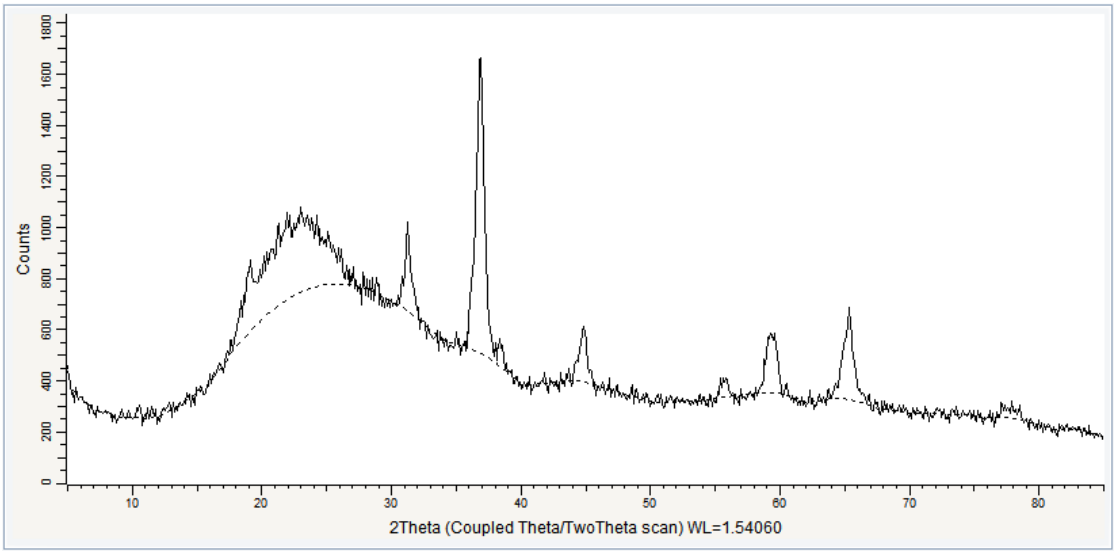


Figure 9.4: Original scan replaced with the corrected scan

9.3 Step 3: Saving

1. Click **Save As** on the **File** menu.
   ➨ The **Save EVA File As** dialog box will be displayed.
2. Select the appropriate disc drive and directory.
3. Type in the file name. (To overwrite an **.EVA** file, use the same name).
4. Click **Save**.

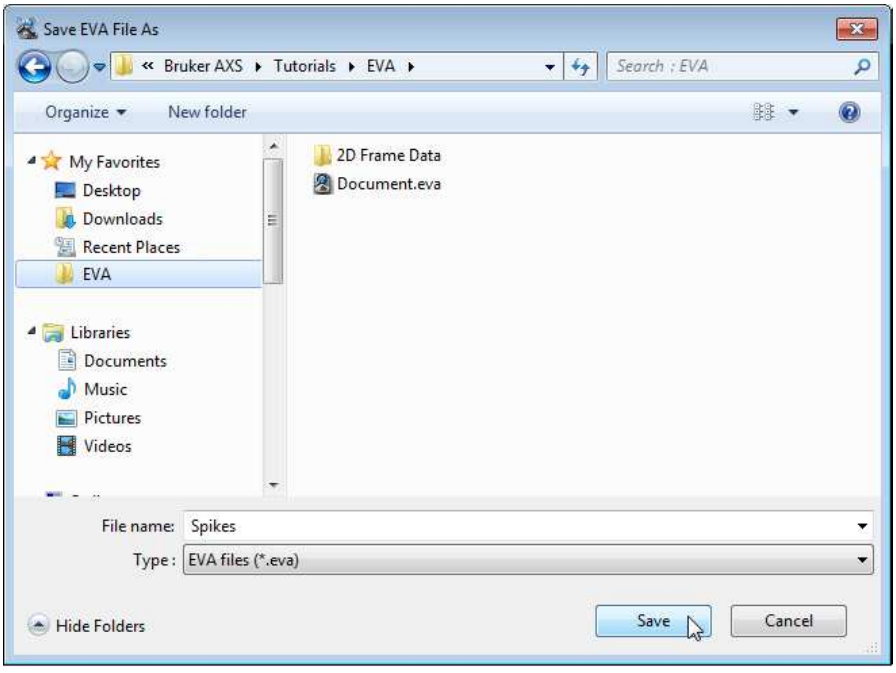


Figure 9.5: Saving the Spikes.EVA document

10 Computing Areas

The following procedure describes the basic procedure for computing an area.

The scan used is held as a tutorial file, ET20.RAW, found in the Tutorial directory. ET20 is a mixture of Corundum and Boehmite.

Steps

1. Creating a new EVA document and importing ET20.RAW.
2. Selecting and computing an area.
3. Saving the EVA document containing the scan.

10.1 Step 1: Creating a New EVA Document and Importing ET20.RAW

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   - ➨ The EVA document is empty.

2. Click the **Import from files** data command or the **Import from files** button.
   - ➨ The **Import From Files** dialog box will be displayed.
3. Search the Tutorials/EVA* directory and select the ET20.RAW file.
4. Click **Open**.
   - ➨ The scan ET20 will be added to the Data tree and displayed in the graphical view of the EVA document.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

Figure 10.1: Importing ET20.raw

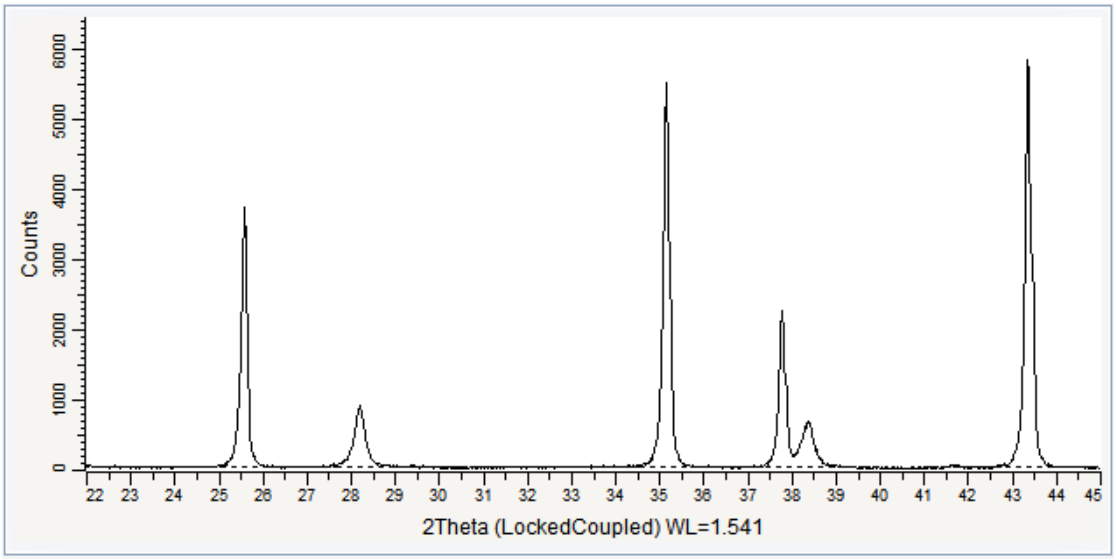


Figure 10.2: ET20.RAW file imported in the graphical view

10.2 Step 2: Selecting and Computing an Area

▷ Make certain the scan is selected; if not, select it either in the data tree or in the 1D view.

1. Click **Create Area** in the Tool list of the Data Command panel,
   — or —
   click the **Create Area** button on the Peak /Area toolbar,
   — or —
   right-click the scan, and then click **Tool** on the context menu. Click **Create Area** on the Tool submenu.

   ➨ The **Create Area** dialog box will be displayed.

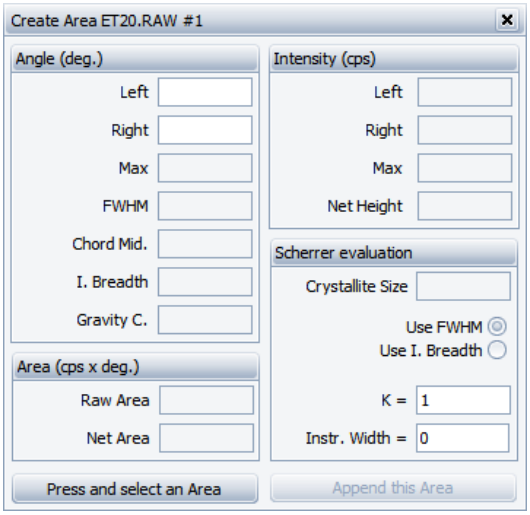


Figure 10.3: Create Area dialog box

2. Click **Press and select an Area** to select an area with the mouse (press and hold the left mouse button with the pointer on one end of the selection, then point to the opposite end and release the button). In the example the first peak (Corundum peak) has been chosen.

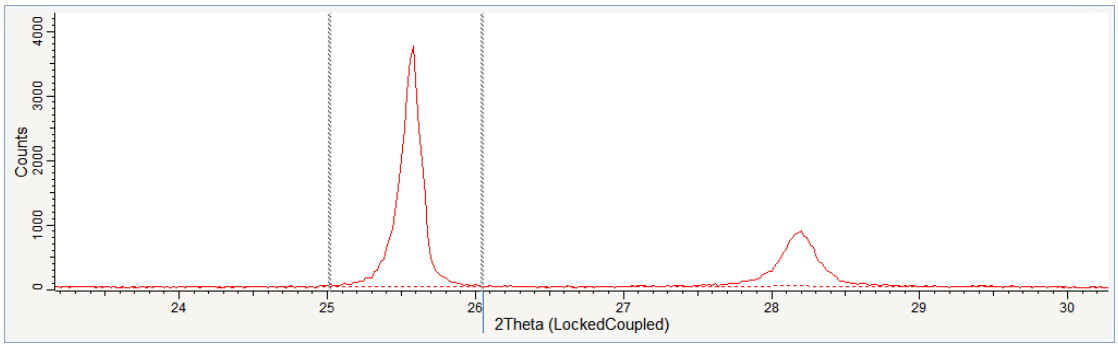


Figure 10.4: Selecting an area

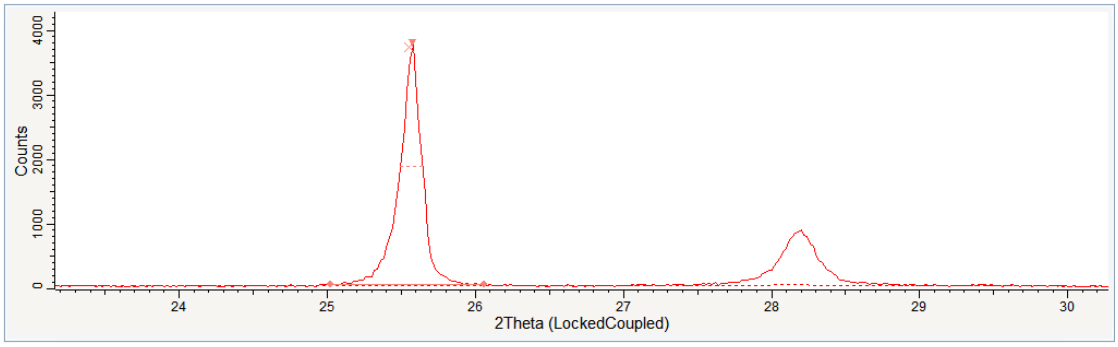


Figure 10.5: Area selected

3. You can modify the area by dragging any filled circle of the area bottom line.
   ➨ The results are displayed in the dialog box.

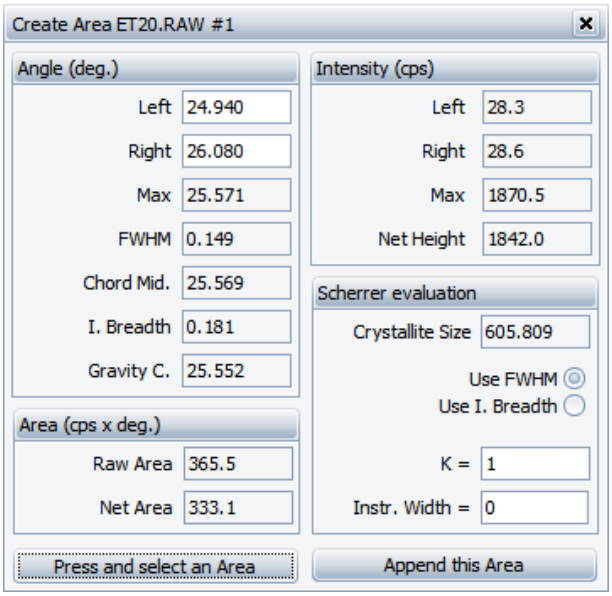


Figure 10.6: Results of the area computation

4. Once the selection is satisfactory, click **Append this Area** to add the area to an Area list in the Data tree.

⇨ The results will be displayed in the Area Property table.

10.3 Step 3: Saving

1. Click **Save As** on the **File** menu.
   ➨ The **Save EVA File As** dialog box will be displayed.
2. Select the appropriate disc drive and directory.
3. Type in the file name. (To overwrite an **.EVA** file, use the same name).
4. Click **Save**.

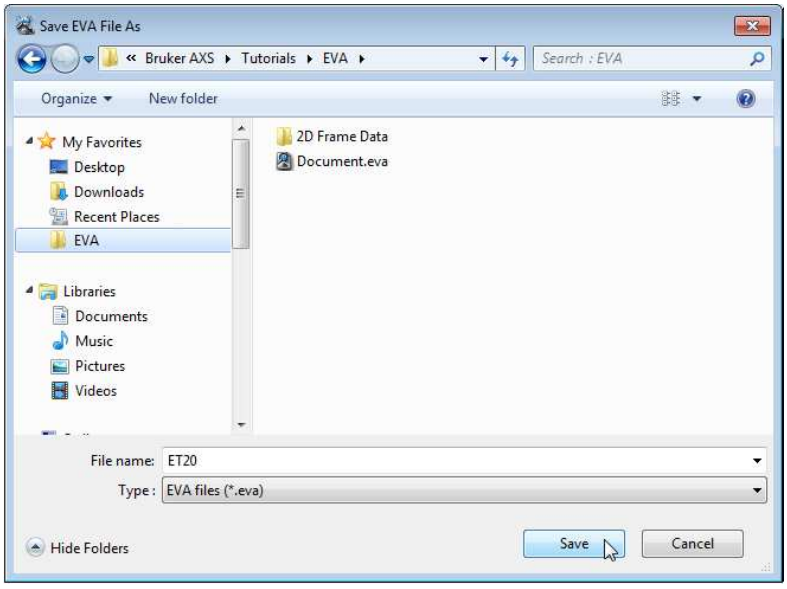


Figure 10.7: Saving ET20.EVA document

11 Adding Scans

The following procedure describes the basic procedure for adding scans.

The scans used are held as tutorial files, ET20.RAW, ET50.RAW, ET80.RAW, found in the Tutorial directory. They are mixtures of Corundum and Boehmite.

Steps

1. Creating a new EVA document and importing ET20.RAW, ET50.RAW and ET80.RAW.
2. Adding the scans.
3. Saving the EVA document containing the scans.

11.1 Step 1: Creating a New EVA Document and Importing ET20.RAW, ET50.RAW and ET80.RAW

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   ➨ The EVA document is empty.

2. Click the **Import from files** data command or the **Import from files** button.
   ➨ The **Import From Files** dialog box will be displayed.
3. Search the Tutorials/EVA* directory and multi-select the ET20.RAW, ET50.RAW and ET80.RAW files.
4. Click **Open**.

⇨ The scan ET20, ET50 and ET80 will be added to the Data tree and displayed in the graphical view of the EVA document.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

Figure 11.1: Importing the 3 scans

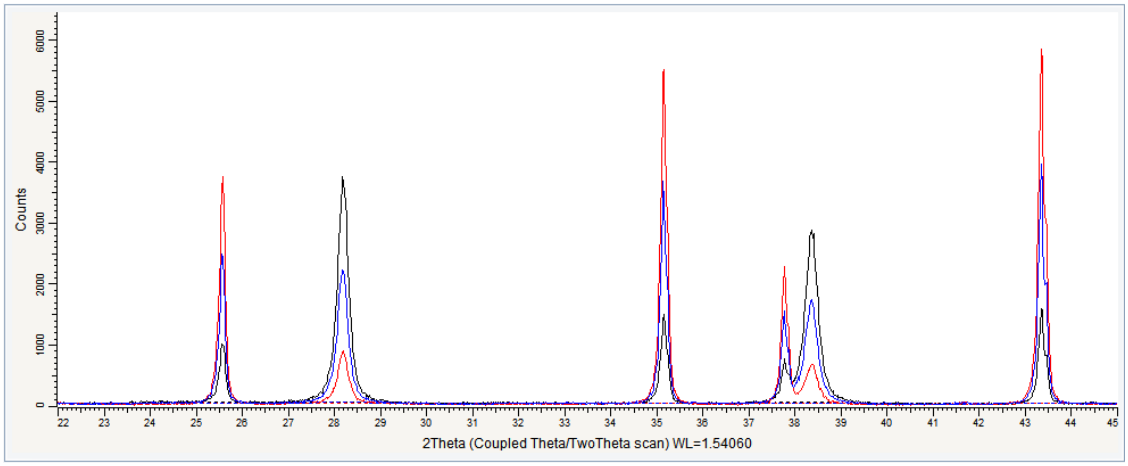


Figure 11.2: ET20.RAW, ET50.RAW and ET80.RAW files imported in the graphical view

11.2 Step 2: Adding the Scans

1. Multi-select the scans in the data tree.
2. Click **Add** in the Tool list of the Data Command panel
   — or —
   click the **Add** button on the Scan toolbar
   — or —
   right-click the multi-selection, and then click **Tool** on the context menu. Click **Add** on the Tool submenu.

   ➨ The resulting scan will be displayed in the graphical view and added to the scan list in the data tree. The resulting scan will inherit the name of the first selected scan.

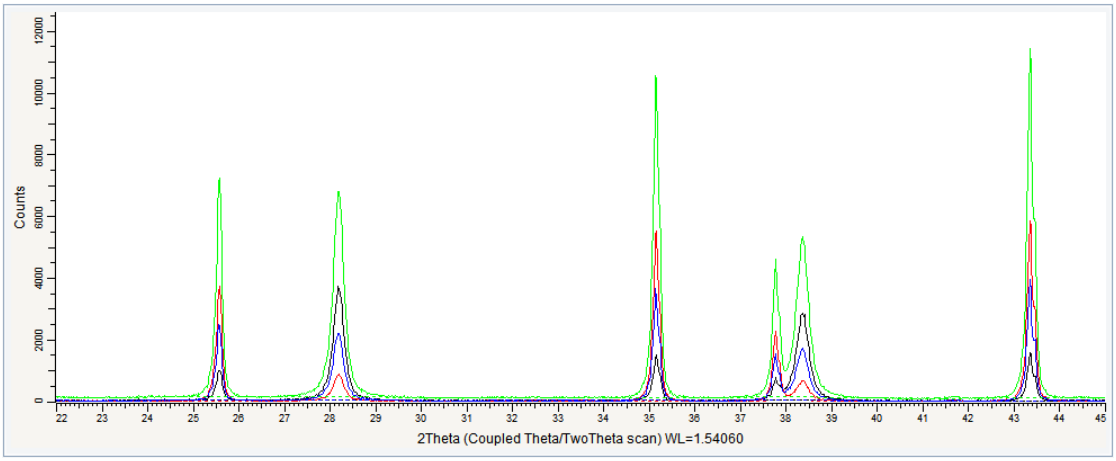


Figure 11.3: Original scans and the scan resulting from the addition

11.3 Step 3: Saving

1. Click **Save As** on the **File** menu.
   ➨ The **Save EVA File As** dialog box will be displayed.
2. Select the appropriate disc drive and directory.
3. Type in the file name. (To overwrite an **.EVA** file, use the same name).
4. Click **Save**.

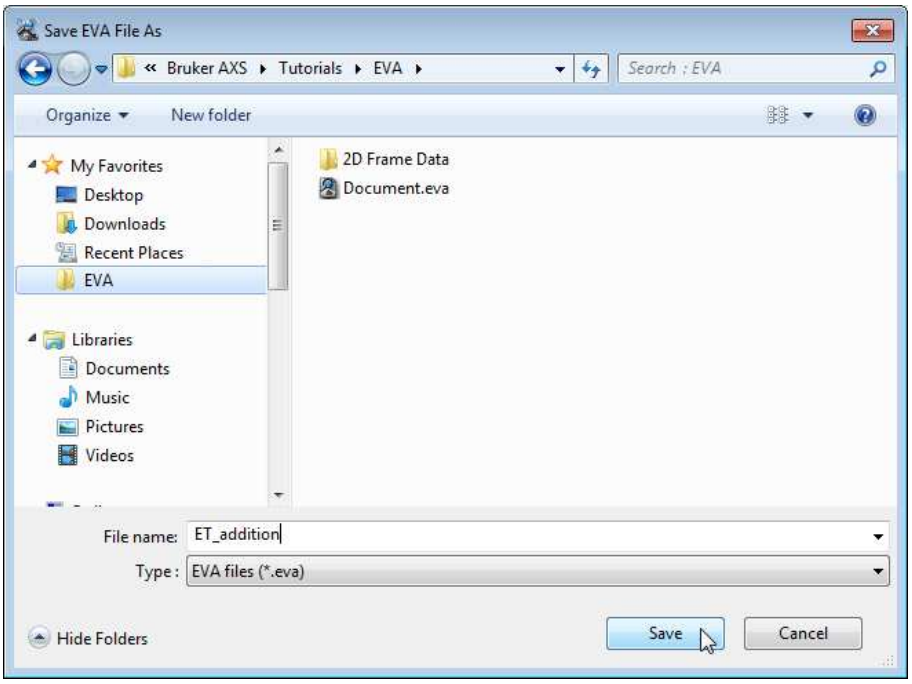


Figure 11.4: Saving ET_addition.EVA document

12 Subtracting Scans

The following procedure describes the basic procedure for subtracting scans. It can be applied on two scans only.

The scans used are held as tutorial files, ET20.RAW and ET50.RAW, found in the Tutorial directory. They are mixtures of Corundum and Boehmite.

Steps

1. Creating a new EVA document and importing ET20.RAW and ET50.RAW.
2. Subtracting the scans.
3. Saving the EVA document containing the scans.

12.1 Step 1: Creating a New EVA Document and Importing ET20.RAW and ET50.RAW

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   - ➨ The EVA document is empty.

2. Click the **Import from files** data command or the **Import from files** button.
   - ➨ The **Import From Files** dialog box will be displayed.
3. Search the Tutorials/EVA* directory and multi-select the files ET20.RAW and ET50.RAW.
4. Click **Open**.
   - ➨ The scans ET20 and ET50 will be added to the Data tree and displayed in the graphical view of the EVA document.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

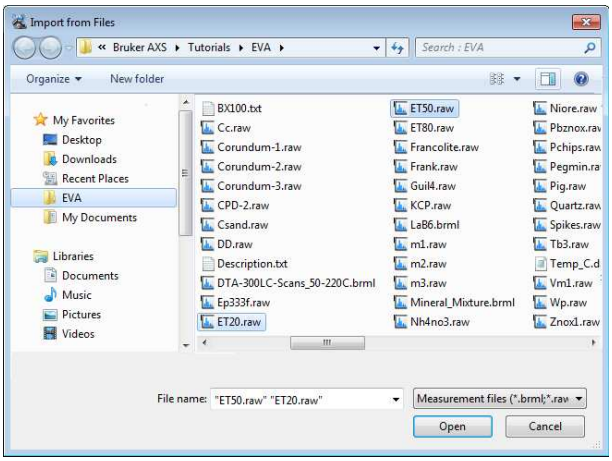


Figure 12.1: Importing ET50.raw and ET20.raw

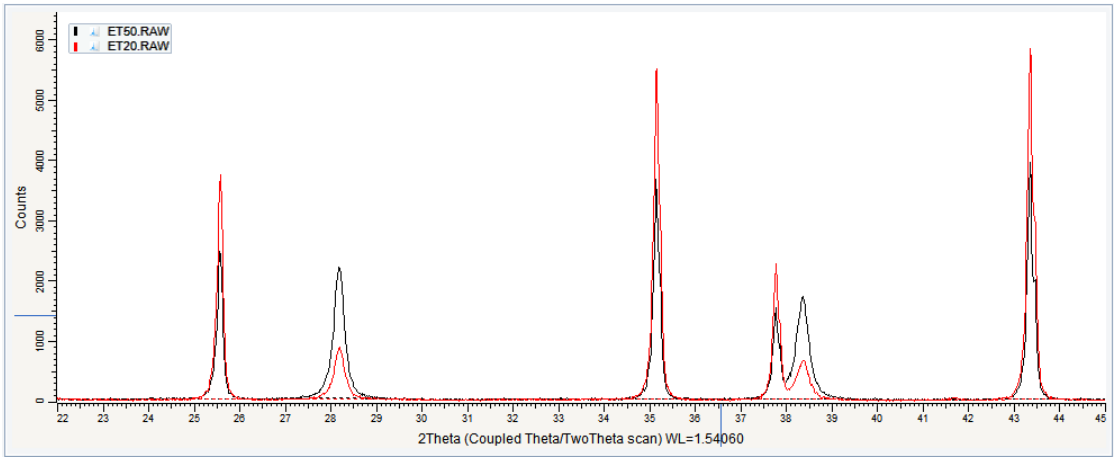


Figure 12.2: ET20.RAW and ET50.RAW files imported in the graphical view

12.2 Step 2: Subtracting the Scans

Case #1: Subtraction result with positive values

1. Multi-select the scans in the data tree (select ET50.RAW first).

2. Click **Subtract** in the Tool list of the Data Command panel
   — or —
   click the **Subtract** button on the Scan toolbar
   — or —
   right-click (the multi-selection), and then click **Tool** on the context menu. Click **Subtract** on the Tool submenu.
   ➨ The resulting scan is displayed in the graphical view and added to the scan list in the data tree. The resulting scan is given the name of the first selected scan.

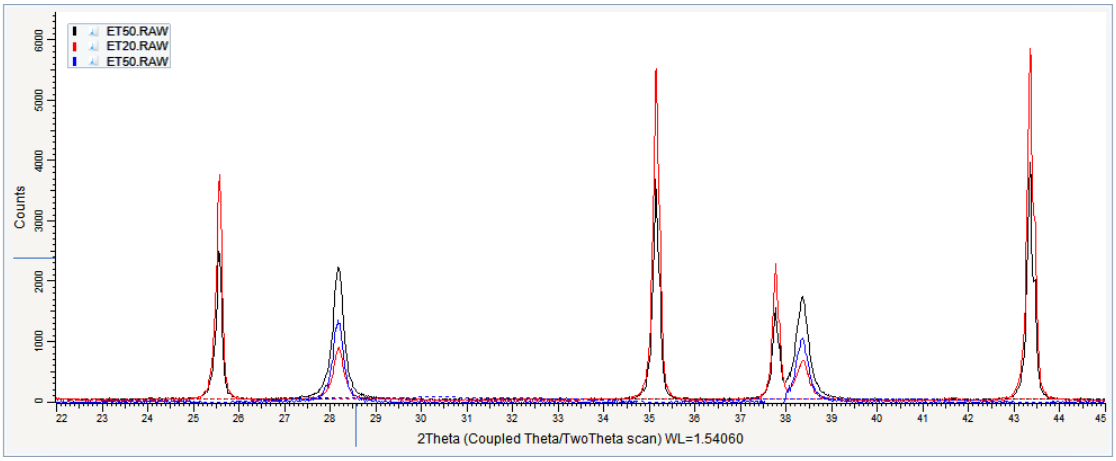


Figure 12.3: Original scans and the scan resulting from the subtraction

Case #2: Subtraction result with negative values

1. Multi-select the scans in the data tree (select ET20.RAW first).

2. Click **Subtract** in the Tool list of the Data Command panel
   — or —
   click the **Subtract** button on the Scan toolbar
   — or —
   right-click (the multi-selection), and then click **Tool** on the context menu. Click **Subtract** on the Tool submenu.

➨ The difference curve is automatically displayed in the extended view and added to the scan list in the data tree. The resulting scan is given the name of the first selected scan and is visible only in the extended view.

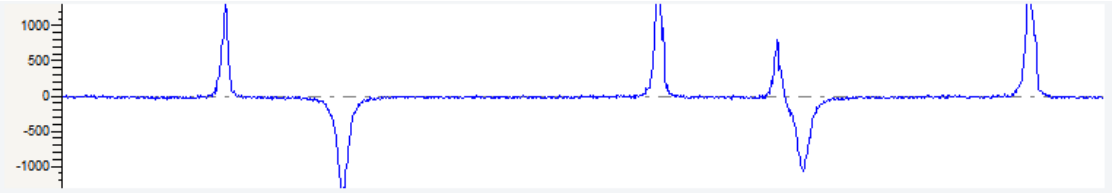


Figure 12.4: Difference curve displayed in the extended view

3. Adjust the extended view scale by clicking on it and dragging up or down to zoom in or out.

12.3 Step 3: Saving

1. Click **Save As** on the **File** menu.
   ➨ The **Save EVA File As** dialog box will be displayed.
2. Select the appropriate disc drive and directory.
3. Type in the file name. (To overwrite an **.EVA** file, use the same name).
4. Click **Save**.

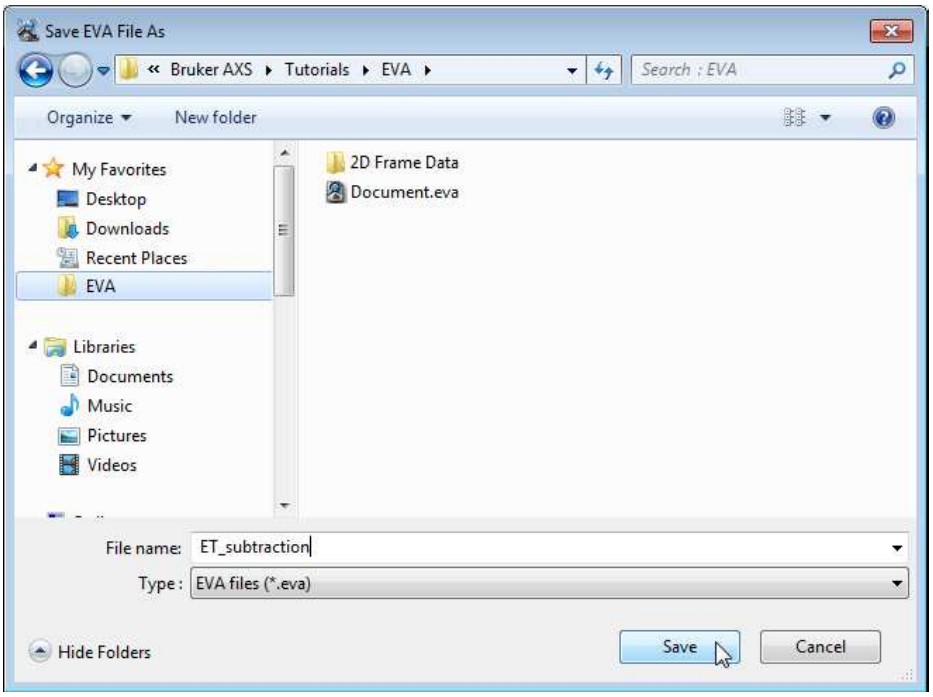


Figure 12.5: Saving ET_subtraction.EVA document

13 Merging Scans

The following procedure describes the basic procedure for subtracting scans. It can be applied on several scans.

The scans used are held as tutorial files, Corundum-1.RAW, Corundum-2.RAW and Corundum-3.RAW, found in the Tutorial directory.

Steps

1. Creating a new EVA document and importing Corundum-1.RAW, Corundum-2.RAW and Corundum-3.RAW.
2. Merging the scans.
3. Saving the EVA document containing the scans.

13.1 Step 1: Creating a New EVA Document and Importing Corundum-1.RAW, Corundum-2.RAW and Corundum-3.RAW

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   - ➨ The EVA document is empty.

2. Click the **Import from files** data command or the **Import from files** button.
   - ➨ The **Import From Files** dialog box will be displayed.
3. Search the Tutorials/EVA1 directory and multi-select the files Corundum-1.RAW, Corundum-2.RAW and Corundum-3.RAW.
4. Click **Open**.

⇨ The scans Corundum-1, Corundum-2 and Corundum-3 will be added to the Data tree and displayed in the graphical view of the EVA document.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

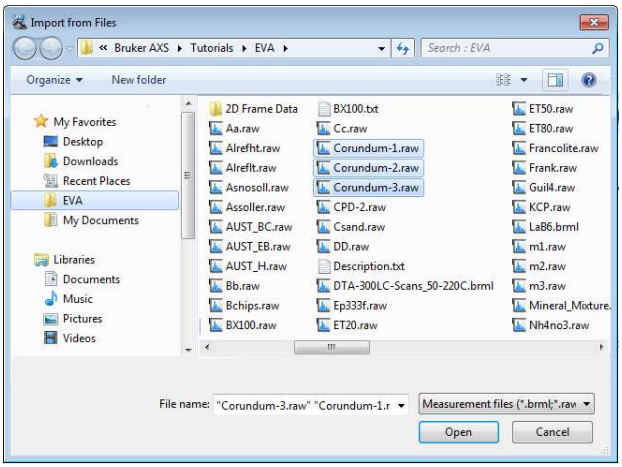


Figure 13.1: Import the 3 scans

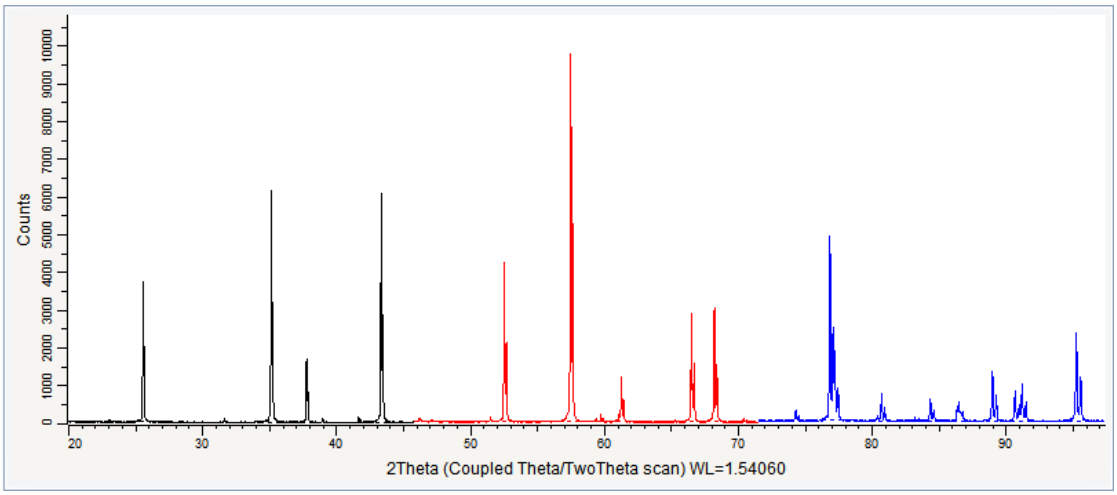


Figure 13.2: Corundum-1.RAW, Corundum-2.RAW and Corundum-3 files imported in the graphical view

13.2 Step 2: Merging the Scans

1. Multi-select the scans from Corundum-1 to Corundum-3 in the data tree; the Corundum-1 is taken as the reference.

2. Click **Merge** in the Tool list of the Data Command panel
   — or —
   click the **Merge** button on the Scan Toolbar
   — or —
   right-click the multi-selection, and then click **Tool** on the context menu. Click **Merge** on the Tool submenu.

   ➨ The resulting scan is displayed in the graphical view and added to the scan list in the data tree. The resulting scan is given the name of the first selected scan.

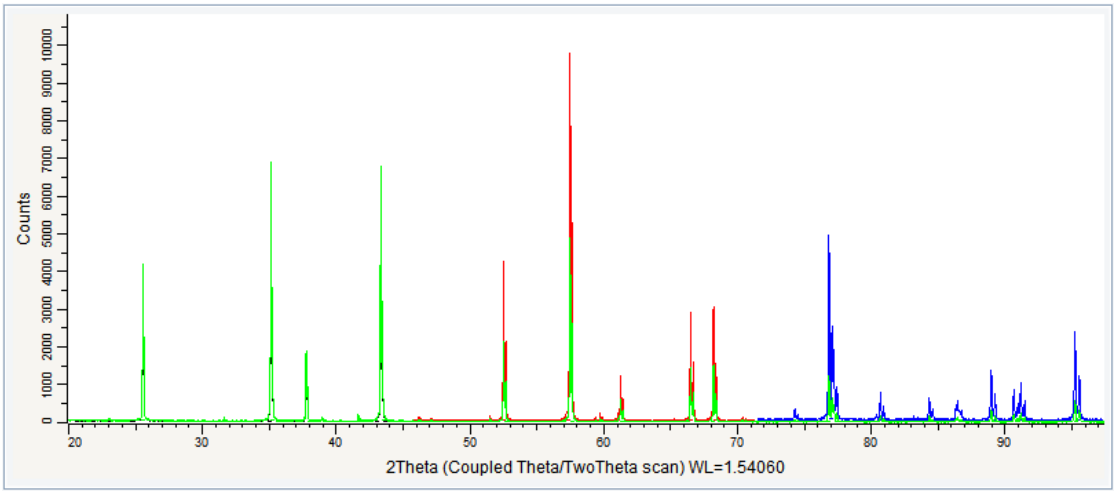


Figure 13.3: Original scans and the scan resulting from the merging

13.3 Step 3: Saving

1. Click **Save As** on the **File** menu.
   ➨ The **Save EVA File As** dialog box will be displayed.
2. Select the appropriate disc drive and directory.
3. Type in the file name. (To overwrite an **.EVA** file, use the same name).
4. Click **Save**.

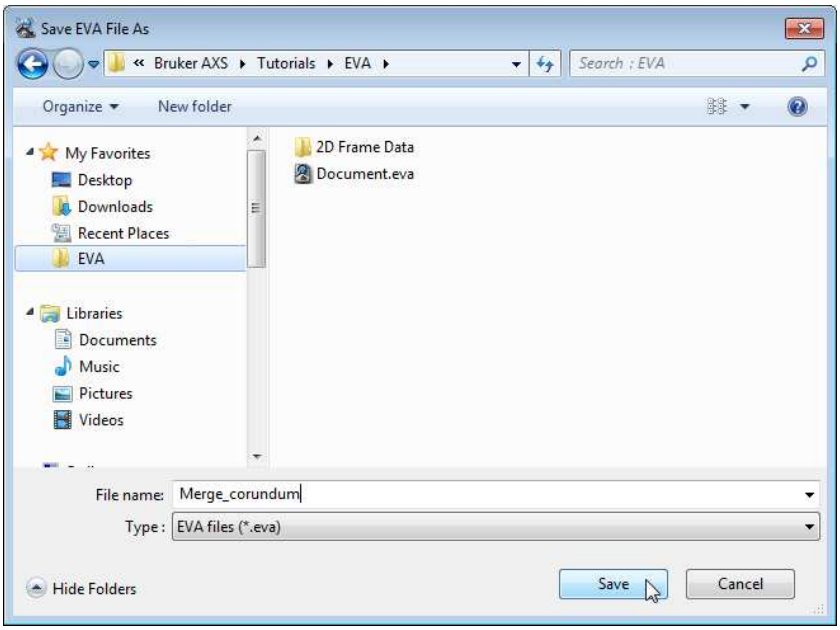


Figure 13.4: Saving Merge_corundum.EVA document

14 Normalizing Scans

The following procedure describes the basic procedure for normalizing scans.

The scans used are held as tutorial files, Znox1.RAW and Znox2.RAW, found in the Tutorial directory. They are zinc minerals.

Steps

1. Creating a new EVA document and importing Znox1.RAW and Znox2.RAW.
2. Normalizing the scans.
3. Saving the EVA document containing the scans.

14.1 Step 1: Creating a New EVA Document and Importing Znox1.RAW and Znox2.RAW

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   - ➨ The EVA document is empty.

2. Click the **Import from files** data command or the **Import from files** button.
   - ➨ The **Import From Files** dialog box will be displayed.
3. Search the Tutorials/EVA* directory and multi-select the Znox1.RAW and Znox2.RAW.
4. Click **Open**.
   - ➨ The scans Znox1.RAW and Znox2.RAW will be added to the Data tree and displayed in the graphical view of the EVA document.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

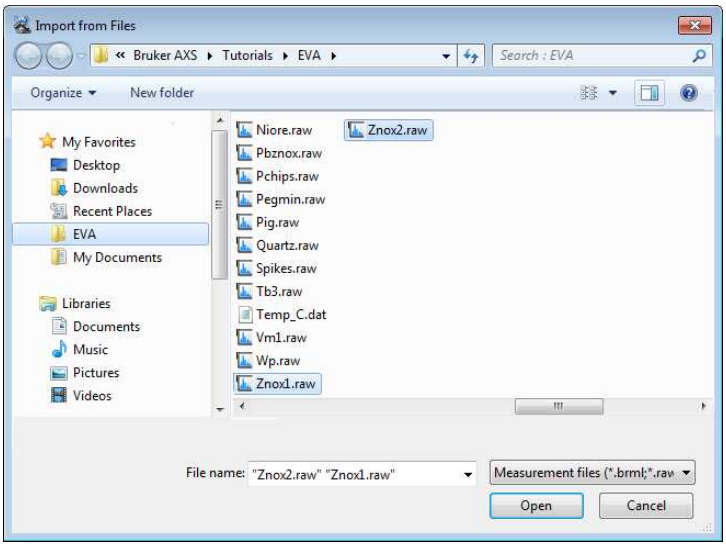


Figure 14.1: Importing the scans

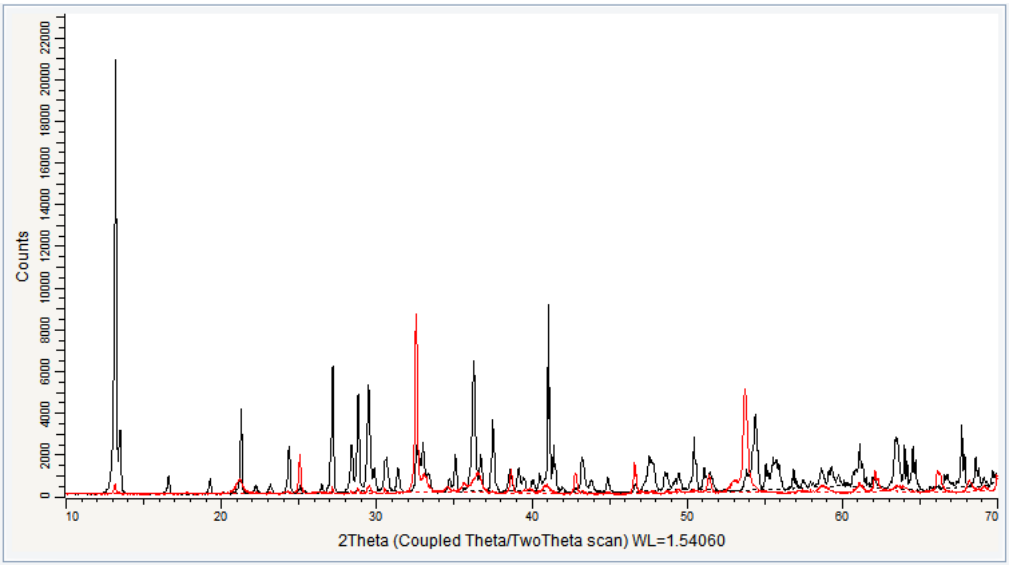


Figure 14.2: Znox1.RAW (in red) and Znox2.RAW (in black) files imported in the graphical view

14.2 Step 2: Normalizing the Scans

There are three different ways of normalizing scans: scans can be normalized to share the same maximum intensity, to share a common point or to share the maximum of a certain scan. All the scans displayed in the graphical view are normalized. Note that normalization is only available in CPS. Therefore if the display is in Counts, you have to switch to CPS to be able to normalize.

To normalize on the Znox2 scan:

1. The Y-scale unit is Counts by default. Select CPS for the Y-scale in the 2 Theta View Property table.
2. Right-click the Znox2 scan.
3. The related context menu is displayed.
4. Point to **Normalize all visible scans** and on the sub-menu, click the **Normalize on scan Znox2.RAW** command.
   - ➨ The scans are normalized on the maximum of the Znox2 scan.

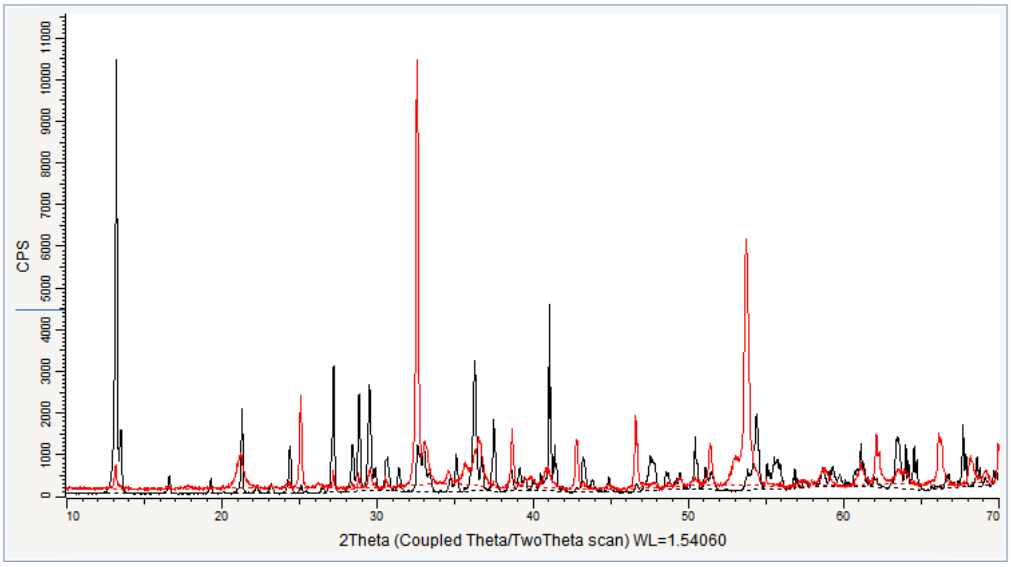


Figure 14.3: Original scans and the scan resulting from normalizing

14.3 Step 3: Saving

1. Click **Save As** on the **File** menu.
   ➨ The **Save EVA File As** dialog box will be displayed.
2. Select the appropriate disc drive and directory.
3. Type in the file name. (To overwrite an **.EVA** file, use the same name).
4. Click **Save**.

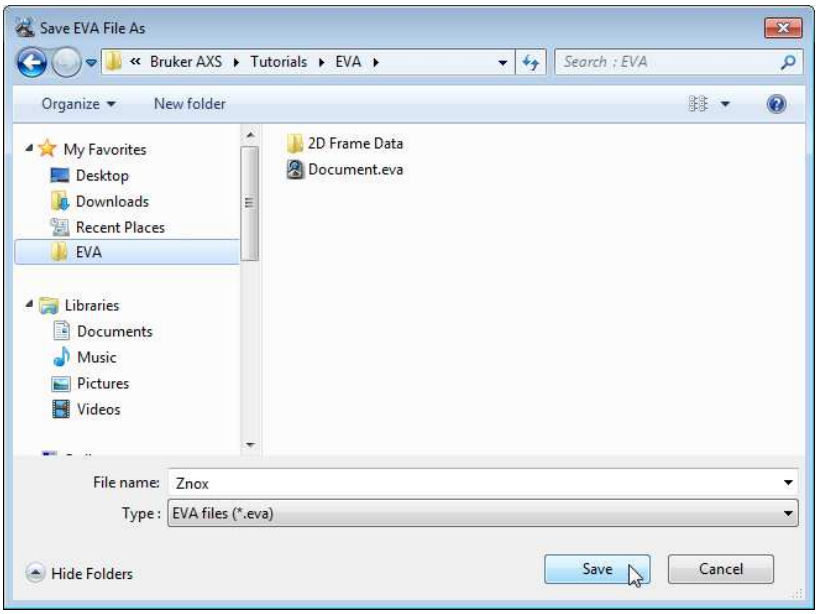


Figure 14.4: Saving Znox.EVA document

15 Computing the Crystallinity

The following procedure describes the basic procedure for computing the crystallinity of a sample.

The scan used is held as a tutorial file, m2.RAW, found in the Tutorial directory.

Steps

1. Creating a new EVA document and importing m2.RAW.
2. Computing the crystallinity.
3. Checking the calculation.
4. Saving the EVA document containing the scans.

15.1 Step 1: Creating a New EVA Document and Importing m2.RAW

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   - ➨ The EVA document is empty.

2. Click the **Import from files** data command or the **Import from files** button.
   - ➨ The **Import From Files** dialog box will be displayed.
3. Search the Tutorials/EVA* directory and select the m2.RAW file.
4. Click **Open**. The scan m2 will be added to the Data tree and displayed in the graphical view of the EVA document.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

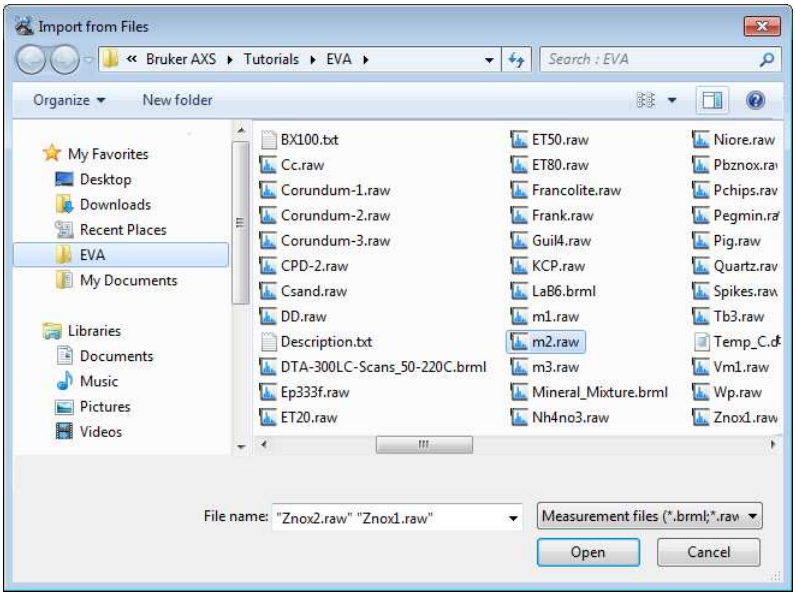


Figure 15.1: Importing m2.raw

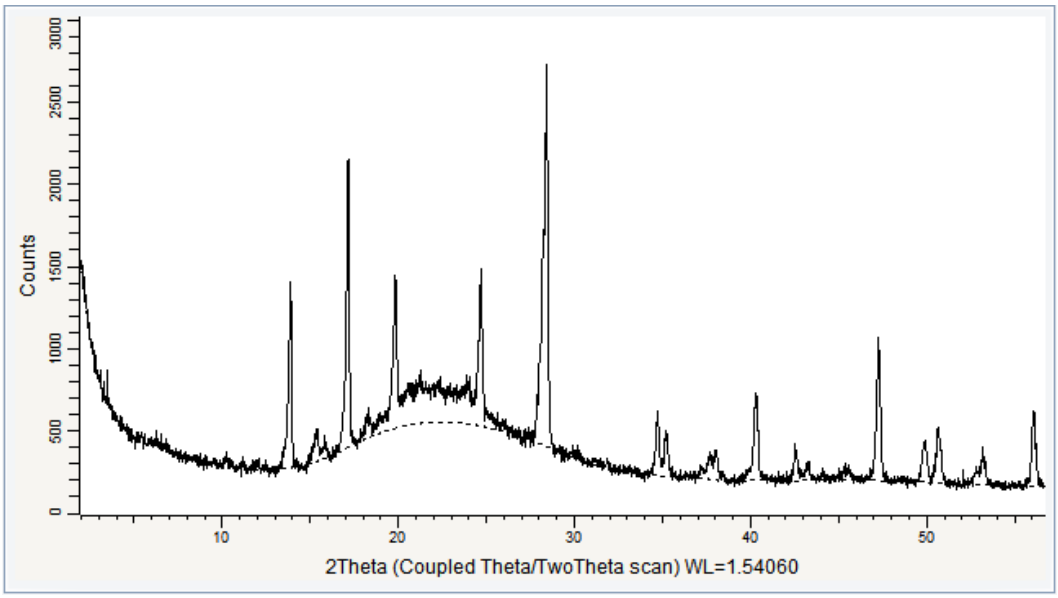


Figure 15.2: m2 file imported in the graphical view

15.2 Step 2: Computing the Crystallinity

▷ Make certain the m2 scan is selected in the data tree.

1. Adjust the background. To do so:

2. Click **Background** in the Tool list of the Data Command panel
   — or —
   click the **Background** button on the Scan toolbar
   — or —
   right-click the scan in the data tree and then click **Tool** on the context menu. Click **Background** on the Tool submenu.
   ➨ The background dialog box will be displayed.
3. Adjust the background curvature as shown below.

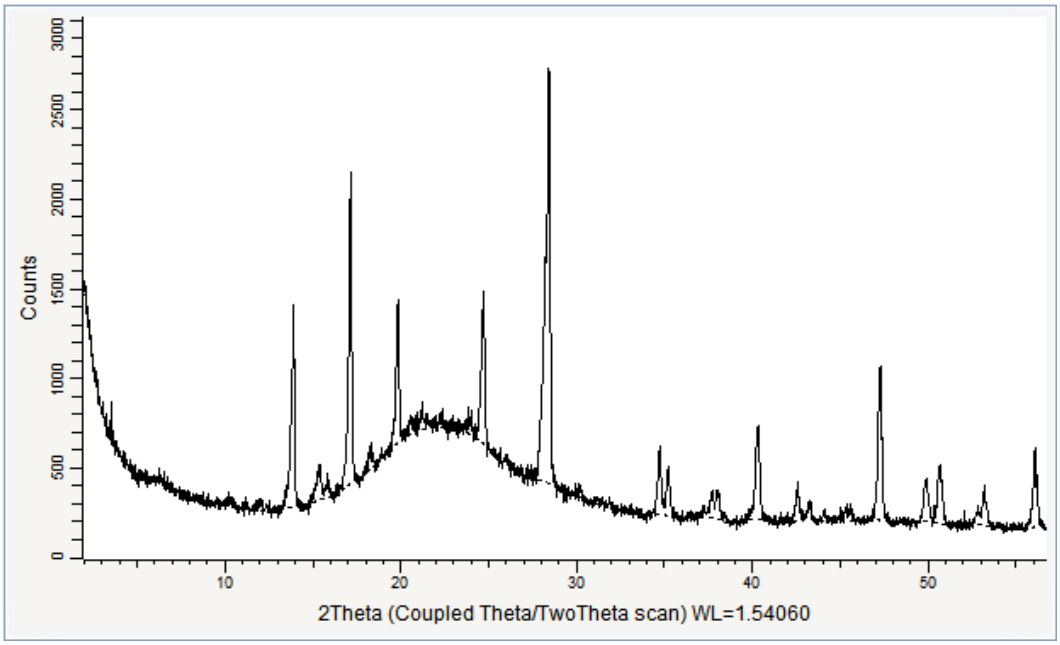
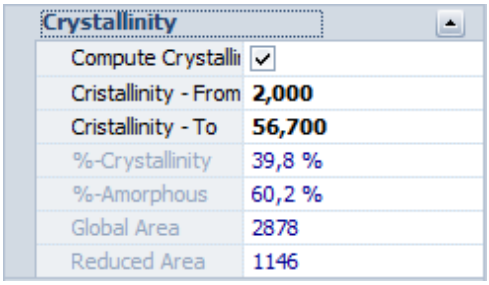


Figure 15.3: Background adjusted

4. Select the **Compute Crystallinity** check box in the Scan Property table

⇨ The crystallinity percentage is automatically computed and given below in the table.



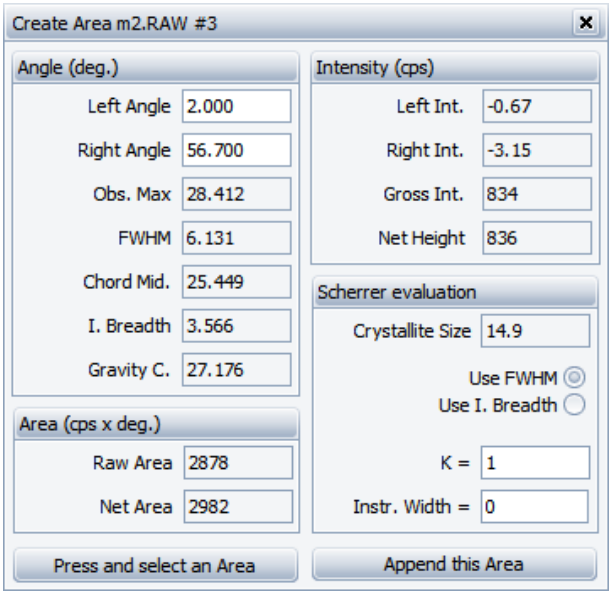
15.3 Step 3: Checking the Results

You can check the results by computing the global area “manually”.

▷ Make certain the m2 scan is selected in the data tree.

1. Click **Background** in the Tool list of the Data Command panel
   — or —
   click the **Background** button on the Scan toolbar
   — or —
   right-click the scan in the data tree and then click **Tool** on the context menu. Click **Background** on the Tool submenu.
2. Set the curvature to the minimum of 0.01.
3. Click the **Append Background** button to create a scan from the background line.
   ➨ This scan will be named m2.RAW #2 by default.
4. Subtract this scan (m2.RAW #2) from the initial m2.RAW scan (m2.RAW #1). See the tutorial chapter *Subtracting Scans [▷ 73]* to know how to operate.
   ➨ It gives you a new scan which is listed in the data tree as m2.RAW #3.
5. Select the scan resulting from the subtraction if it is not already selected. Compute the area on the whole range. To do so:

6. Click **Create Area** in the Tool list of the Data Command panel
   — or —
   click the **Create Area** button on the Peak / Area toolbar
   — or —
   right-click the multi-selection, and then click **Tool** on the context menu. Click **Create Area** on the Tool submenu.
   ➨ The Create Area dialog box will be displayed.
7. Enter the left and right angle values (2 and 56.7) of the scan to compute the corresponding area. The value to look at is the raw area.



8. You can check if this value is equal to the global area value given automatically by the program which is 2878 cps x deg.
9. You can compute the **Reduced area** the same way but using the adjusted background. The raw area value found is equal to the reduced area value which is 1125 cps x deg.
10. From this you can finally compute the crystallinity using the following formulas:

$$\%Amorphous = \frac{\text{Global area - Reduced area}}{\text{Global area}} \times 100$$

$$\%Crystallinity = 100 - \%Amorphous$$

15.4 Step 4: Saving

1. Click **Save As** on the **File** menu.
   ➨ The **Save EVA File As** dialog box will be displayed.
2. Select the appropriate disc drive and directory.
3. Type in the file name. (To overwrite an **.EVA** file, use the same name).
4. Click **Save**.

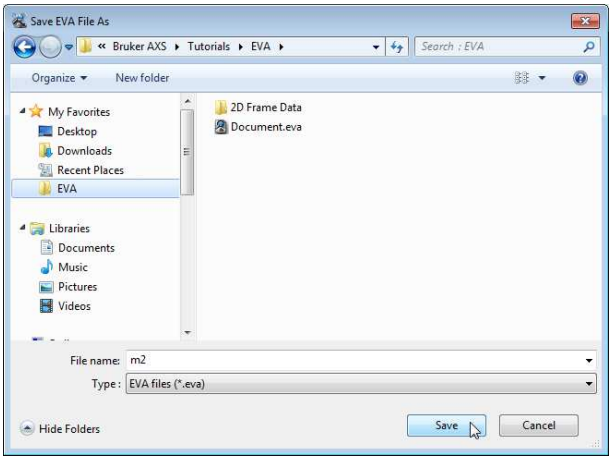


Figure 15.4: Saving m2.EVA document

16 Simulating a Slit Mode

A reference database is required to perform a **Search/Match** operation.

This tutorial was prepared using **PDF 4+ 2016** as a reference database. You may have another reference database.

If you have no database, you cannot perform this part of the tutorial concerning the **Search/Match**.

The following chapter describes the basic procedure for simulating a slit mode.

The scan used is held as a tutorial file, LaB6.BRML, found in the Tutorial directory.

LaB6 was measured using variable slits.

Steps

1. Creating a new EVA document and importing LaB6.BRML.
2. Performing the Search/Match operation.
3. Simulating a slit mode.
4. Saving the EVA document containing the scans.

16.1 Step 1: Creating a New EVA Document and Importing LaB6.BRML

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   - ➨ The EVA document is empty.
2. Click the **Import from files** data command or the **Import from files** button.
   - ➨ The **Import From Files** dialog box will be displayed.
3. Search the Tutorials/EVA* directory and select the LaB6.BRML file.
4. Click **Open**.
   - ➨ The scan LaB6 will be added to the Data tree and displayed in the graphical view of the EVA document.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

Figure 16.1: Importing LaB6.brml

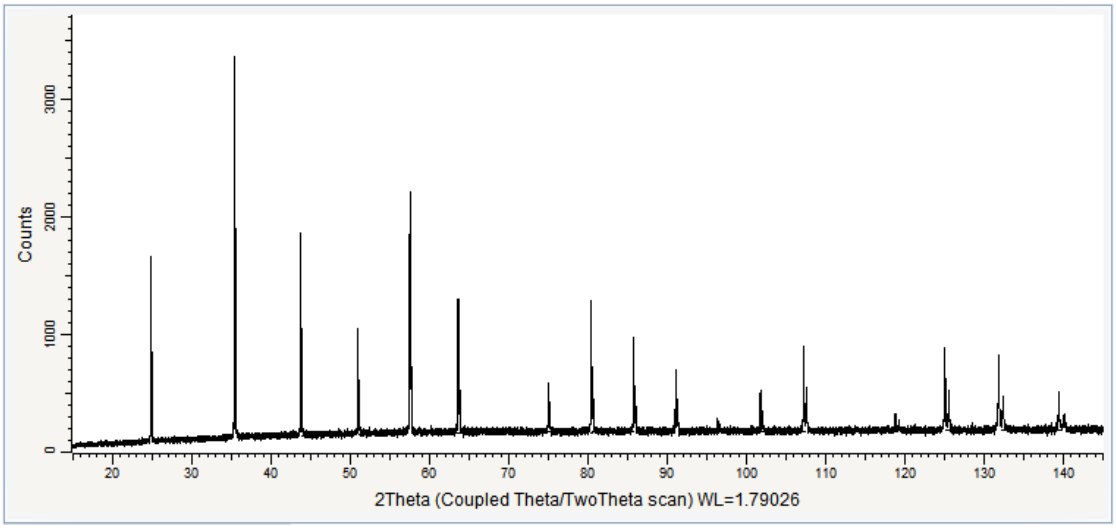
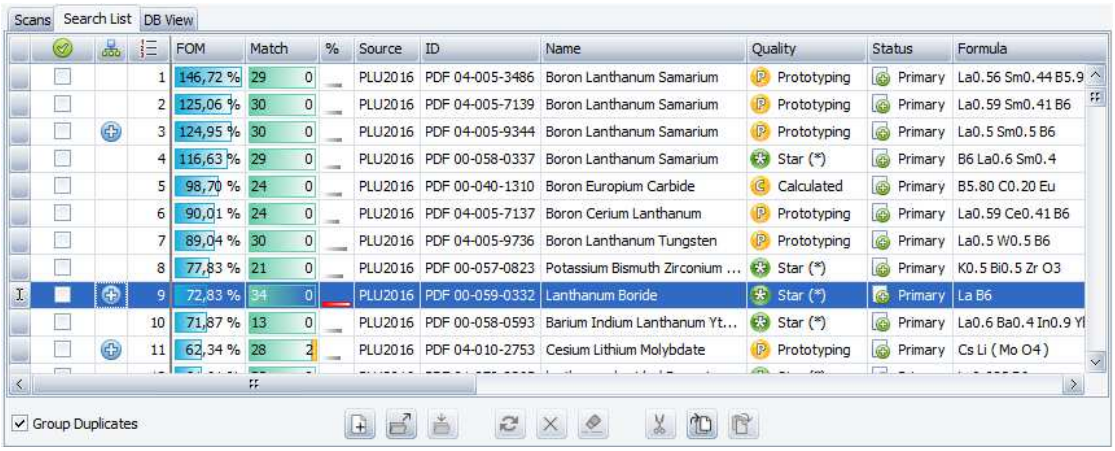


Figure 16.2: LaB6 file imported in the graphical view

16.2 Step 2: Performing the Search/Match Operation

▷ Make certain the LaB6 scan is selected in the data tree.

1. Keep the default search parameters and run a search.
   ➨ Here are the results obtained:



2. Lanthanum Boride (PDF 00-059-0332) can easily be identified.
3. Mark this pattern by selecting the corresponding check box. The pattern is displayed in the graphical view and added to the data tree.
4. Adjust the Y-scale on the strongest peak: press the **Ctrl key** and point to the pattern stick corresponding to the strongest peak. Adjust it to the peak height.

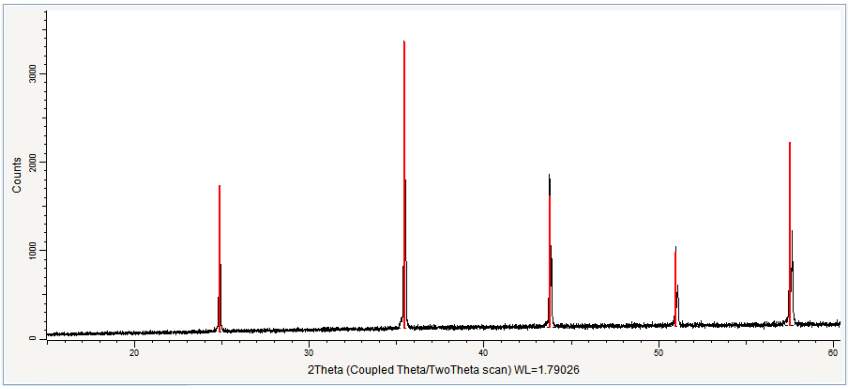


Figure 16.3: Zoom on the scan and the pattern (2θ=20° to 60°)

16.3 Step 3: Simulating a Slit Mode

▷ Make certain the LaB6 scan is selected in the data tree.

▶ In the Scan Property Table, change the **Simul. Slit Mode** property from **Variable** to **Fixed**.

➨ The intensities of the scan will be recalculated. The other scan related data, a pattern in this example, will be projected as well.

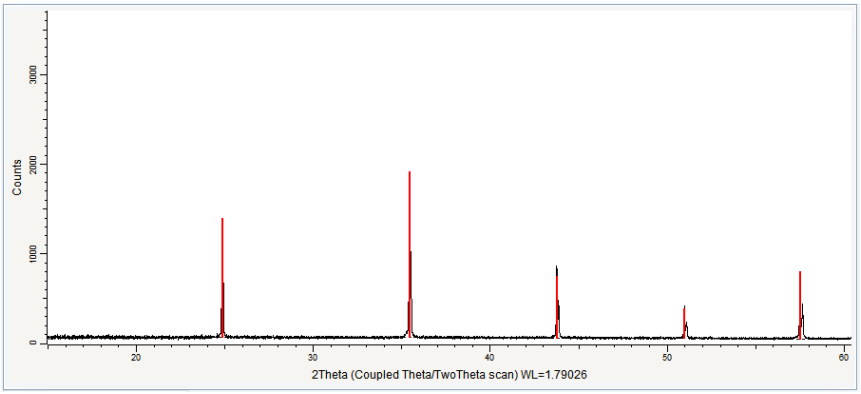


Figure 16.4: Zoom on the scan and the pattern (2θ=20° to 60°)

16.4 Step 4: Saving

1. Click **Save As** on the **File** menu.
   ➨ The **Save EVA File As** dialog box will be displayed.
2. Select the appropriate disc drive and directory.
3. Type in the file name. (To overwrite an **.EVA** file, use the same name).
4. Click **Save**.

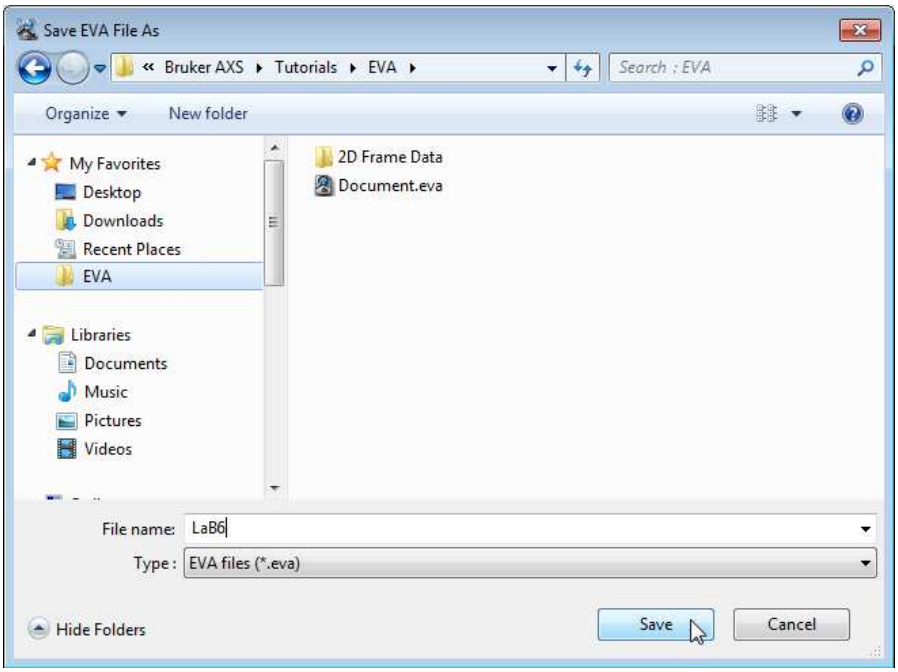


Figure 16.5: Saving LaB6.EVA document

17 Performing the Semi-Quantitative Phase-Analysis and Comparing with a Chemical Analysis

A reference database is required to perform a **Search/Match** operation.

This tutorial was prepared using **PDF 4+ 2016** as a reference database. You may have another reference database.

If you have no database, you cannot perform this part of the tutorial concerning the **Search/Match**.

The following procedure describes the semi-quantitative phase-analysis on a scan and the comparison of the results with the results of a chemical analysis.

The document used is held as a tutorial file, BX100.RAW, found in the Tutorial directory.

Steps

1. Creating a new EVA document and importing BX100.RAW.
2. Performing the Search/Match operation.
3. Exploiting the semi-quantitative phase-analysis.
4. Comparing the Results with the Results of a Chemical Analysis
5. Saving.

17.1 Step 1: Creating a New EVA Document and Importing BX100.RAW

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   - ➨ The EVA document is empty.

2. Click the **Import from files** data command or the **Import from files** button.
   - ➨ The **Import From Files** dialog box will be displayed.
3. Search the Tutorials/EVA* directory and select the BX100.RAW file.
4. Click **Open**.
   - ➨ The scan BX100 will be added to the Data tree and displayed in the graphical view of the EVA document.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

Figure 17.1: Importing BX100.raw

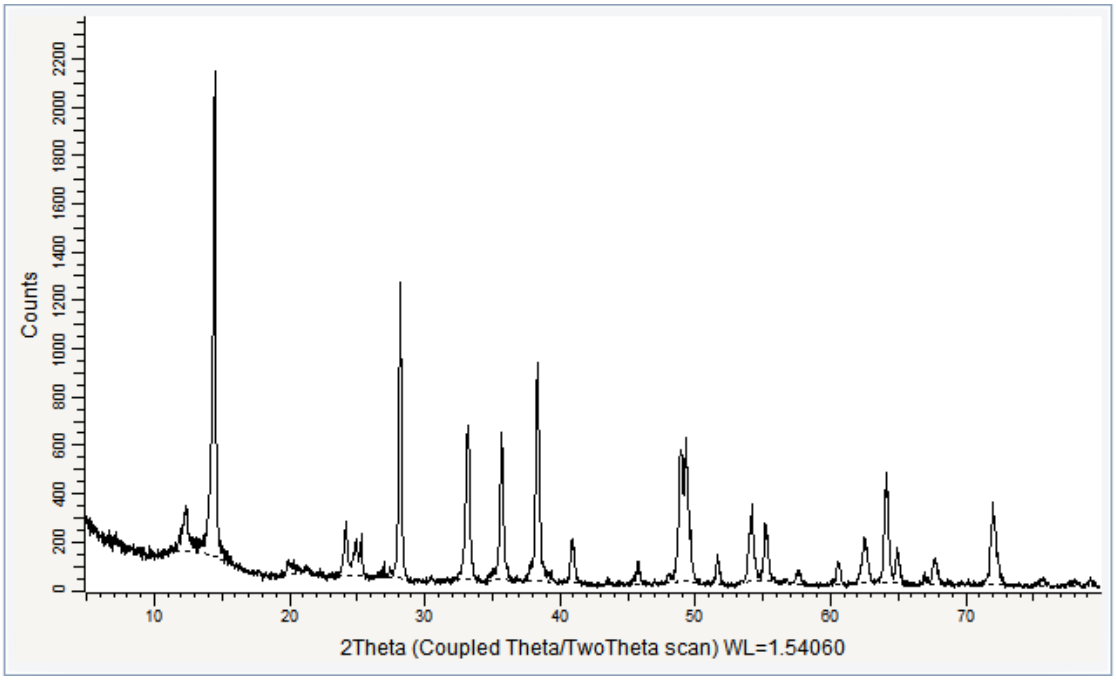


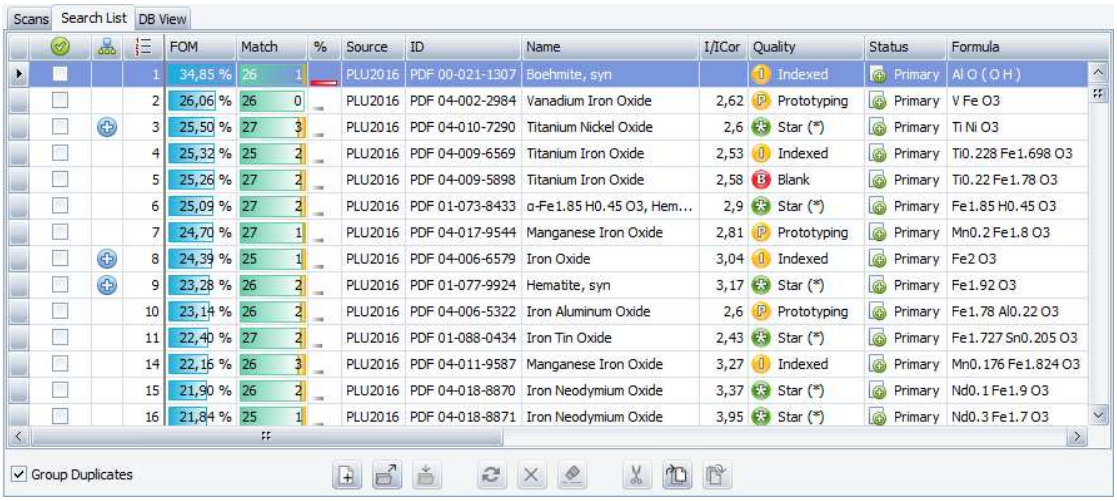
Figure 17.2: BX100.RAW imported in the graphical view

17.2 Step 2: Performing the Search/Match Operation

Before the semi-quantitative phase analysis, all phases must be identified. We will choose patterns with I/Icor values and which belong to a structure database as their I/Icor values are more reliable.

Here, we will describe briefly the search/match operation. For more details about how to proceed see the tutorial chapter *Performing a Search/Match Operation [▶ 3]* or the EVA Manual.

1. Keep the default search parameters and run a first search.
   ➨ Here are the results obtained:



2. Boehmite and Iron Oxide can be easily identified. Nevertheless, the first Boehmite candidate has no I/Icor value. We select another candidate, the Boehmite pattern PDF 01-074-6248. Moreover, the search results show several types of iron oxide, we select pure iron oxide and mark the pattern PDF 04-006-6579.

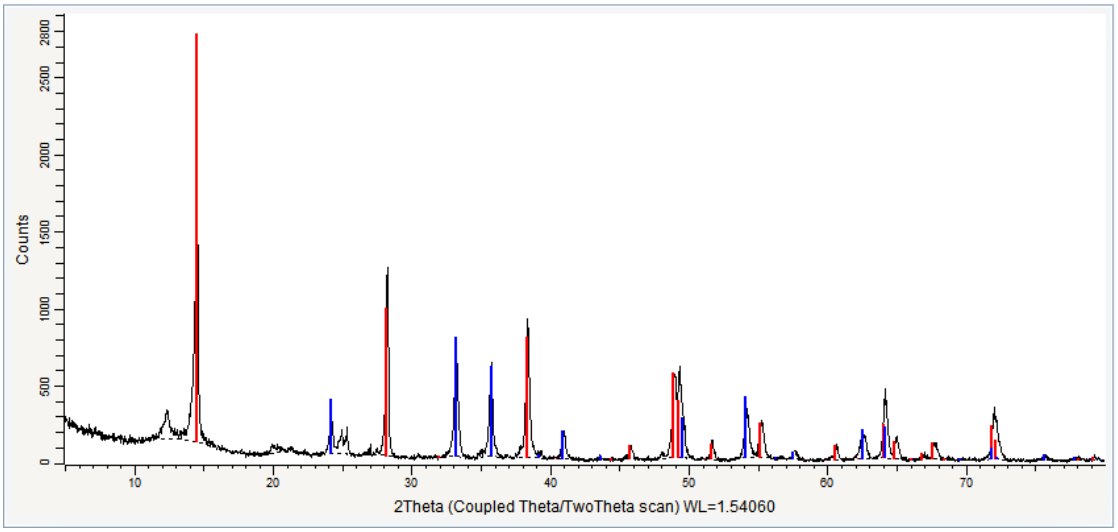
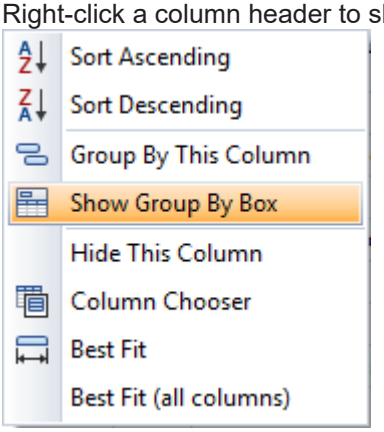


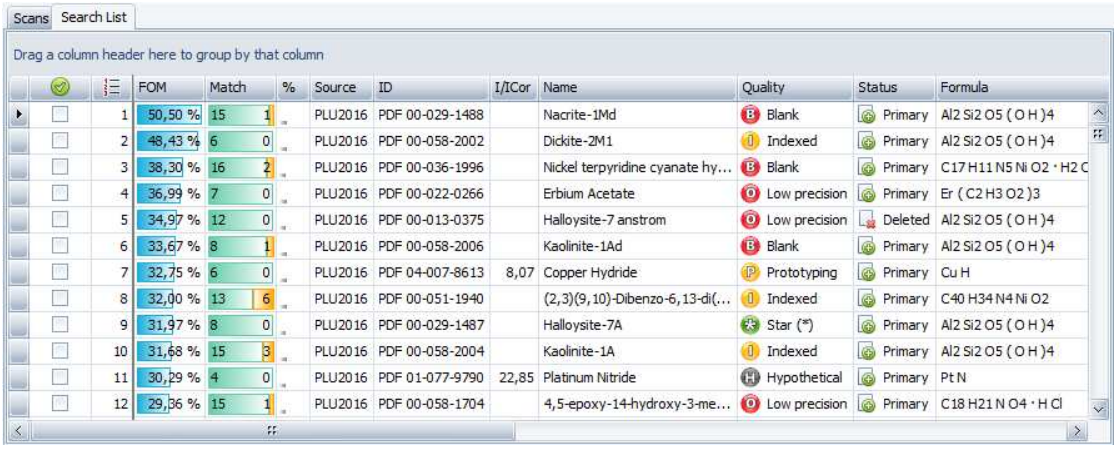
Figure 17.3: Boehmite pattern in red and Iron Oxide pattern in blue

3. Remove the already explained regions by preparing a residual scan using the **Auto Residue**. See *Performing a Search/Match Operation [▶ 3]* | *Step 4: Preparing the Residual Scan [▶ 7]* to know to do.
4. Another run on the residual scan makes it possible to identify Kaolinite-1A. In the first candidates, no pattern has an I/Icor value. We will group candidates by columns to find one.

5. Right-click a column header to show the related contextual menu.

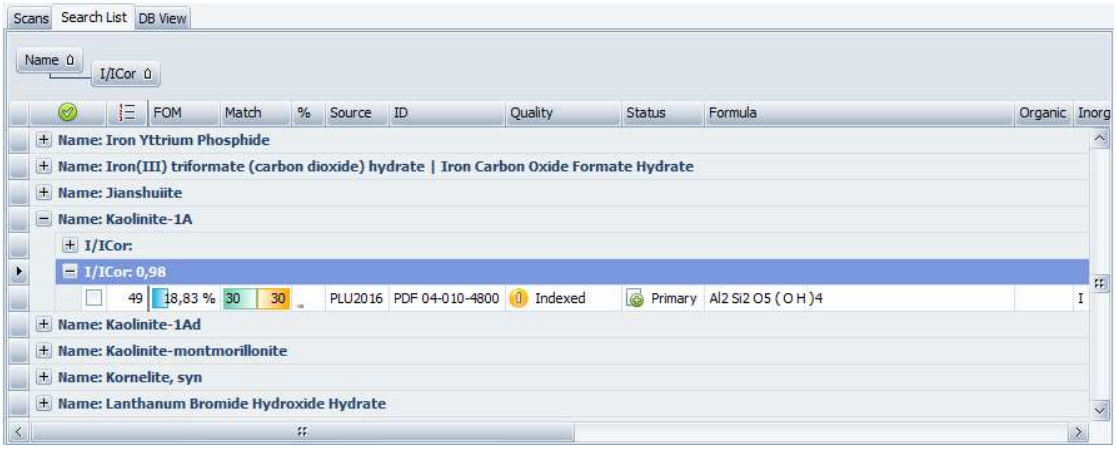


6. Click the **Show Group By Box** command to display the grouping area above the table.



		FOM	Match	%	Source	ID	I/ICor	Name	Quality	Status	Formula
	1	50,50 %	15	1	PLU2016	PDF 00-029-1488		Nacrite-1Md	Blank	Primary	Al2 Si2 O5 (O H)4
	2	48,43 %	6	0	PLU2016	PDF 00-058-2002		Dickite-2M1	Indexed	Primary	Al2 Si2 O5 (O H)4
	3	38,30 %	16	2	PLU2016	PDF 00-036-1996		Nickel terpyridine cyanate hy...	Blank	Primary	C17 H11 N5 Ni O2 · H2 C
	4	36,99 %	7	0	PLU2016	PDF 00-022-0266		Erbium Acetate	Low precision	Primary	Er (C2 H3 O2)3
	5	34,97 %	12	0	PLU2016	PDF 00-013-0375		Halloysite-7 anstrom	Low precision	Deleted	Al2 Si2 O5 (O H)4
	6	33,67 %	8	1	PLU2016	PDF 00-058-2006		Kaolinite-1Ad	Blank	Primary	Al2 Si2 O5 (O H)4
	7	32,75 %	6	0	PLU2016	PDF 04-007-8613	8,07	Copper Hydride	Prototyping	Primary	Cu H
	8	32,00 %	13	6	PLU2016	PDF 00-051-1940		(2,3)(9,10)-Dibenzo-6,13-di(...	Indexed	Primary	C40 H34 N4 Ni O2
	9	31,97 %	8	0	PLU2016	PDF 00-029-1487		Halloysite-7A	Star (*)	Primary	Al2 Si2 O5 (O H)4
	10	31,68 %	15	3	PLU2016	PDF 00-058-2004		Kaolinite-1A	Indexed	Primary	Al2 Si2 O5 (O H)4
	11	30,29 %	4	0	PLU2016	PDF 01-077-9790	22,85	Platinum Nitride	Hypothetical	Primary	Pt N
	12	29,36 %	15	1	PLU2016	PDF 00-058-1704		4,5-epoxy-14-hydroxy-3-me...	Low precision	Primary	C18 H21 N O4 · H Cl

7. Drag first the **Name** column header and then the **I/ICor** column to the grouping area.
   - Candidates will be grouped first by Name and then by I/ICor value.



8. Look for Kaolinite patterns with an I/ICor value. Thre is one: pattern PDF 01-010-4800. Select the corresponding check box.

To terminate the grouping, right click **I/Icor** in the grouping area, and select **Ungroup** from the contextual menu. Repeat the operation for **Name**.

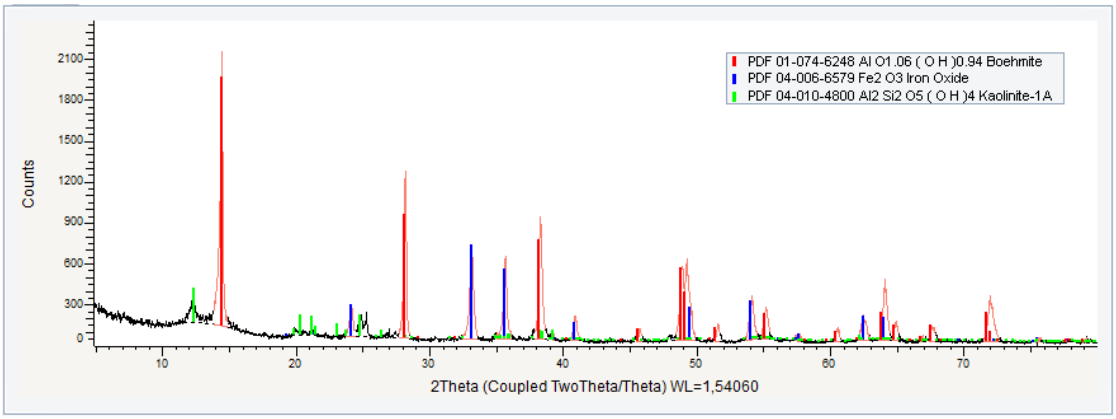


Figure 17.4: Boehmite pattern in red, Iron Oxide pattern in blue and Kaolinite-1A pattern in green.

Removing the regions explained by Kaolinite-1A would not be useful as the Kaolinite-1A peaks are very numerous. Using the results of a chemical analysis of the sample can help to complete the identification:

1. Select the scan BX100.RAW either in the data tree or in the graphical view.
2. Click **Import XRF Results** in the Data Command panel
   — or —
   Right-click the scan, then click **Import XRF Results** on the context menu.
   ➨ The Open an XRF results filename dialog box will be displayed.
3. Select the BX100.txt file in the Open an XRF results filename dialog box and click **Open**.
   ➨ The results of the chemical analysis will be displayed in the element list in the data tree next to the SQD results.

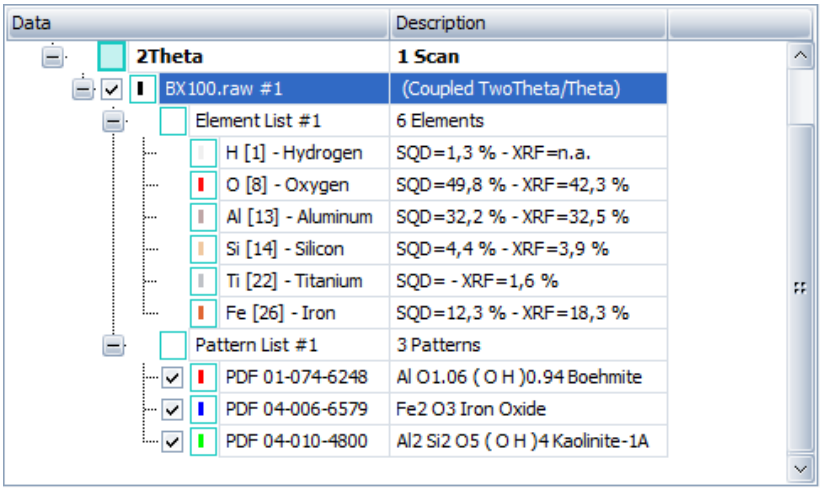


Figure 17.5: The chemical analysis indicates that the sample contains titanium.

Create a chemical filter from Titanium. To do so:

1. Select the Titanium in the data tree.
2. Click **Green Filter data** in the Data Command panel.
   — or —
   Right-click the scan, then click **Create|Green Filter data** on the context menu.
   ➨ A new chemical filter is created: BX100.RAW #1 Green Filter.
3. Another run using this new chemical filter makes it then possible to identify Anatase (PDF 04-014-0491).

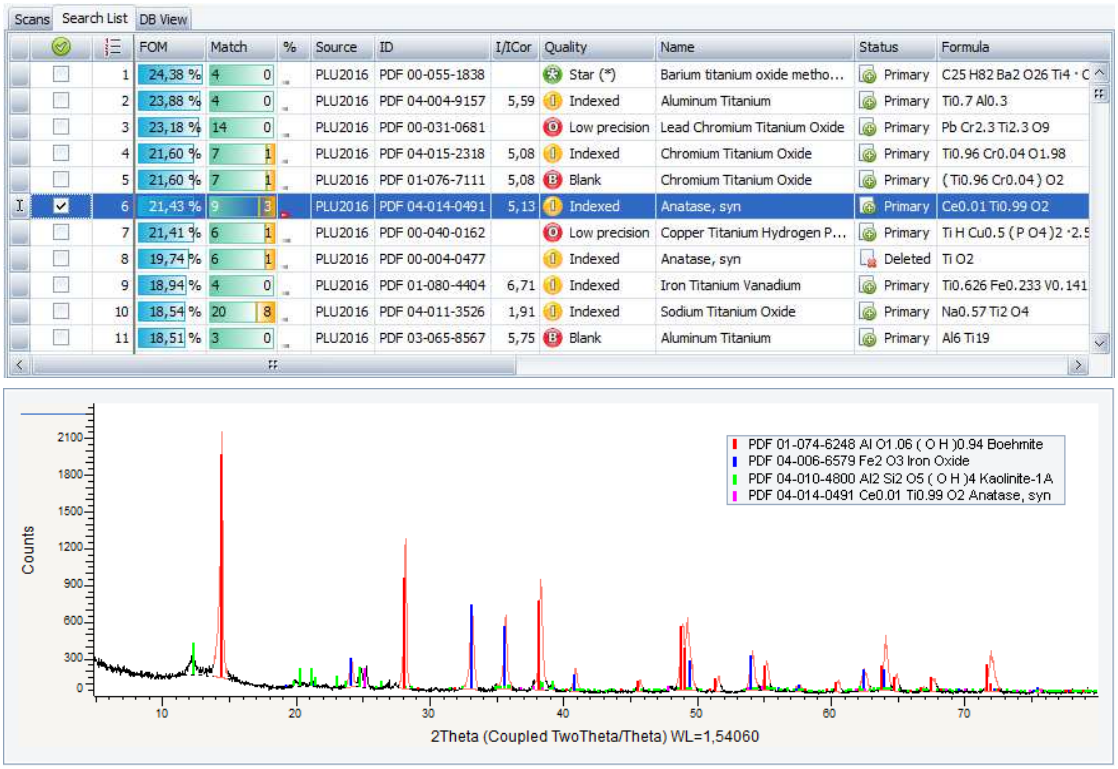


Figure 17.6: Boehmite pattern in red, Iron Oxide pattern in blue, Kaolinite-1A pattern in green and Anatase pattern in pink.

17.3 Step 3: Performing the Semi-Quantitative Phase Analysis

Once all the phases have been identified, the semi-quantitative analysis can be performed

The first phase identified in the list is Boehmite.

1. Zoom in on the strongest peak of the Boehmite, and then change the Y-Scale of the pattern to adjust the stick height to the peak.
2. To adjust the Y-Scale, point to the stick of interest and press the control key to change the pointer into a hand. Move it up or down to adjust the Y-Scale.

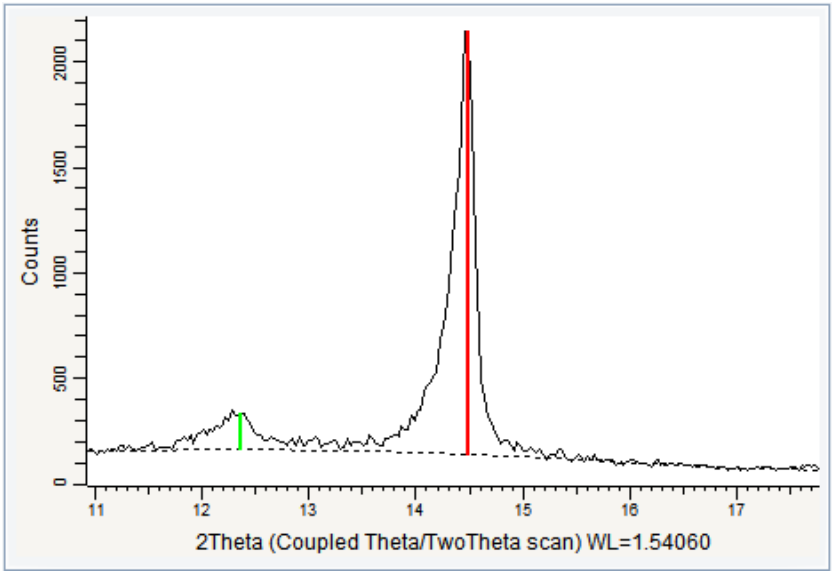
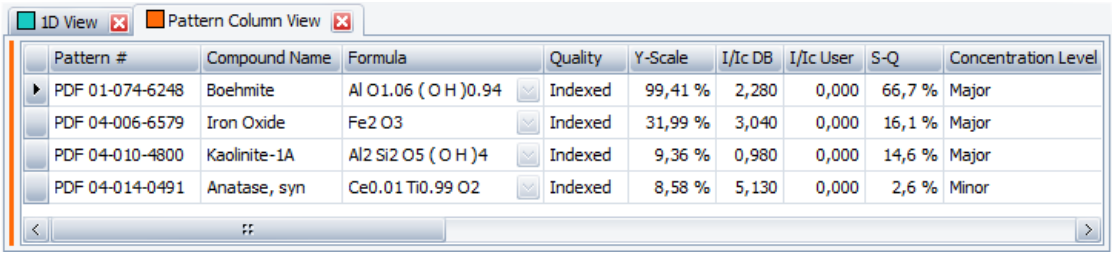


Figure 17.7: Zoom on the peaks (2θ=38° to 48°)

3. Proceed the same way for the other phases.
4. Select the BX100 scan either in the data tree or in the 1D view.
5. Click **Pattern Column View** in the Create list of the Data Command panel
   — or —
   click the **Pattern Column View** button on the Create View toolbar.
   — or —
   right-click and then click **Create.** Click **Pattern Column View** on the submenu.
   ➨ The phases' concentrations are listed in the **S-Q** column of the pattern column view.



Pattern #	Compound Name	Formula	Quality	Y-Scale	I/Ic DB	I/Ic User	S-Q	Concentration Level
PDF 01-074-6248	Boehmite	Al O1.06 (O H)0.94	Indexed	99,41 %	2,280	0,000	66,7 %	Major
PDF 04-006-6579	Iron Oxide	Fe2 O3	Indexed	31,99 %	3,040	0,000	16,1 %	Major
PDF 04-010-4800	Kaolinite-1A	Al2 Si2 O5 (O H)4	Indexed	9,36 %	0,980	0,000	14,6 %	Major
PDF 04-014-0491	Anatase, syn	Ce0.01 Ti0.99 O2	Indexed	8,58 %	5,130	0,000	2,6 %	Minor

Figure 17.8: Semi-quantitative analysis results in the Pattern Column view

To display the results as a pie or bar chart:

1. Select the pattern list in the data tree.
2. Click **Pattern Chart View** in the Create list of the Data Command panel
   — or —
   click the **Pattern Chart View** button on the Create View toolbar.
   — or —
   Right-click and then click **Create.** Click **Pattern Chart View** on the submenu.
3. Select either **Pie Chart** or **Bar Chart** in the Pattern Chart View table.

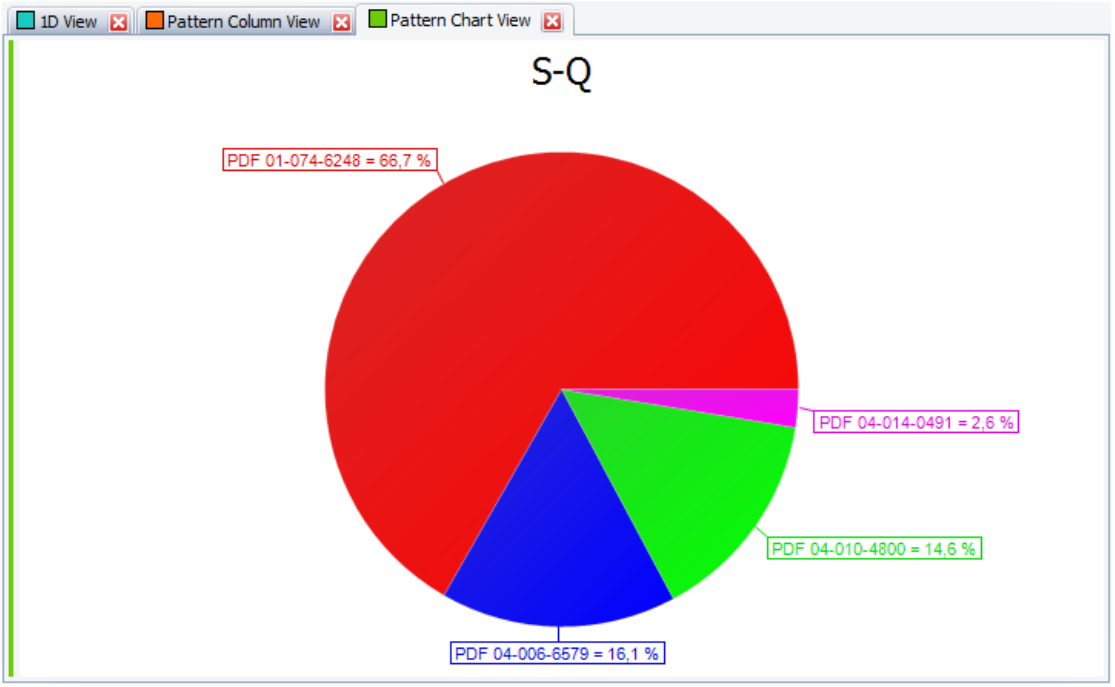


Figure 17.9: Semi-quantitative analysis results as a pie chart

17.4 Step 4: Saving

1. Click **Save As** on the **File** menu.

➨ The **Save EVA File As** dialog box will be displayed.

2. Select the appropriate disc drive and directory.
3. Type in the file name. (To overwrite an **.EVA** file, use the same name).
4. Click **Save**.

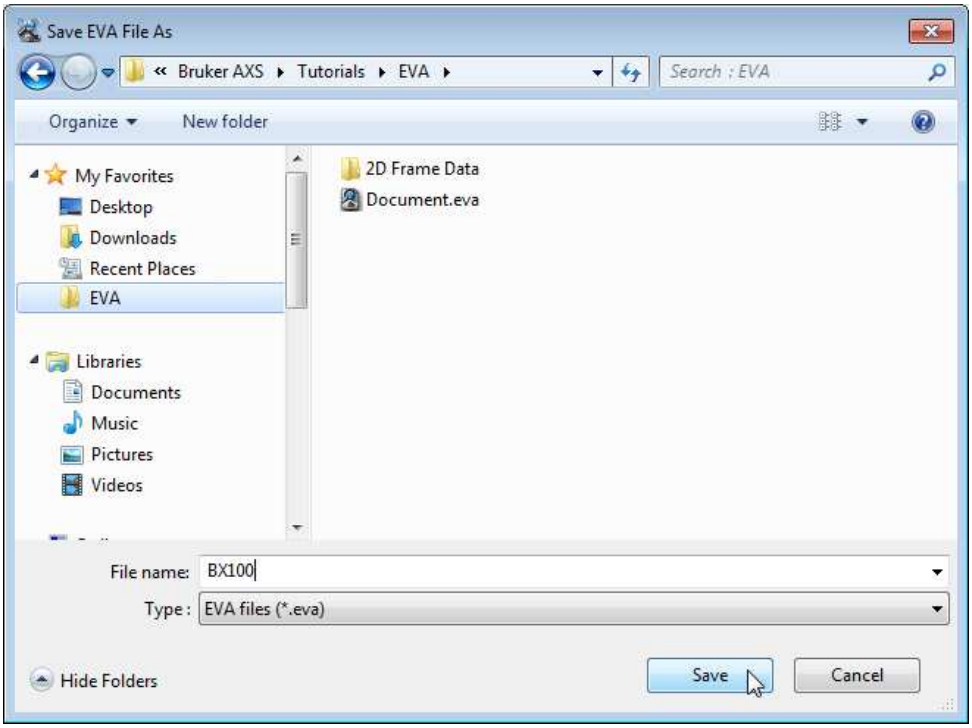


Figure 17.10: Saving BX100.EVA document

18 Using the d Multiplied By Tool

A reference database is required to perform a **Search/Match** operation.

This tutorial was prepared using **PDF 4+ 2016** as a reference database. You may have another reference database.

If you have no database, you cannot perform this part of the tutorial concerning the **Search/Match**.

The following procedure describes how to use the d Multiplied By tool.

The document used is held as a tutorial file, CSand.RAW, found in the Tutorial directory.

Csand is white coral sand from a beach in Hawaii.

The coral sand consists of three types of Carbonates, Aragonite, Calcite and Magnesian calcite. The calcite peaks are shifted to slightly larger angles, indicating minor Mg for Ca solid solution replacement. The Magnesian calcite peaks show large shifts.

Steps

1. Creating a new EVA document and importing Csand.RAW.
2. Performing the Search/Match operation.
3. Using the d Multiplied By Tool.
4. Saving.

18.1 Step 1: Creating a New EVA Document and Importing Csand.RAW

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   ➨ The EVA document is empty.
2. Click the **Import from files** data command or the **Import from files** button.
   ➨ The **Import From Files** dialog box will be displayed.
1. Search the Tutorials/EVA* directory and select the Csand.RAW file.
2. Click **Open**. The scan Csand.RAW will be added to the Data tree and displayed in the graphical view of the EVA document.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

Figure 18.1: Importing Csand.raw

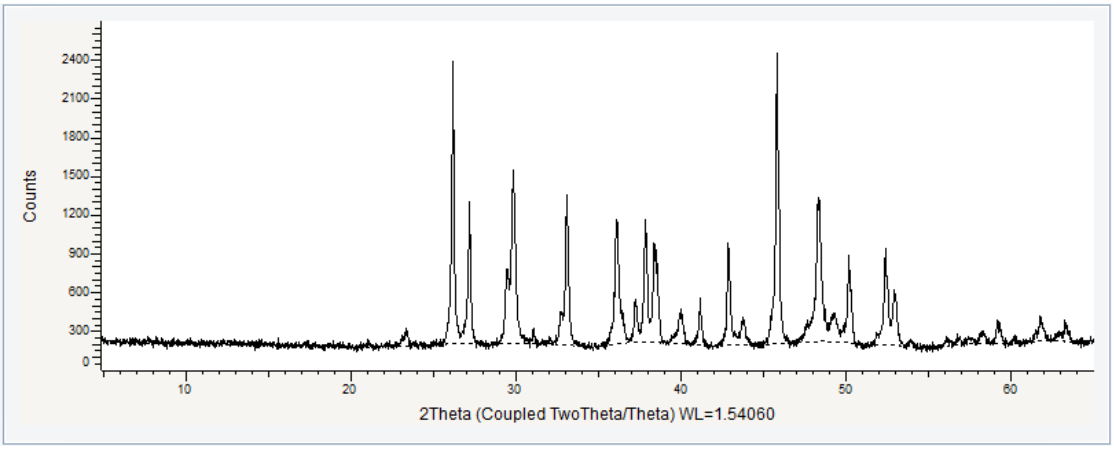
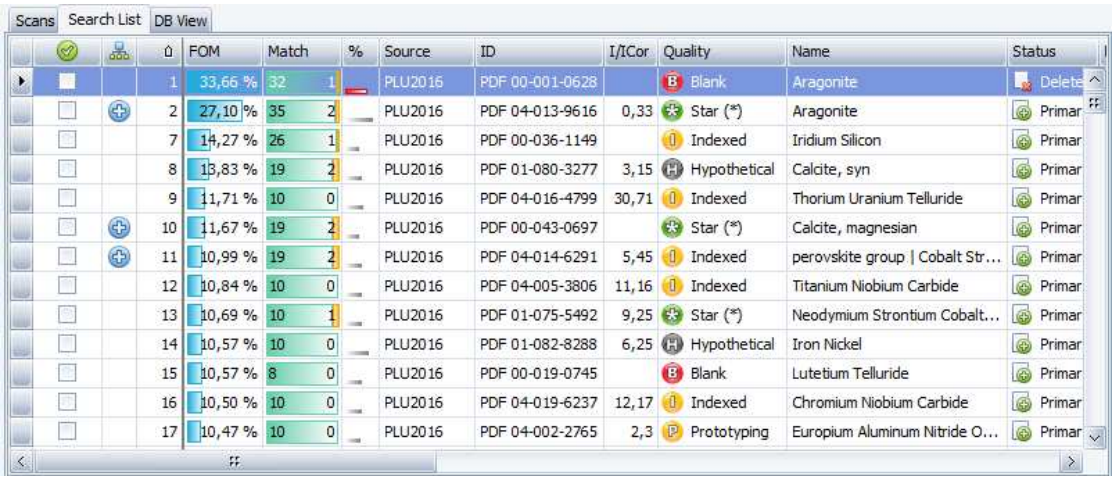


Figure 18.2: Csand scan imported in the graphical view

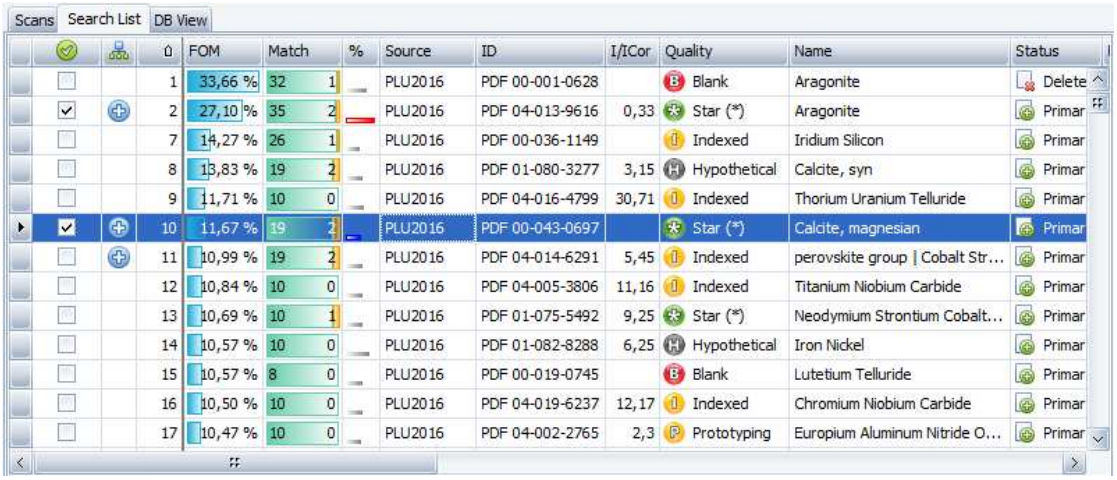
18.2 Step 2: Performing the Search/Match Operation

1. Keep the default search parameters and run a first search.
   ➥ Here are the results obtained:



	FOM	Match	%	Source	ID	I/ICor	Quality	Name	Status
1	33,66 %	32 1		PLU2016	PDF 00-001-0628		Blank	Aragonite	Delete
2	27,10 %	35 2		PLU2016	PDF 04-013-9616	0,33	Star (*)	Aragonite	Primar
7	14,27 %	26 1		PLU2016	PDF 00-036-1149		Indexed	Iridium Silicon	Primar
8	13,83 %	19 2		PLU2016	PDF 01-080-3277	3,15	Hypothetical	Calcite, syn	Primar
9	11,71 %	10 0		PLU2016	PDF 04-016-4799	30,71	Indexed	Thorium Uranium Telluride	Primar
10	11,67 %	19 2		PLU2016	PDF 00-043-0697		Star (*)	Calcite, magnesian	Primar
11	10,99 %	19 2		PLU2016	PDF 04-014-6291	5,45	Indexed	perovskite group | Cobalt Str...	Primar
12	10,84 %	10 0		PLU2016	PDF 04-005-3806	11,16	Indexed	Titanium Niobium Carbide	Primar
13	10,69 %	10 1		PLU2016	PDF 01-075-5492	9,25	Star (*)	Neodymium Strontium Cobalt...	Primar
14	10,57 %	10 0		PLU2016	PDF 01-082-8288	6,25	Hypothetical	Iron Nickel	Primar
15	10,57 %	8 0		PLU2016	PDF 00-019-0745		Blank	Lutetium Telluride	Primar
16	10,50 %	10 0		PLU2016	PDF 04-019-6237	12,17	Indexed	Chromium Niobium Carbide	Primar
17	10,47 %	10 0		PLU2016	PDF 04-002-2765	2,3	Prototyping	Europium Aluminum Nitride O...	Primar

2. Aragonite can be easily identified. We select pattern PDF 04-013-9616.



	FOM	Match	%	Source	ID	I/ICor	Quality	Name	Status
1	33,66 %	32 1		PLU2016	PDF 00-001-0628		Blank	Aragonite	Delete
2	27,10 %	35 2		PLU2016	PDF 04-013-9616	0,33	Star (*)	Aragonite	Primar
7	14,27 %	26 1		PLU2016	PDF 00-036-1149		Indexed	Iridium Silicon	Primar
8	13,83 %	19 2		PLU2016	PDF 01-080-3277	3,15	Hypothetical	Calcite, syn	Primar
9	11,71 %	10 0		PLU2016	PDF 04-016-4799	30,71	Indexed	Thorium Uranium Telluride	Primar
10	11,67 %	19 2		PLU2016	PDF 00-043-0697		Star (*)	Calcite, magnesian	Primar
11	10,99 %	19 2		PLU2016	PDF 04-014-6291	5,45	Indexed	perovskite group | Cobalt Str...	Primar
12	10,84 %	10 0		PLU2016	PDF 04-005-3806	11,16	Indexed	Titanium Niobium Carbide	Primar
13	10,69 %	10 1		PLU2016	PDF 01-075-5492	9,25	Star (*)	Neodymium Strontium Cobalt...	Primar
14	10,57 %	10 0		PLU2016	PDF 01-082-8288	6,25	Hypothetical	Iron Nickel	Primar
15	10,57 %	8 0		PLU2016	PDF 00-019-0745		Blank	Lutetium Telluride	Primar
16	10,50 %	10 0		PLU2016	PDF 04-019-6237	12,17	Indexed	Chromium Niobium Carbide	Primar
17	10,47 %	10 0		PLU2016	PDF 04-002-2765	2,3	Prototyping	Europium Aluminum Nitride O...	Primar

3. Going down in the list, we can find the Magnesian Calcite (PDF 00-043-0697).

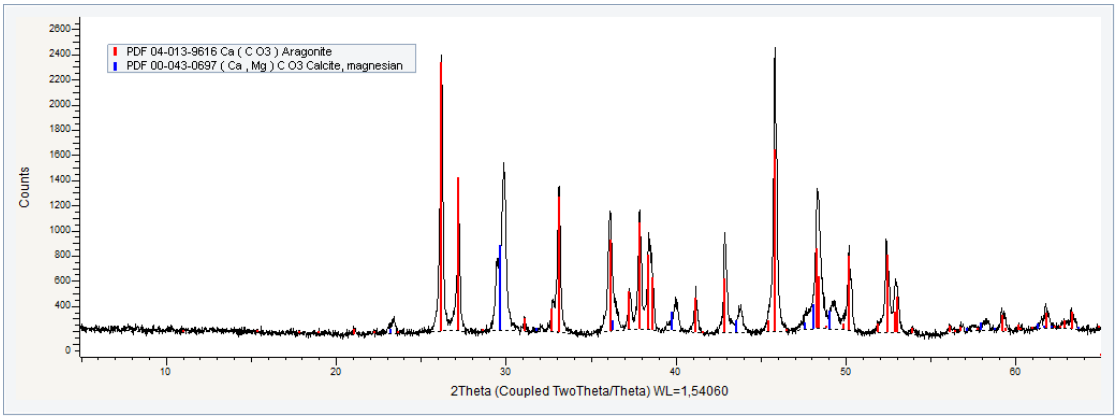


Figure 18.3: Aragonite pattern in red and Magnesian calcite in blue

18.3 Step 3: Using the d Multiplied By Tool

1. Insert the pure Calcite pattern (PDF 00-005-0586) by using the Search by name tool.
2. Zoom in around the location of the 100% line of pure Calcite.
3. Select the Calcite pattern in the data tree.

1. Click **d x by** in the Data Command panel
   — or —
   click the **d x by** command on the Pattern toolbar
   — or —
   right-click the pattern, then click **d x by** on the context menu.
   ➨ The **d x by** dialog box will be displayed.
2. Set the **d Multiplied by value** to 0.990 using the slider. It shows the Magnesian calcite pattern (PDF 00-043-0697) corresponds to the pure Calcite d-spacing multiplied by about 0.990.

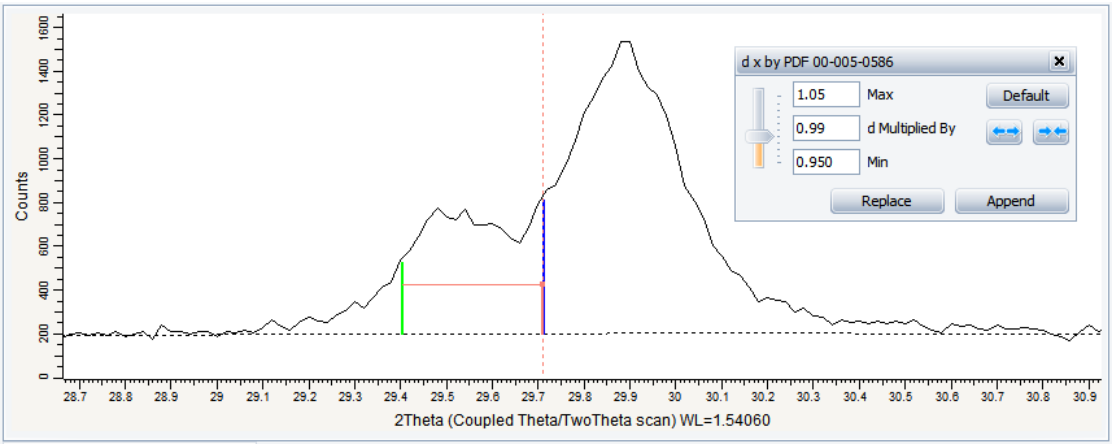
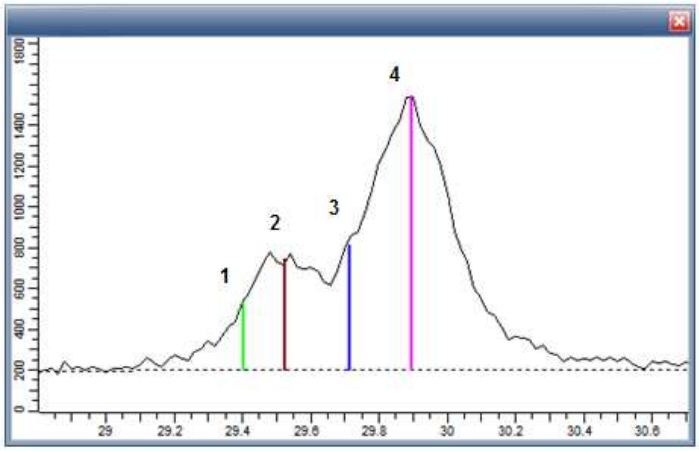


Figure 18.4: Adjusting the d Multiplied by value to 0.990 using the slider

But the file shows a mixture of two solid solutions exactly on both sides. Thus, the perfect explanation of this unknown scan requires two modified Calcite patterns. We can, for instance, make use of the pure Calcite (pattern 00-005-586) and modify it by means of the **d x By** tool. The adjustment of the slider leads to a *d* times value of 0.984 for matching the modified Calcite pattern having the stronger peaks, and of 0.996 for the second pattern as shown in the figure below.



1 Calcite pattern 00-005-0586
2 Calcite pattern 00-005-0586 multiplied by 0.996.
3 Magnesian Calcite pattern 00-043-0687
4 Calcite pattern 00-005-0586 multiplied by 0.984.

18.4 Step 4: Saving

1. Click **Save As** on the **File** menu.
   ➨ The **Save EVA File As** dialog box will be displayed.
2. Select the appropriate disc drive and directory.
3. Type in the file name. (To overwrite an **.EVA** file, use the same name).
4. Click **Save**.

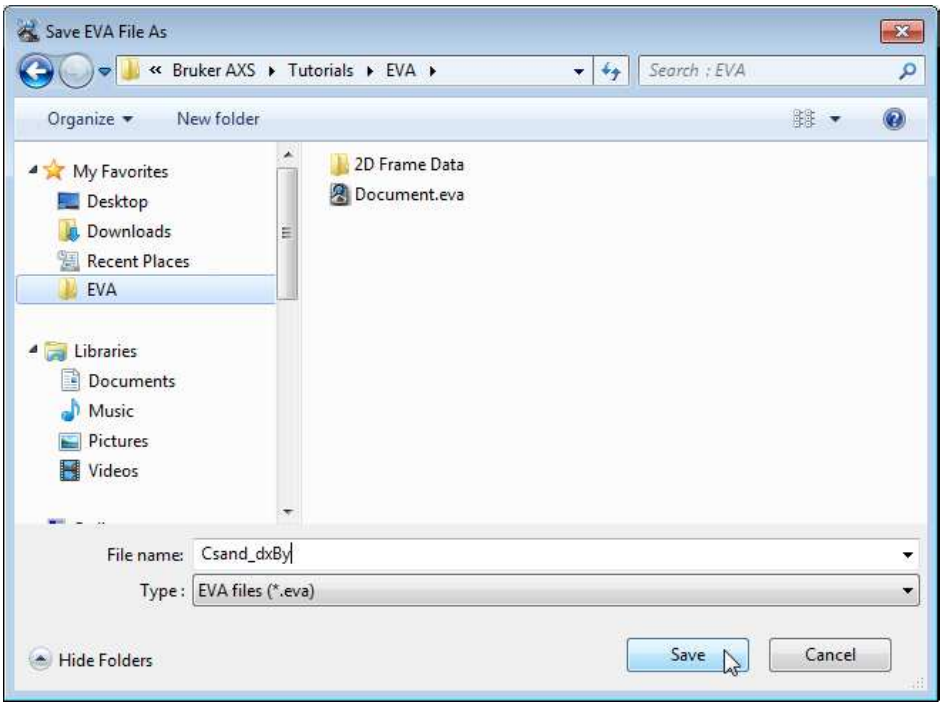


Figure 18.5: Saving Csand_dxBy.EVA document

19 Using the Tune Cell Tool

A reference database is required to perform a **Search/Match** operation.

This tutorial was prepared using **PDF 4+ 2016** as a reference database. You may have another reference database.

If you have no database, you cannot perform this part of the tutorial concerning the **Search/Match**.

The following procedure describes how use the Tune Cell tool.

The document used is held as a tutorial file, Francolite.RAW, found in the Tutorial directory.

The measured sample is a Carbonate-fluoroapatite (its mineral name is Francolite) and the difference from the Fluorapatite Ca10(PO4)6F2 is that P is partly replaced by C.

The replacement of P5+ (ionic radius 0.35) by the smaller C4+ (0.16) is expressed by deformation of the PO4-tetraeder, with shorter P-O-distances and the reduction of *a*o cell parameter (X-Ray Powder Diffraction Study of Francolite by the Rietveld Method, B. Perdikatsis, Materials Science Forum Vols. 79-82 (1991), pp. 809-814.).

Steps

1. Creating a new EVA document and importing Francolite.RAW.
2. Performing the Search/Match operation.
3. Performing the Tune cell operation.
4. Saving.

19.1 Step 1: Creating a New EVA Document and Importing Francolite.RAW

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   ➨ The EVA document is empty.

2. Click the **Import from files** data command or the **Import from files** button.
   ➨ The **Import From Files** dialog box will be displayed.
3. Search the Tutorials/EVA* directory and select the Francolite.RAW file.
4. Click **Open**.
5. The scan Francolite will be added to the Data tree and displayed in the graphical view of the EVA document.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

Figure 19.1: Importing Francolite.raw

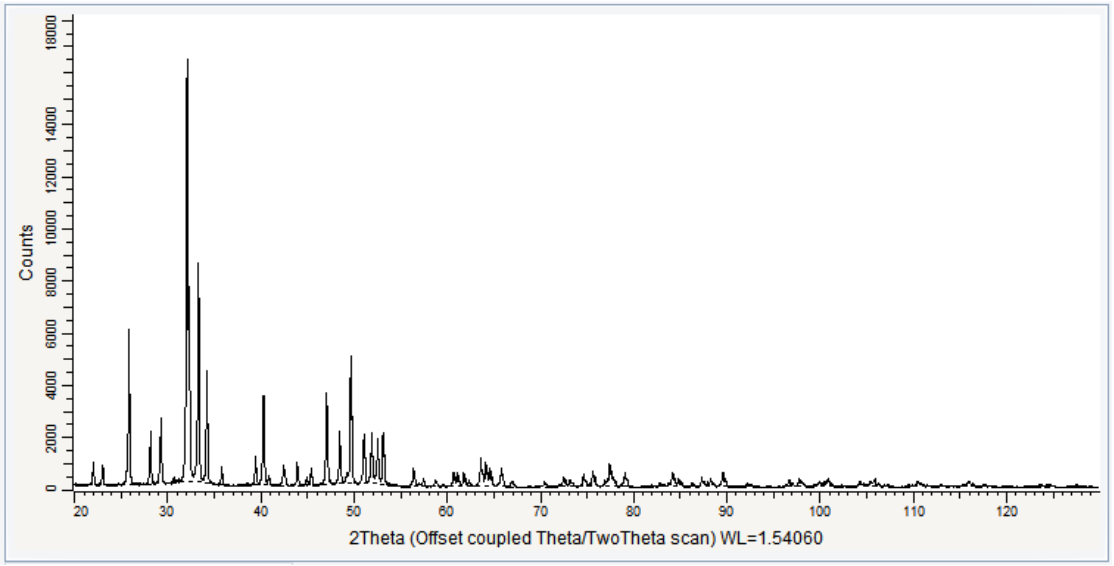
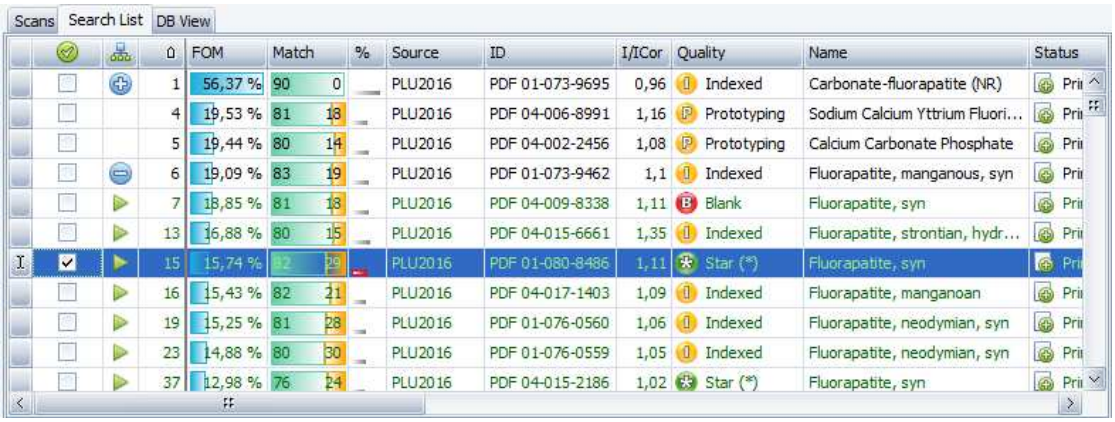


Figure 19.2: Francolite.RAW imported in the graphical view

19.2 Step 2: Performing the Search/Match Operation

1. Keep the default search parameters and run a search.
   ➥ Here are the results obtained:



		FOM	Match	%	Source	ID	I/ICor	Quality	Name	Status
	1	56,37 %	90	0	PLU2016	PDF 01-073-9695	0,96	Indexed	Carbonate-fluorapatite (NR)	Pri
	4	19,53 %	81	18	PLU2016	PDF 04-006-8991	1,16	Prototyping	Sodium Calcium Yttrium Fluori...	Pri
	5	19,44 %	80	14	PLU2016	PDF 04-002-2456	1,08	Prototyping	Calcium Carbonate Phosphate	Pri
	6	19,09 %	83	19	PLU2016	PDF 01-073-9462	1,1	Indexed	Fluorapatite, manganous, syn	Pri
	7	18,85 %	81	18	PLU2016	PDF 04-009-8338	1,11	Blank	Fluorapatite, syn	Pri
	13	16,88 %	80	15	PLU2016	PDF 04-015-6661	1,35	Indexed	Fluorapatite, strontian, hydr...	Pri
✓	15	15,74 %	82	29	PLU2016	PDF 01-080-8486	1,11	Star (*)	Fluorapatite, syn	Pri
	16	15,43 %	82	21	PLU2016	PDF 04-017-1403	1,09	Indexed	Fluorapatite, manganoan	Pri
	19	15,25 %	81	28	PLU2016	PDF 01-076-0560	1,06	Indexed	Fluorapatite, neodymian, syn	Pri
	23	14,88 %	80	30	PLU2016	PDF 01-076-0559	1,05	Indexed	Fluorapatite, neodymian, syn	Pri
	37	12,98 %	76	24	PLU2016	PDF 04-015-2186	1,02	Star (*)	Fluorapatite, syn	Pri

2. Carbonatefluoroapatite is easily identified but we select Fluorapatite (PDF 01-080-8486) for the need of the example.

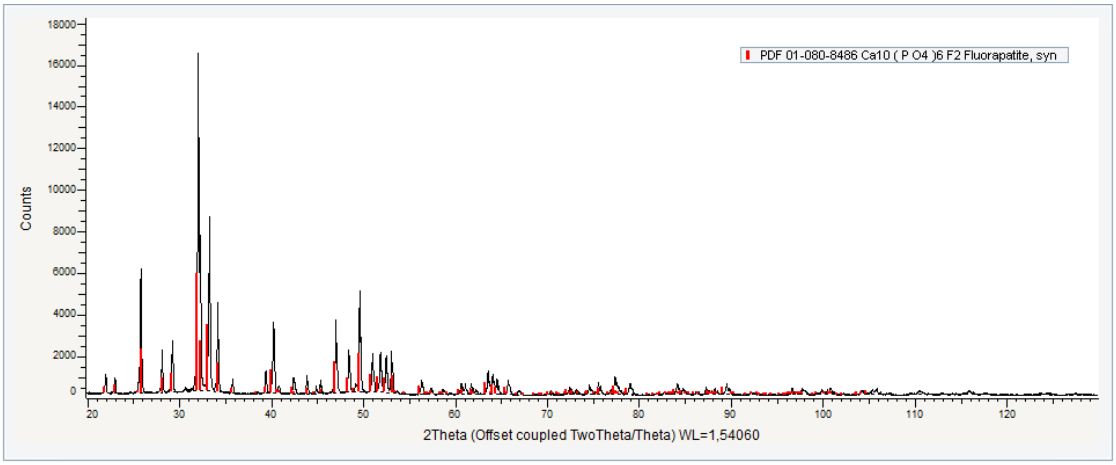
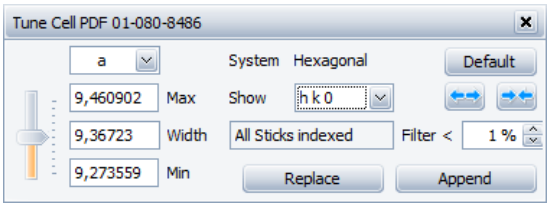


Figure 19.3: Fluorapatite pattern in blue

19.3 Step 3: Performing the Tune Cell Operation

1. Select the Fluorapatite pattern in the data tree.

2. Click **Tune Cell** in the Data Command panel
   — or —
   click the **Tune Cell** button on the Pattern toolbar
   — or —
   right-click the pattern, then click **Tune Cell** on the context menu.
   ➥ The Tune cell dialog box will be displayed.
3. In the list of parameters, click **a**, and then click **hk0** in the **Show** drop-down list to see lines which position depend only on *a*.



4. Zoom in on one of the (hk0)-peaks.
5. The ghosts of pattern sticks are displayed in the graphical view. Use the slider to fine-tune *a* in order to fit the peak.

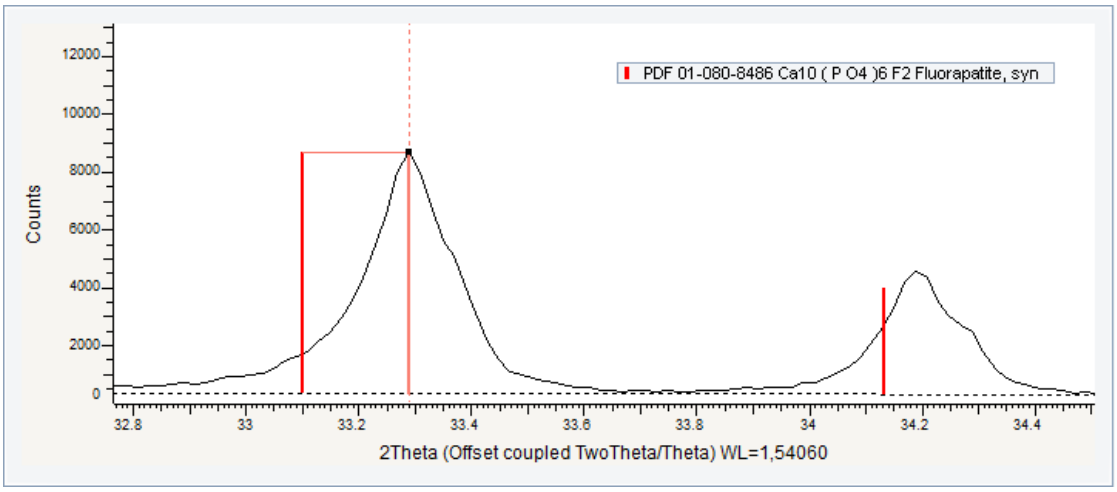


Figure 19.4: (300) stick (located at 2theta=33.129°) of the pattern PDF 00-015-0876 shifted to fit the corresponding peak.

6. Check whether all peaks fit the pattern.
7. Repeat steps 3 through 6 for *c* by selecting **00l** in the **Show** drop-down list.
8. Use the **Replace** or **Append** buttons to either replace the current pattern or append the modified one to the data tree.

19.4 Step 4: Saving

1. Click **Save As** on the **File** menu.
   ➨ The **Save EVA File As** dialog box will be displayed.
2. Select the appropriate disc drive and directory.
3. Type in the file name. (To overwrite an **.EVA** file, use the same name).
4. Click **Save**.

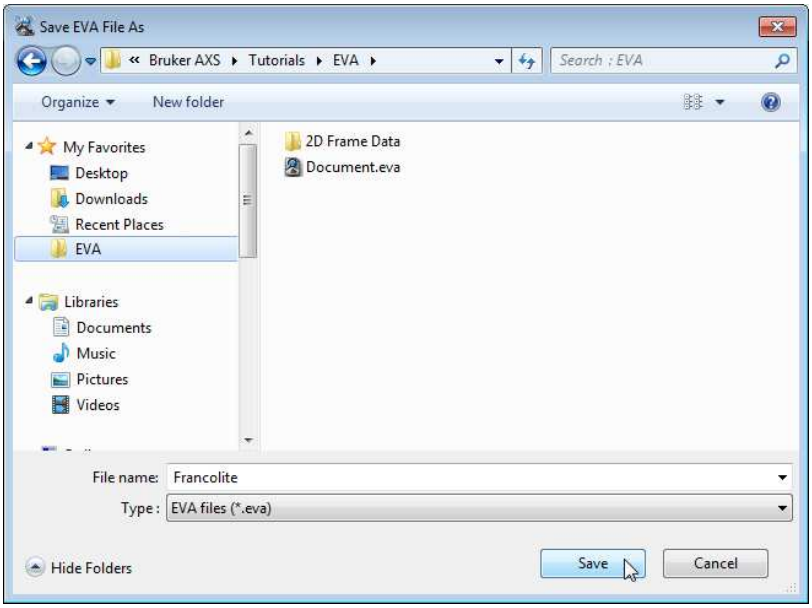


Figure 19.5: Saving Francolite.EVA document

20 Displaying a Pattern with Another Wavelength

A reference database is required to perform a **Search/Match** operation.

This tutorial was prepared using **PDF 4+ 2016** as a reference database. You may have another reference database.

If you have no database, you cannot perform this part of the tutorial concerning the **Search/Match**.

The following procedure describes how to display a pattern with another wavelength.

The document used is held as a tutorial file, Francolite.RAW, found in the Tutorial directory.

The measured sample is a Carbonate-fluoroapatite (its mineral name is Francolite). We are going to check the pollution of the X-ray tube is suspected.

Steps

1. Creating a new EVA document and importing Francolite.RAW.
2. Performing the Search/Match operation.
3. Changing the wavelength.
4. Saving.

20.1 Step 1: Creating a New EVA Document and Importing Francolite.RAW

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   ➨ The EVA document is empty.
2. Click the **Import from files** data command or the **Import from files** button.
   ➨ The **Import From Files** dialog box will be displayed.
3. Search the Tutorials/EVA* directory and select the Francolite.RAW file.
4. Click **Open**.
5. The scan Francolite will be added to the Data tree and displayed in the graphical view of the EVA document.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

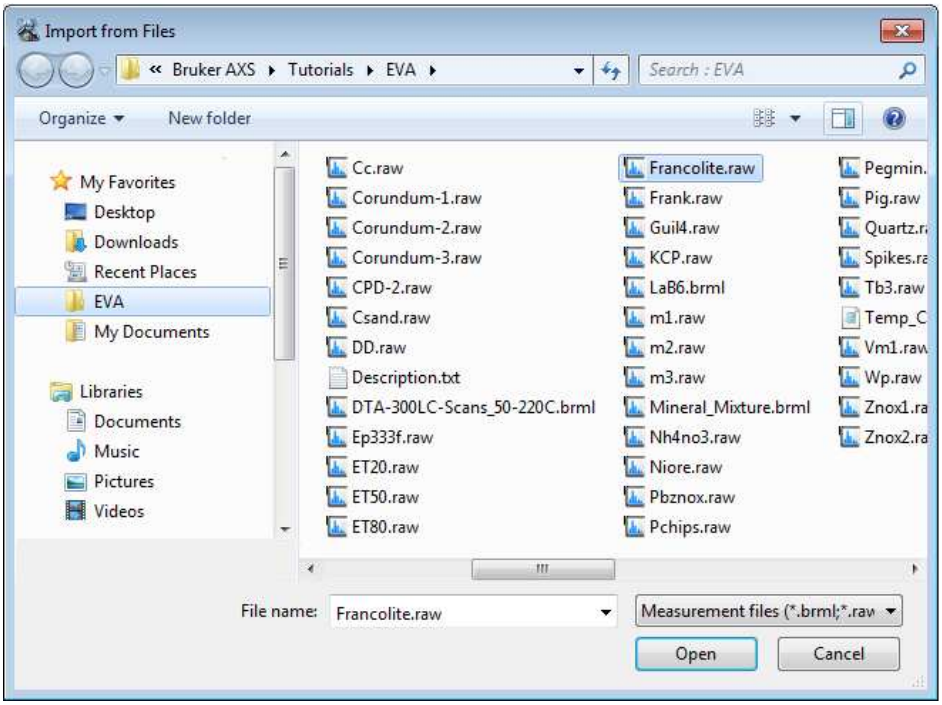


Figure 20.1: Importing Francolite.raw

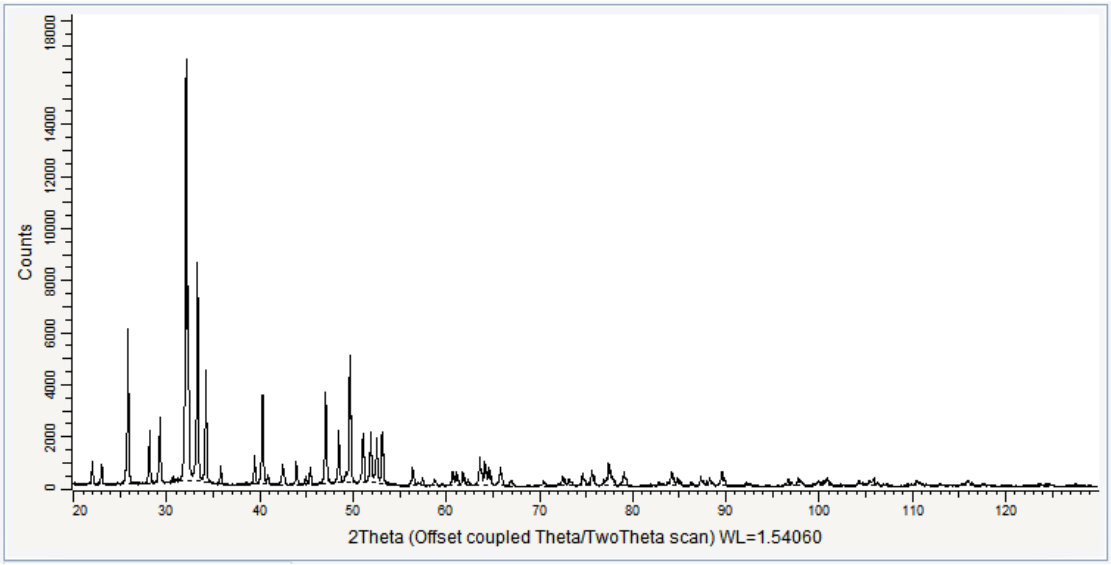
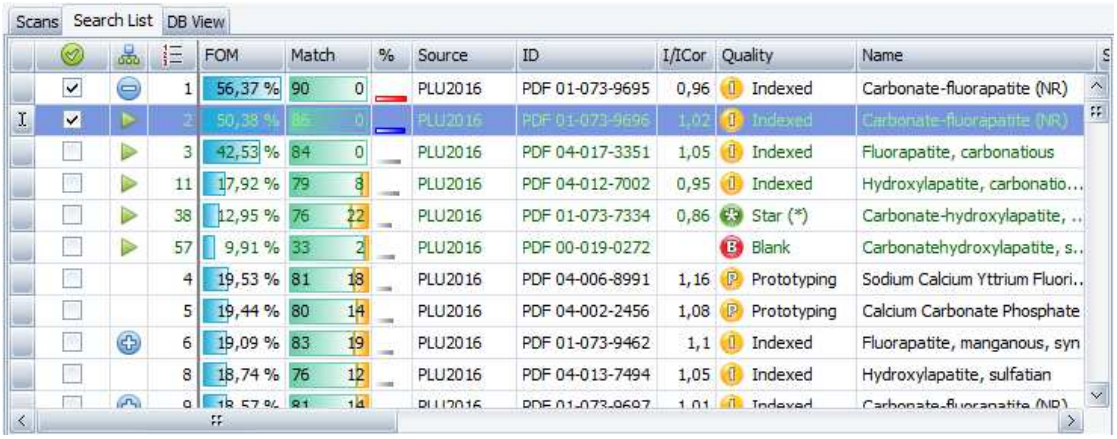


Figure 20.2: Francolite.RAW imported in the graphical view

20.2 Step 2: Performing the Search/Match Operation

1. Keep the default search parameters and run a search.
   ➨ Here are the results obtained:



		FOM	Match	%	Source	ID	I/ICor	Quality	Name
☑	1	56,37 %	90	0	PLU2016	PDF 01-073-9695	0,96	Indexed	Carbonate-fluorapatite (NR)
☑	2	50,38 %	86	0	PLU2016	PDF 01-073-9696	1,02	Indexed	Carbonate-fluorapatite (NR)
☐	3	42,53 %	84	0	PLU2016	PDF 04-017-3351	1,05	Indexed	Fluorapatite, carbonatious
☐	11	17,92 %	79	8	PLU2016	PDF 04-012-7002	0,95	Indexed	Hydroxylapatite, carbonatio...
☐	38	12,95 %	76	22	PLU2016	PDF 01-073-7334	0,86	Star (*)	Carbonate-hydroxylapatite, ..
☐	57	9,91 %	33	2	PLU2016	PDF 00-019-0272		Blank	Carbonatehydroxylapatite, s..
☐	4	19,53 %	81	18	PLU2016	PDF 04-006-8991	1,16	Prototyping	Sodium Calcium Yttrium Fluori..
☐	5	19,44 %	80	14	PLU2016	PDF 04-002-2456	1,08	Prototyping	Calcium Carbonate Phosphate
☐	6	19,09 %	83	19	PLU2016	PDF 01-073-9462	1,1	Indexed	Fluorapatite, manganous, syn
☐	8	18,74 %	76	12	PLU2016	PDF 04-013-7494	1,05	Indexed	Hydroxylapatite, sulfatian

2. Carbonate-fluoroapatite is easily identified. Select both patterns PDF 01-073-9695 and PDF 01-073-9696. It will allow the change to be made.

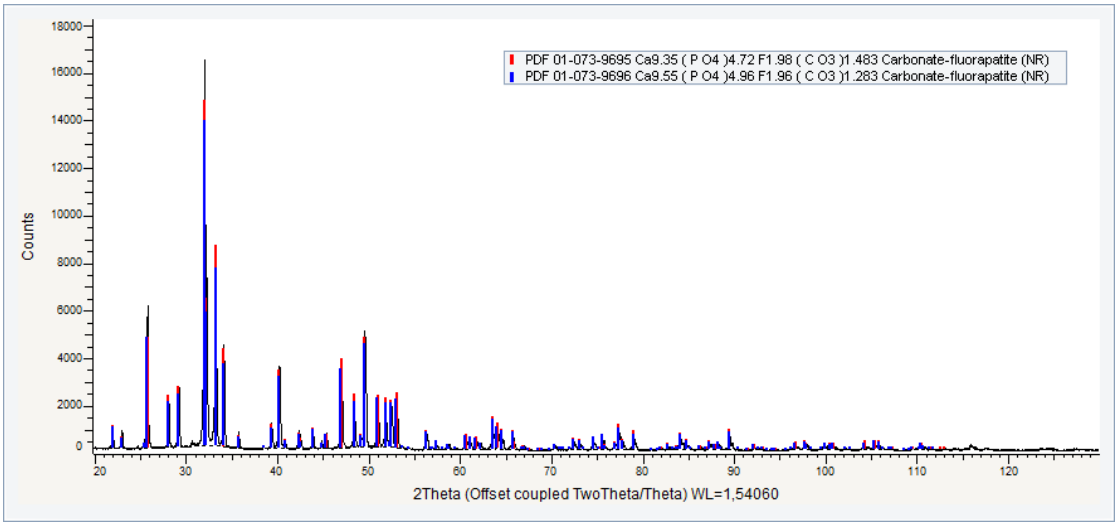


Figure 20.3: The two patterns of Carbonate-fluorapatite are superposed.

20.3 Step 3: Changing the Wavelength

We want to check if there is a pollution of the X-ray tube. The WLα1 radiation is the most frequently encountered spurious X-ray line in sealed X-ray tubes. Therefore, we are going to display the pattern for the WLα1 radiation.

1. Select the pattern PDF 00-073-9696 in the data tree.
2. In the pattern property table, clear the **Scan WL** check box to be able to enter another wavelength.
3. In the **Wavelength** drop-down list below, select the WLα1 wavelength. The pattern PDF 00-021-0141 will be displayed with this new wavelength.
4. Zoom in from 2Theta=20° to 2Theta=55°.

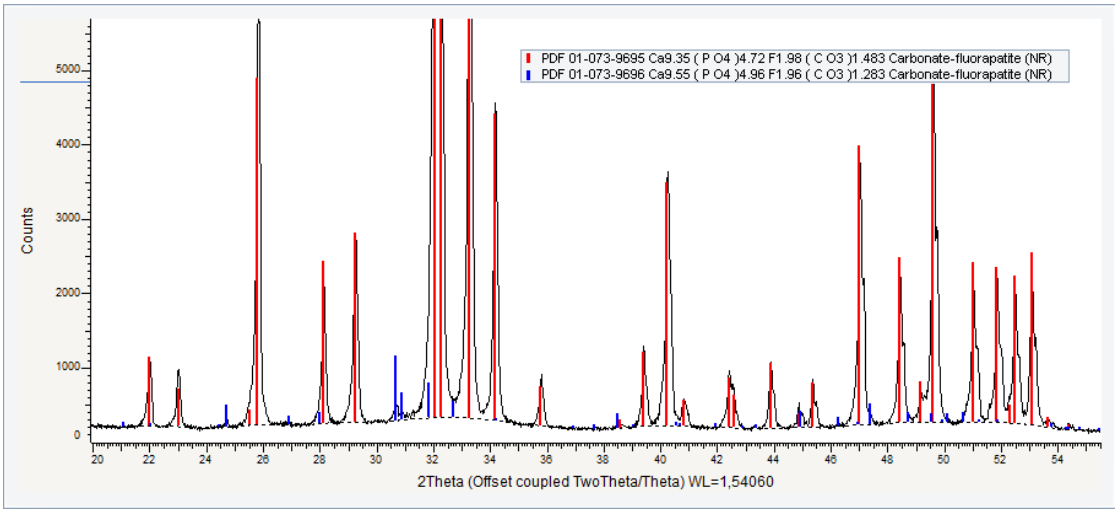


Figure 20.4: Carbonate-fluorapatite pattern displayed with the WLα1 wavelength in blue and original pattern in red.

5. Zoom on the 20-55° 2Theta range. The modified pattern looks to match some parts of the scan.

⇨ It makes it possible to conclude there is likely a pollution of the X-ray tube.

20.4 Step 4: Saving

1. Click **Save As** on the **File** menu.
   ➨ The **Save EVA File As** dialog box will be displayed.
2. Select the appropriate disc drive and directory.
3. Type in the file name. (To overwrite an **.EVA** file, use the same name).
4. Click **Save**.

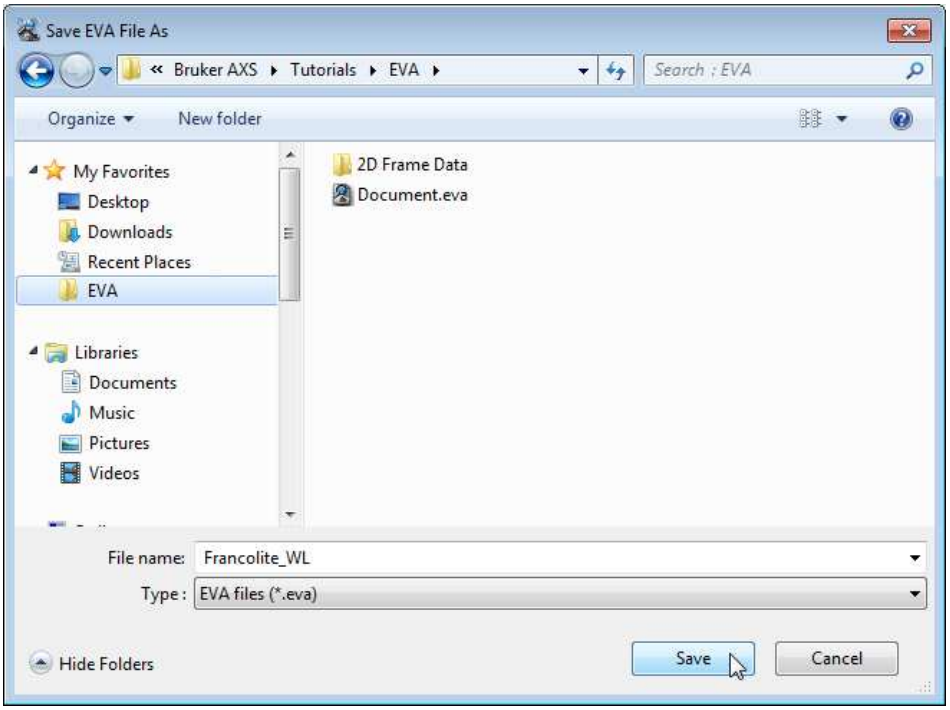


Figure 20.5: Saving Francolite_WL.EVA document

21 Working with the Waterfall View

The following procedure describes how to work with waterfall view.
The scan used is held as a tutorial file, Ep333f.RAW, found in the Tutorial directory.

Steps

1. Creating a new EVA document and importing Ep333f.RAW.
2. Creating and working with the waterfall view.
3. Saving the EVA document containing the scan.

21.1 Step 1: Creating a New EVA Document and Importing Ep333f.RAW

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   - ➨ The EVA document is empty.

2. Click the **Import from files** data command or the **Import from files** button.
   - ➨ The **Import From Files** dialog box will be displayed.
3. Search the Tutorials/EVA* directory and select the Ep333f.RAW file.
4. Click **Open**.
   - ➨ The scan Ep333f will be added to the Data tree and displayed in the graphical view of the EVA document.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

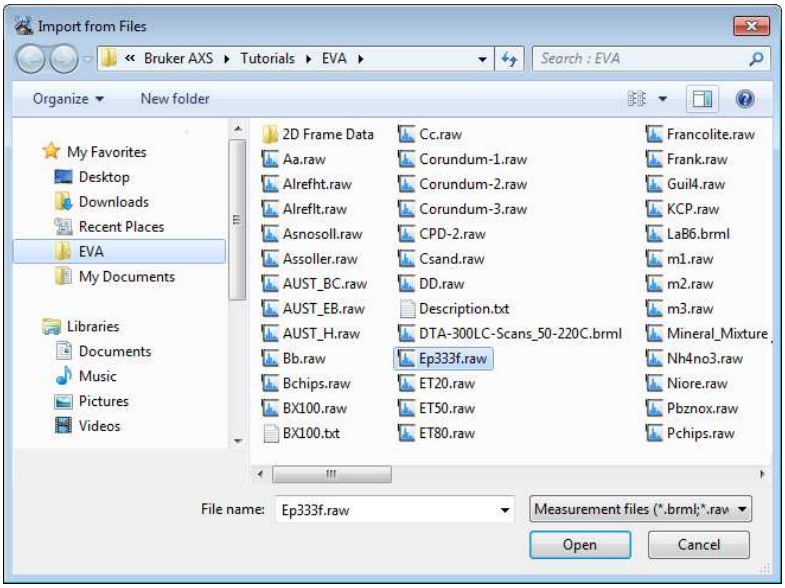


Figure 21.1: Import a Scan File dialog box

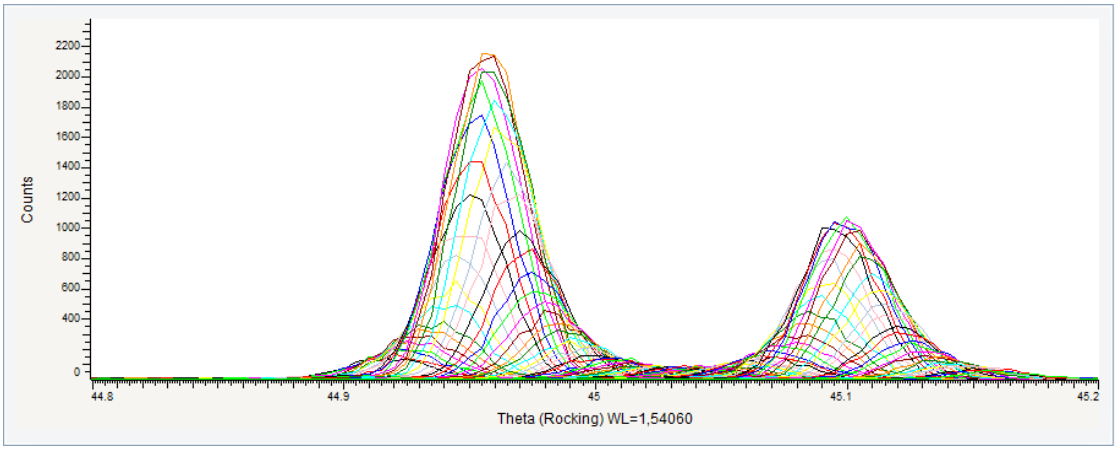


Figure 21.2: Ep333f.RAW file imported in the graphical view

21.2 Step 2: Creating and Working with the Waterfall View

1. Click the **Waterfall Display** button on the 1D View toolbar
   — or —
   select the **Waterfall display** check box in the View property panel.
   ➨ The scans will be displayed as a waterfall.

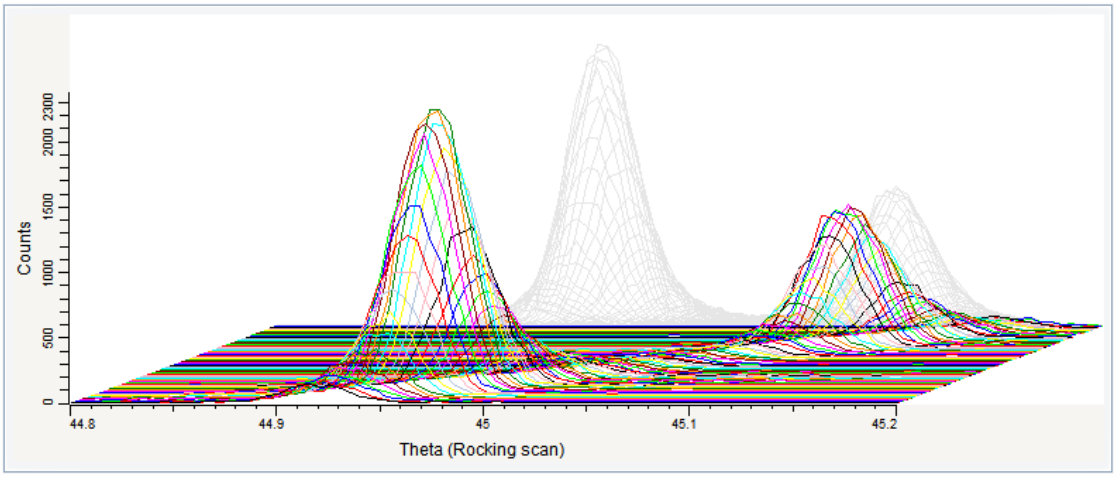


Figure 21.3: Waterfall display

2. Change the perspective of the display.
3. To change the perspective horizontally, click the X-axis to display the horizontal scroll bar.
4. Point to the right end of the scroll bar.
   ➨ The mouse pointer will change into a double arrow.
5. Move the double arrow left or right to reduce or expand the scroll bar.

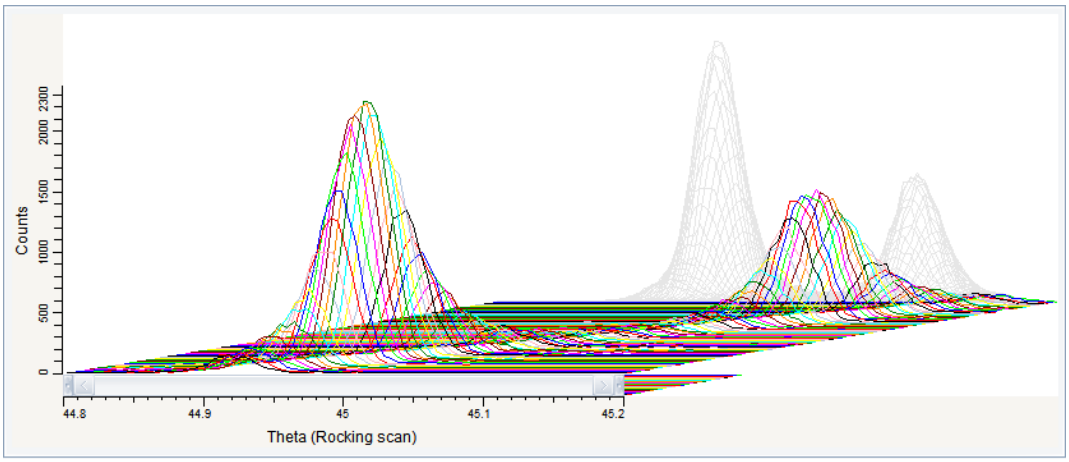


Figure 21.4: Perspective horizontally modified

6. To change the perspective vertically, proceed the same way but start by clicking on the Y-axis.

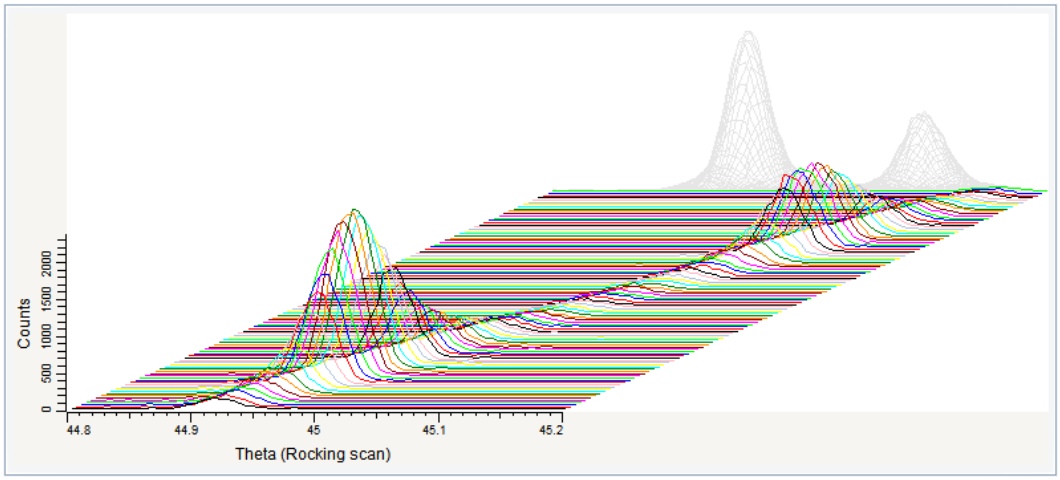


Figure 21.5: Perspective horizontally and vertically modified

7. Zoom in on the right peak. The corresponding zone must be selected in the shadow representation at the back: move the cursor to one end of the targeted zoom area, press and hold the left mouse button while dragging the mouse until the cursor reaches the opposite end, then release the button.

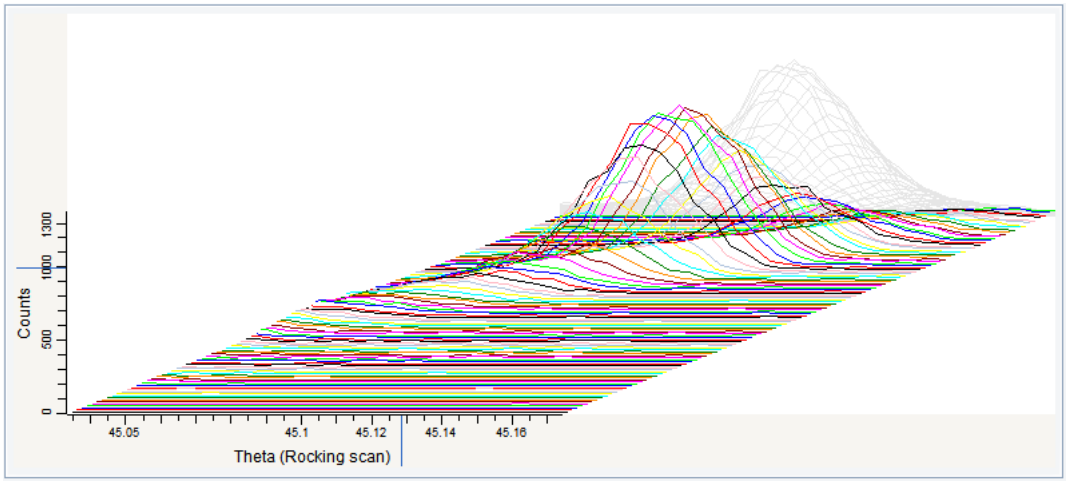


Figure 21.6: Zoom on the right peak

21.3 Step 3: Saving

1. Click **Save As** on the **File** menu.
   ➨ The **Save EVA File As** dialog box will be displayed.
2. Select the appropriate disc drive and directory.
3. Type in the file name. (To overwrite an **.EVA** file, use the same name).
4. Click **Save**.

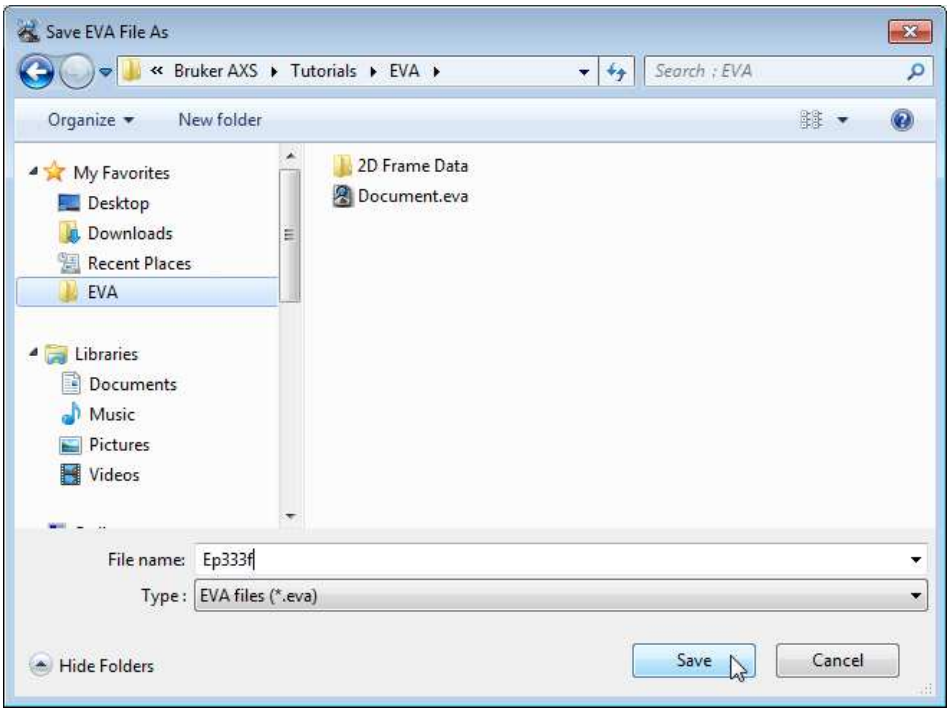


Figure 21.7: Saving Ep333f.EVA document

22 Working with the 2D View

The following procedure describes how to work with the 2D view.
The scan used is held as a tutorial file, Ep333f.RAW, found in the Tutorial directory.

Steps

1. Creating a new EVA document and importing Ep333f.RAW.
2. Creating and working with the 2D view.
3. Saving the EVA document containing the scan.

22.1 Step 1: Creating a New EVA Document and Importing Ep333f.RAW

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   - ➨ The EVA document is empty.

2. Click the **Import from files** data command or the **Import from files** button.
   - ➨ The **Import From Files** dialog box will be displayed.
3. Search the Tutorials/EVA* directory and select the Ep333f.RAW file.
4. Click **Open**.
   - ➨ The scan Ep333f will be added to the Data tree and displayed in the graphical view of the EVA document.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

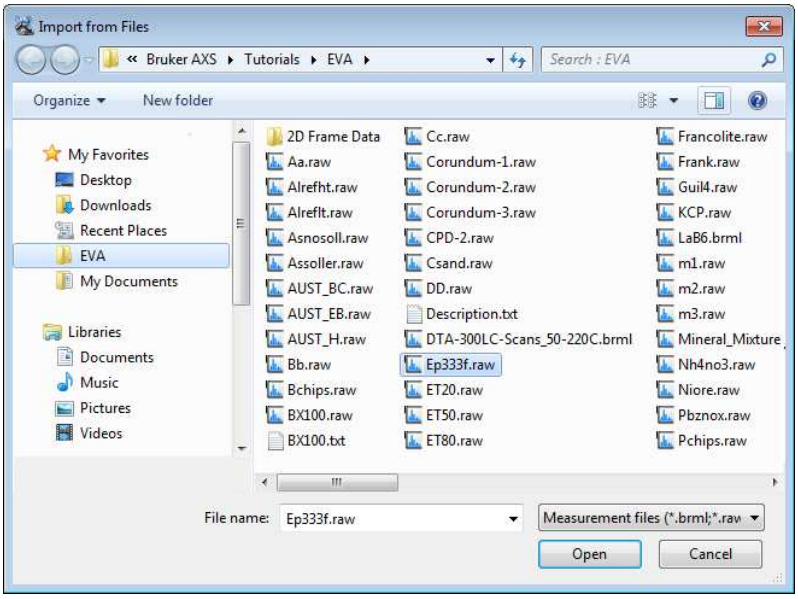


Figure 22.1: Import a Scan File dialog box

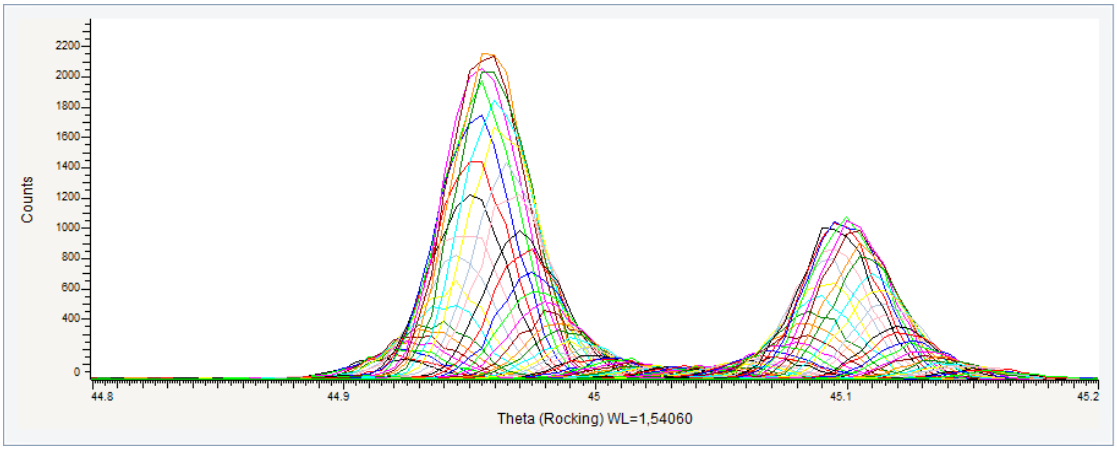


Figure 22.2: Ep333f.RAW file imported in the graphical view

22.2 Step 2: Creating and working with the 2D view.

Case #1: 2D view with intensity map

▷ Make certain the list of scans is selected; if not, select it in the data tree.

1. Click **2D View** in the Create list of the Data Command panel
   — or —
   click the **2D View** button on the Create View toolbar
   — or —
   right-click the scan list in the data tree to display the context menu. Click **Create** and then **2D View** on the related submenu.

   ➨ The 2D View is displayed in a new tab. The Intensity map is displayed by default. Leave the **Intensity map** check box selected.

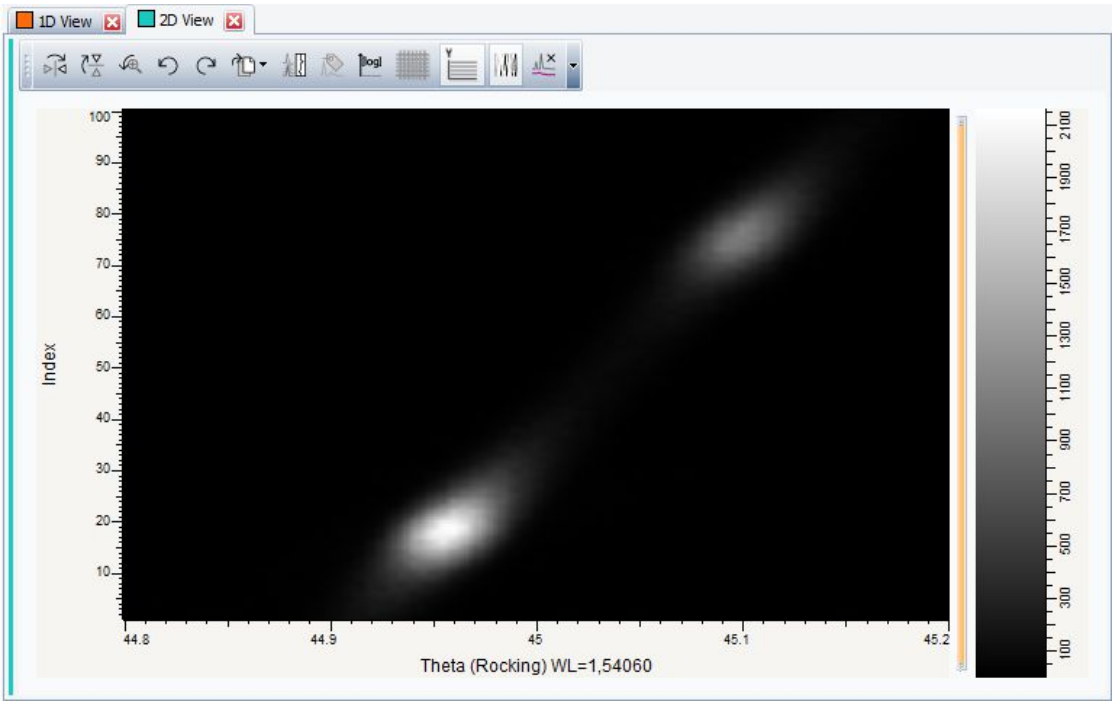


Figure 22.3: 2D view with intensity map

2. Customize the intensity map by right-clicking the color scale on the right and choosing among the offered choices on the context menu. Select for example the **Diffraction Space Viewer** option. You can also click the **Inverse Colors** command to invert the color palette.

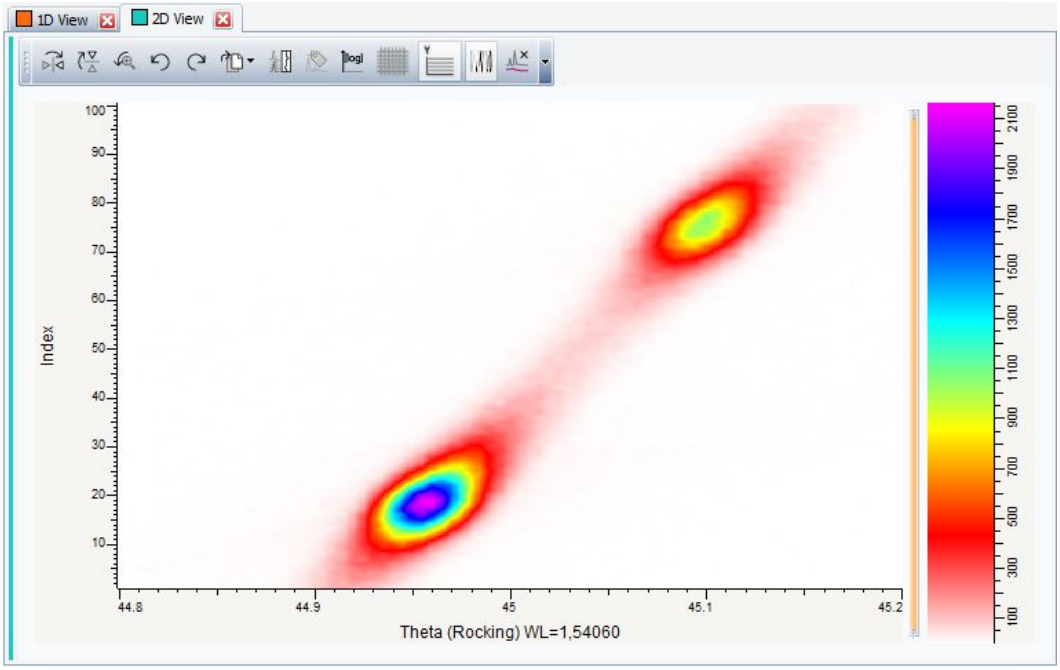


Figure 22.4: 2D view with colored intensity map

Case #2: 2D view with levels

▷ Make certain the list of scans is selected; if not, select it in the data tree.

1. Click **Create Level** in the Tool list of the Data Command panel
   — or —
   right-click the scan list in the data tree to display the context menu. Click **Tool** and then **Create Level** on the related submenu.
   ➨ The Create Level Theta dialog box will be displayed. By default 5 automatic levels will be created. They are displayed as ghost levels on the graphical view.

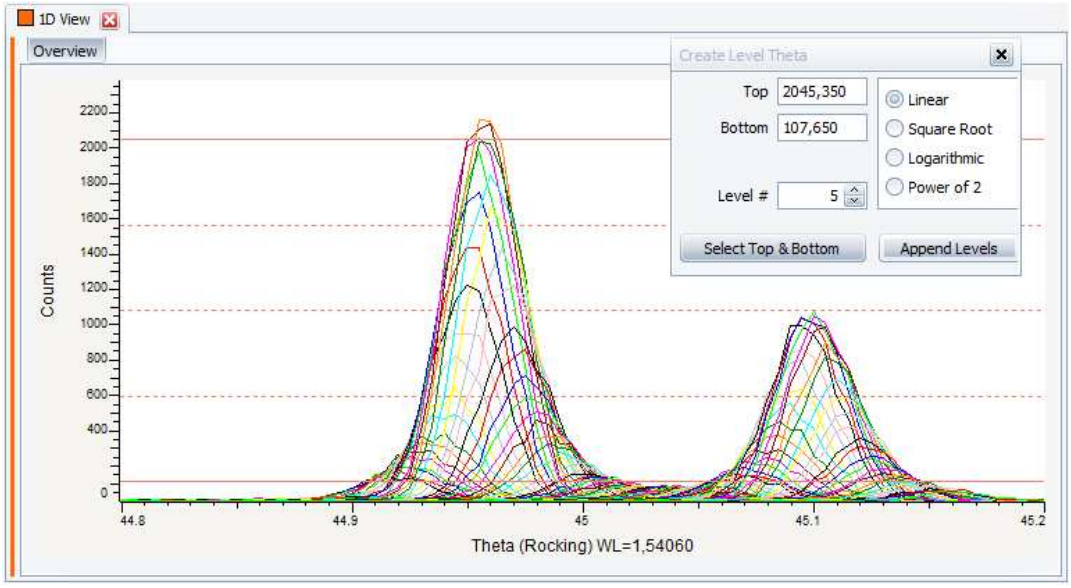


Figure 22.5: Creating levels: Create Level dialog box and ghost levels in the graphical view

2. Click the **Append Levels** button and close the dialog box
   ➨ The levels will be added in the data tree and displayed in the graphical view.

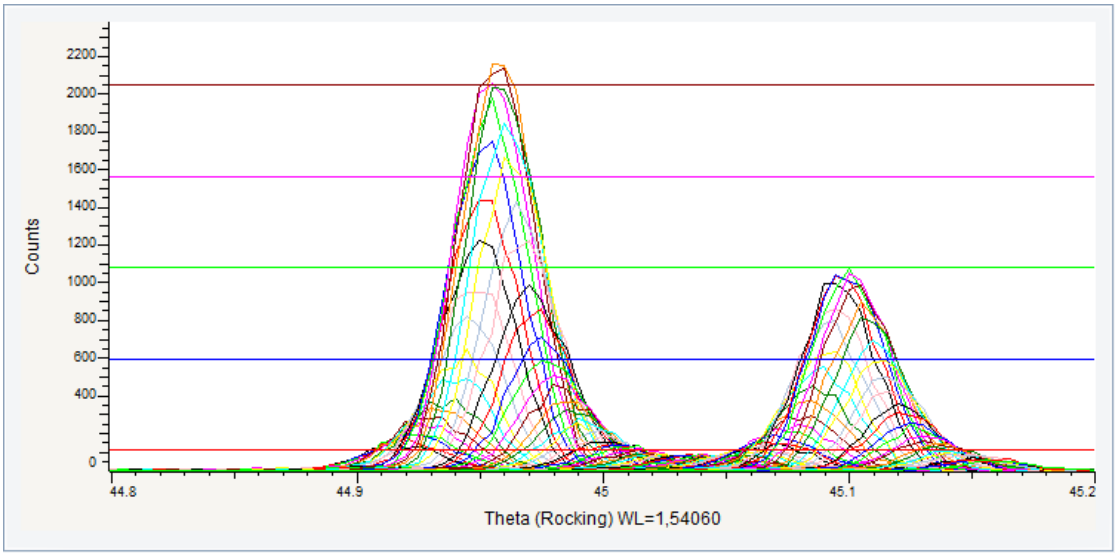


Figure 22.6: Creating levels: levels displayed in the graphical view

3. Click **2D View** in the Create list of the Data Command panel
   — or —
   click the **2D View** button on the Create View toolbar
   — or —
   right-click the scan list in the data tree to display the context menu. Click **Create** and then **2D View** on the related submenu.
   ➨ The 2D View will be displayed in a new tab. The Intensity map and the Levels are displayed by default. Leave the **Intensity map** and the **Levels** check boxes selected.

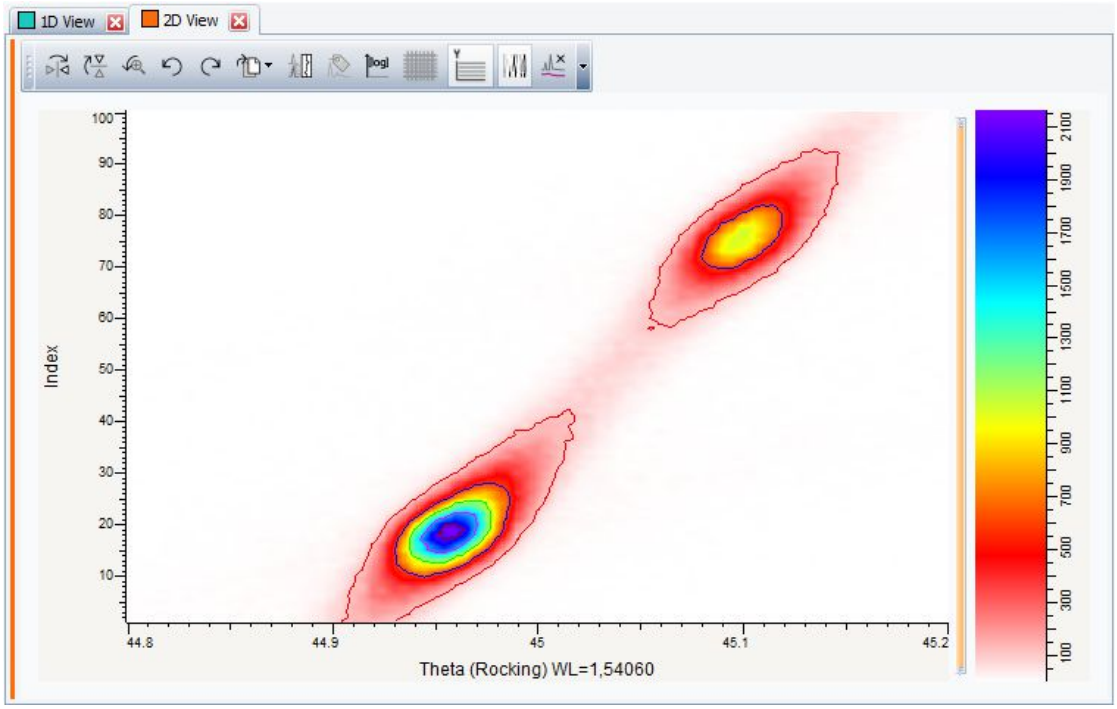


Figure 22.7: 2D view with intensity map and levels

22.3 Step 3: Saving

1. Click **Save As** on the **File** menu.
   ➨ The **Save EVA File As** dialog box will be displayed.
2. Select the appropriate disc drive and directory.
3. Type in the file name. (To overwrite an **.EVA** file, use the same name).
4. Click **Save**.

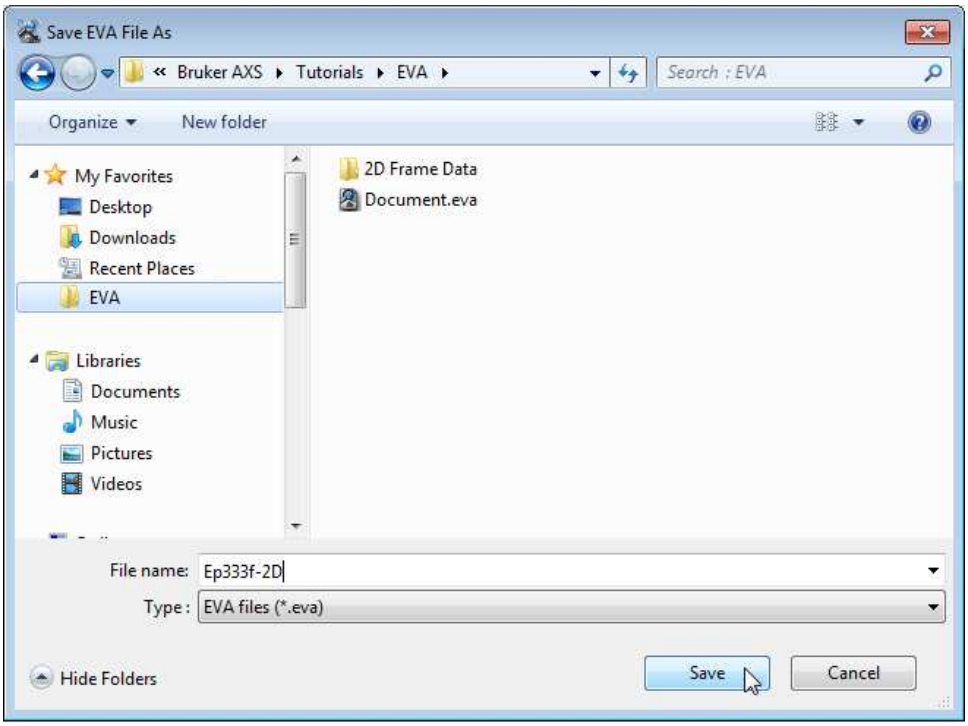


Figure 22.8: Saving Ep333f-2D.EVA document

23 Working with the Side View

The following procedure describes how to work with waterfall view.

The scan used is held as a tutorial file, DTA-300LC-Scans_50-220C.BRML, found in the Tutorial directory.

Steps

1. Creating a new EVA document and importing DTA-300LC-Scans_50-220C.BRML.
2. Creating and working with the side view.
3. Saving the EVA document containing the scan.

23.1 Step 1: Creating a New EVA Document and Importing DTA-300LC-Scans_50-220C.BRML

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   - ➨ The EVA document is empty.

2. Click the **Import from files** data command or the **Import from files** button.
   - ➨ The **Import From Files** dialog box will be displayed.
3. Search the Tutorials/EVA* directory and select the DTA-300LC-Scans_50-220C.BRML file.
4. Click **Open**.
   - ➨ The scan DTA-300LC-Scans_50-220C will be added to the Data tree and displayed in the graphical view of the EVA document.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

Figure 23.1: Importing the scan

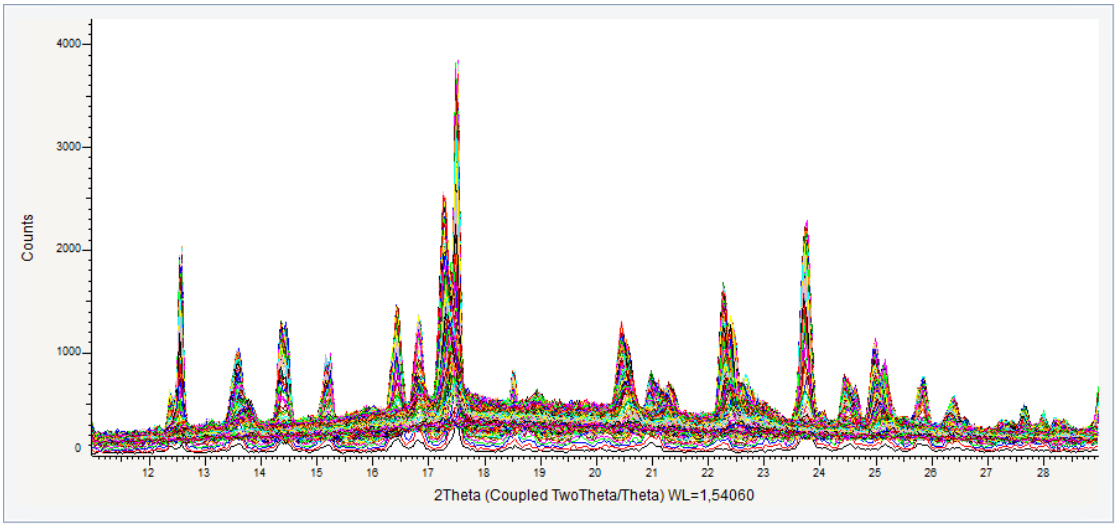


Figure 23.2: DTA-300LC-Scans_50-220C.BRML file imported in the graphical view

23.2 Step 2: Creating and Working with the Side View

1. Click the **Waterfall Display** button on the 1D View toolbar
   — or —
   select the **Waterfall display** check box in the View property panel.
   ➨ The scans will be displayed as a waterfall.

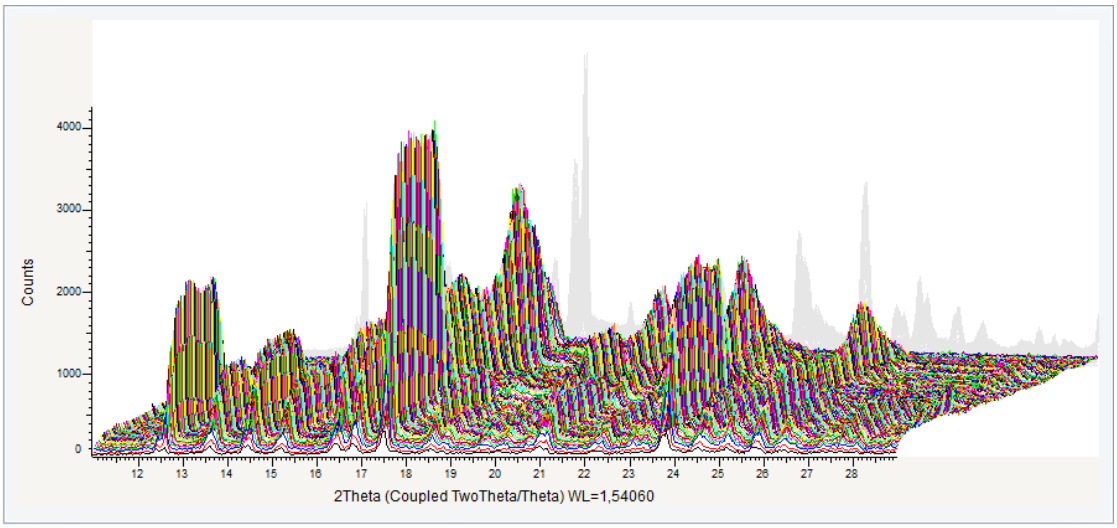


Figure 23.3: Waterfall display

2. Click the **Side View Display** button on the 1D View toolbar
   — or —
   select the **Side View Display** check box in the View property panel.
   ➨ The side view will be displayed at the right of the waterfall view.

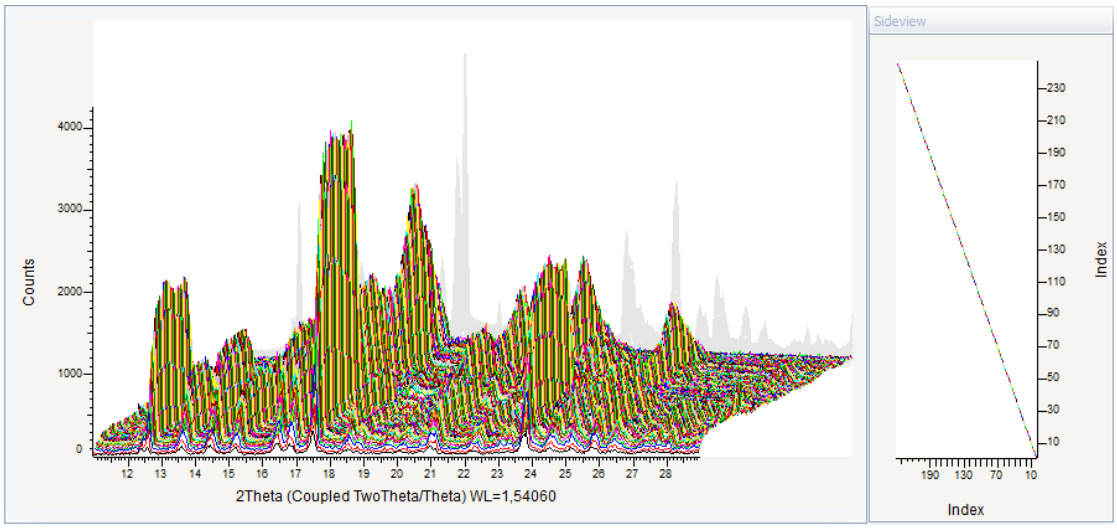


Figure 23.4: Side view added to the waterfall display

Modify the Side view axes in the View property panel and highlight selected scans.

1. In the **Side View X-Axis** drop-down list, select *Temp. Diff*.
2. In the **Side View Y-Axis** drop-down list, select *Temperature.*

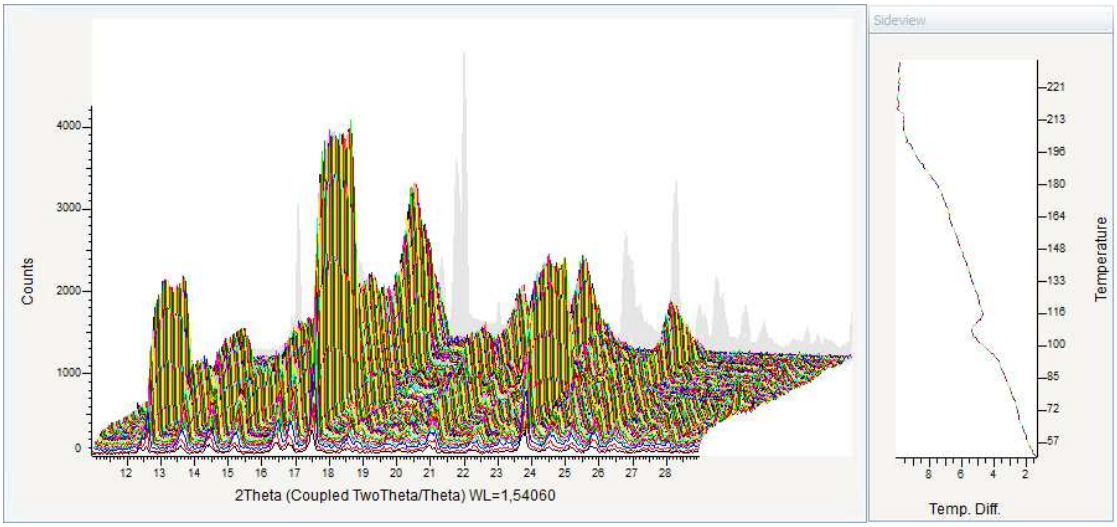


Figure 23.5: Side view with modified axes

3. Select scan #60 to #100 in the Data tree.
4. In the Scan property panel, modify the **Side View Line Thickness** property: enter 4.
   ➨ Selected scans will be highlighted in the Side view.

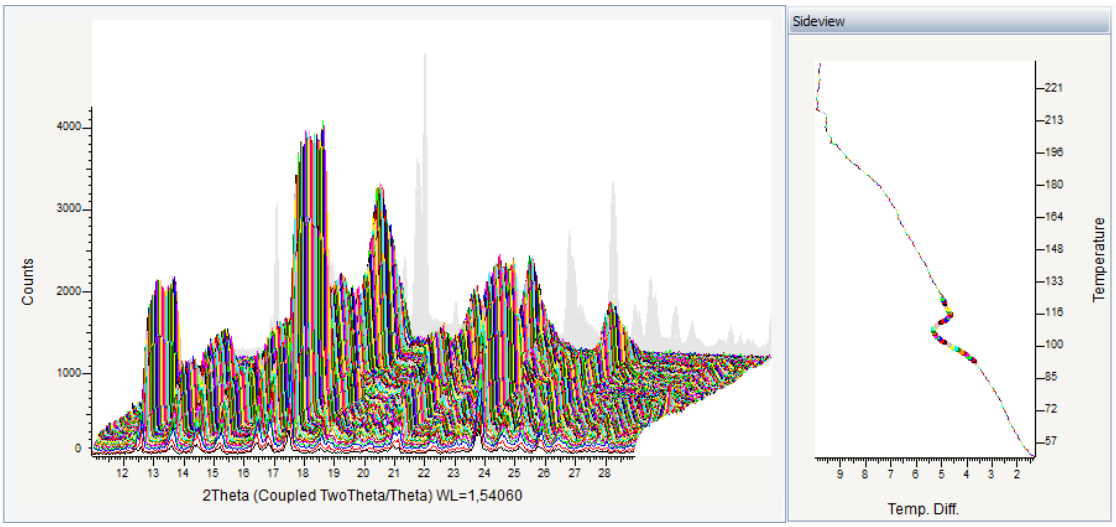


Figure 23.6: Selected scans highlighted in the Side view

23.3 Step 3: Saving

1. Click **Save As** on the **File** menu.
   - ➨ The **Save EVA File As** dialog box will be displayed.
2. Select the appropriate disc drive and directory.
3. Type in the file name. (To overwrite an **.EVA** file, use the same name).
4. Click **Save**.

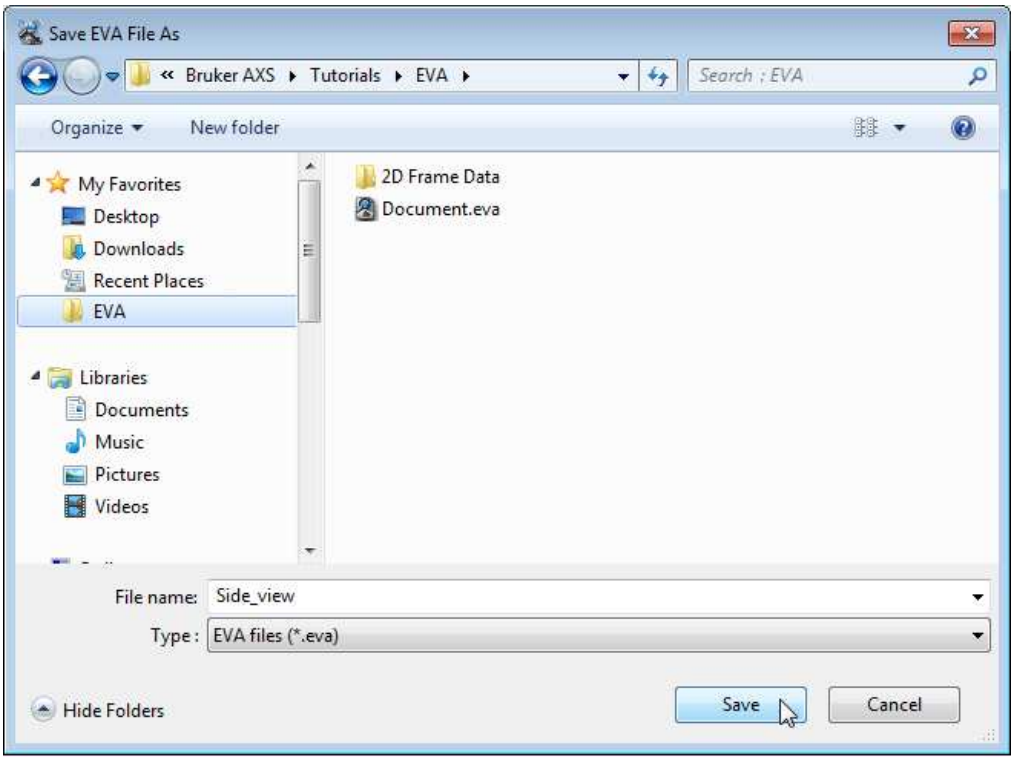


Figure 23.7: Saving Side_view.EVA document

24 Sorting a Multi-range Scan by Temperature in a 2D View

The following procedure describes how to sort scans by temperature from a non-ambient measurement in a 2D view.

The scan used is held as a tutorial file, Guil4.RAW, found in the Tutorial directory.

Steps

1. Creating a new EVA document and importing Guil4.RAW.
2. Creating the 2D view with levels.
3. Sorting the scans on the Y-axis by temperature.
4. Saving the EVA document containing the scan.

24.1 Step 1: Creating a New EVA Document and Importing Guil4.RAW

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   - ➨ The EVA document is empty.

2. Click the **Import from files** data command or the **Import from files** button.
   - ➨ The **Import From Files** dialog box will be displayed.
3. Search the Tutorials/EVA* directory and select the Guil4.RAW file.
4. Click **Open**.
   - ➨ The scan Guil4 will be added to the Data tree and displayed in the graphical view of the EVA document.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

Figure 24.1: Importing Guil4.raw

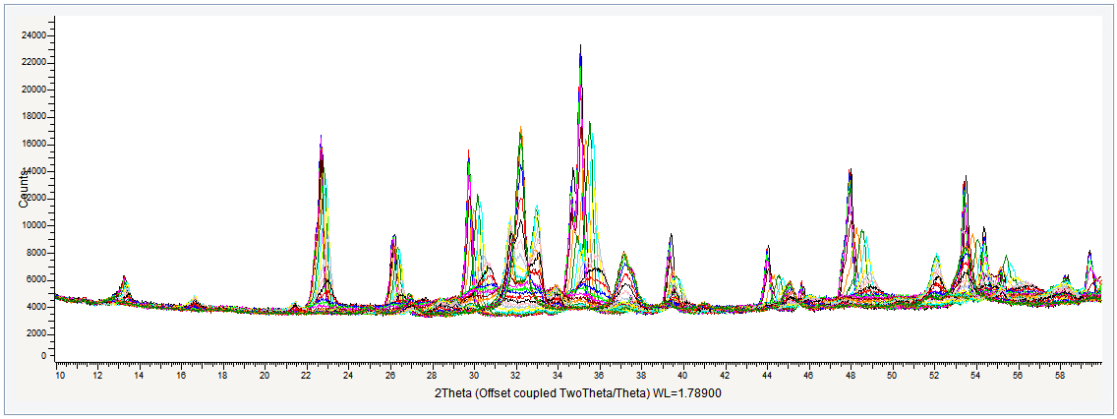
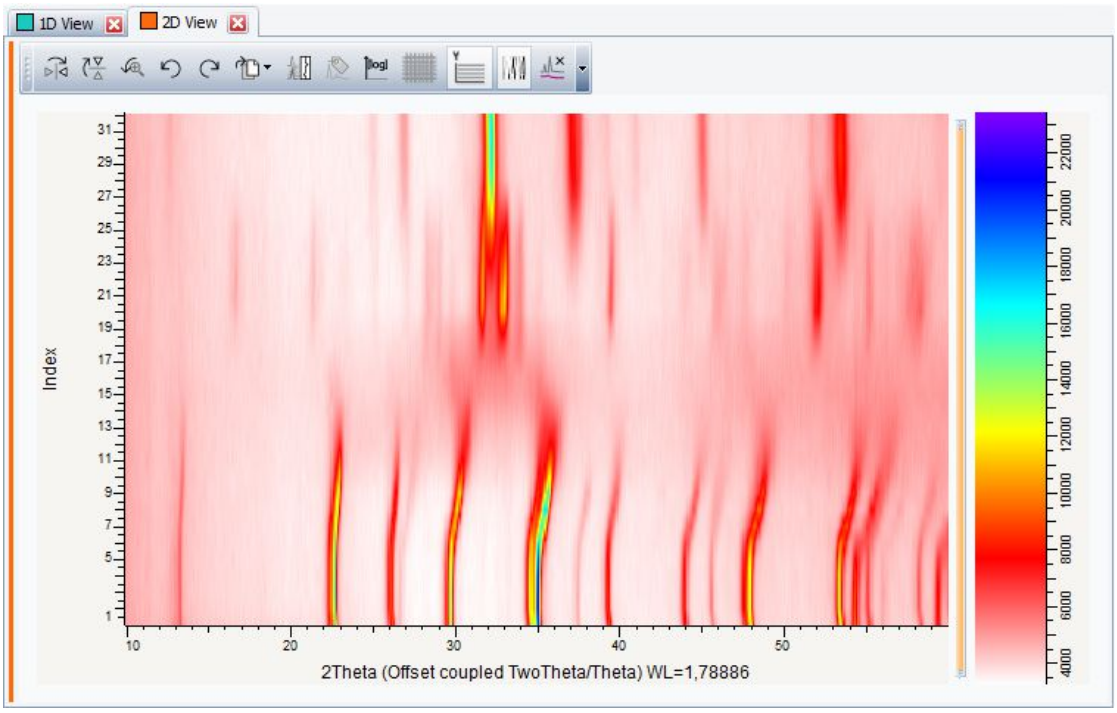


Figure 24.2: Guil4.RAW file imported in the graphical view

24.2 Step 2: Creating the 2D View with Levels

1. Make certain the list of scans is selected. If not, select it in the data tree.
2. Click **2D View** in the Create list of the Data Command panel
   — or —
   click the **2D View** button on the Create View toolbar
   — or —
   right-click the scan list in the data tree to display the context menu. Click **Create** and then **2D View** on the related submenu.
   ➨ The 2D View will be displayed in a new tab.



3. Click **Create Level** in the Tool list of the Data Command panel
   — or —
   right-click the scan list in the data tree to display the context menu. Click **Tool** and then **Create Level** on the related submenu.
   ➨ The Create Level Theta dialog box will be displayed. By default 5 automatic levels will be created.

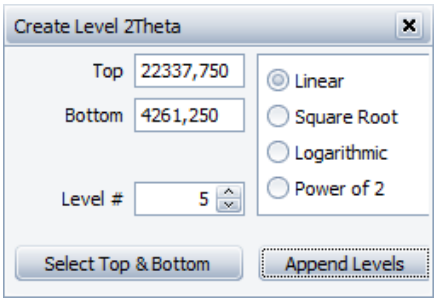


Figure 24.3: Creating levels: Create Level dialog box

4. Click the **Append Levels** button and close the dialog box
   ➨ The levels will be added to the data tree and displayed in the graphical view. The Intensity map and the Levels are displayed by default. Leave the **Intensity map** and the **Levels** check boxes selected.

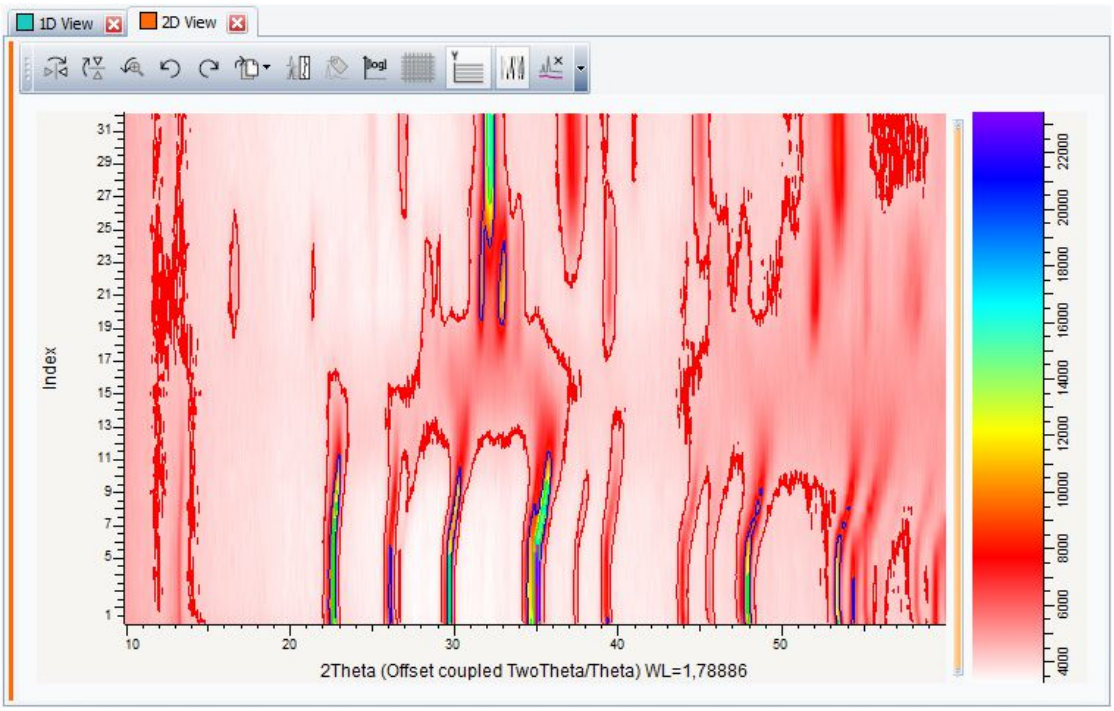


Figure 24.4: 2D view with intensity map and levels, scans sorted by index on the Y-axis

24.3 Step 3: Sorting the Scans on the Y-Axis by Temperature

1. In the 2D View Property table, select {**SORT}** for the Left (Axis) property if necessary.
2. In the 2D View Property table, select **Temperature** in the Y-axis drop-down list.

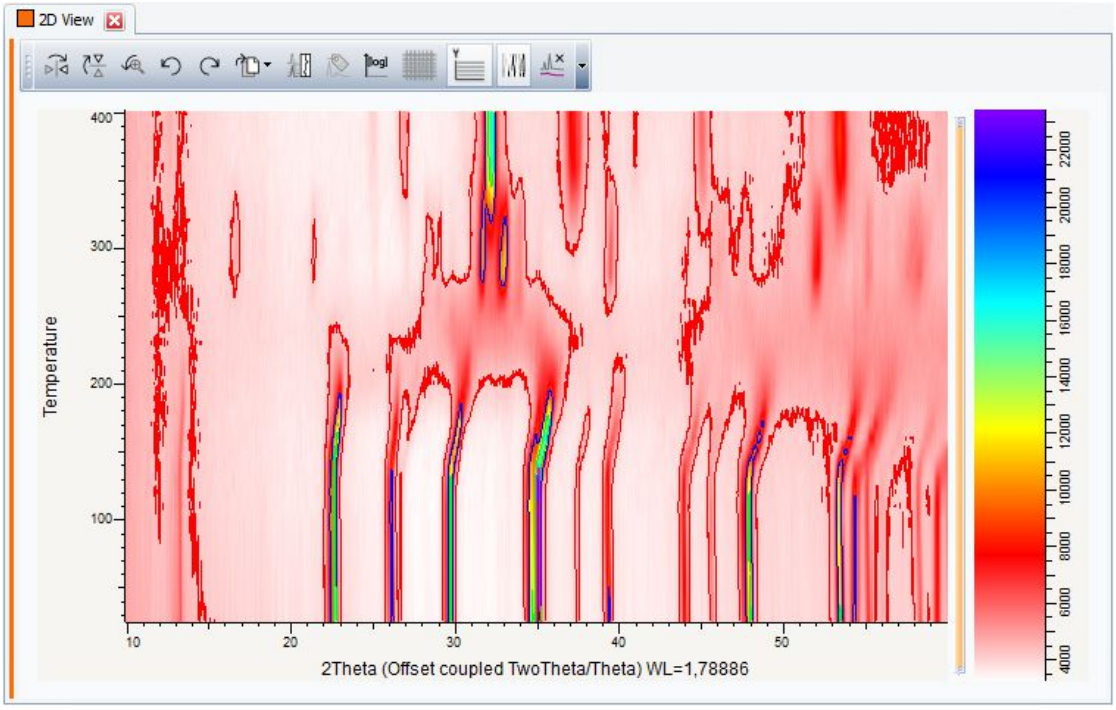


Figure 24.5: 2D view with intensity map and levels - scans sorted by temperature on the Y-axis

24.4 Step 4: Saving

1. Click **Save As** on the **File** menu.
   ➨ The **Save EVA File As** dialog box will be displayed.
2. Select the appropriate disc drive and directory.
3. Type in the file name. (To overwrite an **.EVA** file, use the same name).
4. Click **Save**.

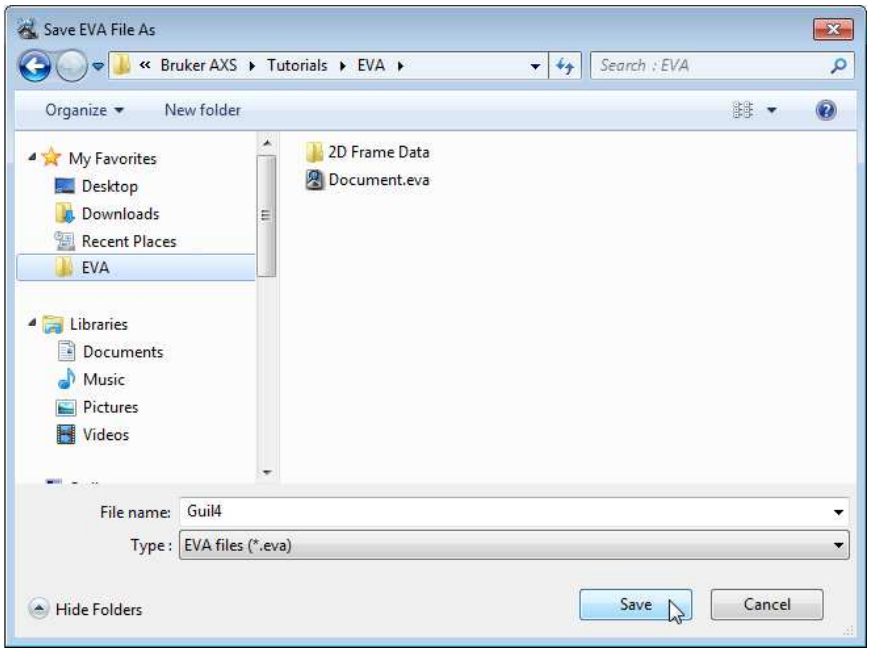


Figure 24.6: Saving Guil4.EVA document

25 Working with the PIP and VIP Views

The following procedure describes how to create and manage PIP and VIP views.
The scan used is held as a tutorial file, m1.RAW, found in the Tutorial directory.
Steps:

1. Creating a new EVA document and importing m1.RAW.
2. Creating and managing the PIP and VIP views.
3. Saving the EVA document containing the scan.

25.1 Step 1: Creating a New EVA Document and Importing m1.RAW

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   - ➨ The EVA document is empty.

2. Click the **Import from files** data command or the **Import from files** button.
   - ➨ The **Import From Files** dialog box will be displayed.
3. Search the **Tutorials/EVA*** directory and select the **m1.RAW file**.
4. Click **Open**.
   - ➨ The scan **m1** will be displayed in the graphical view of the EVA document.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

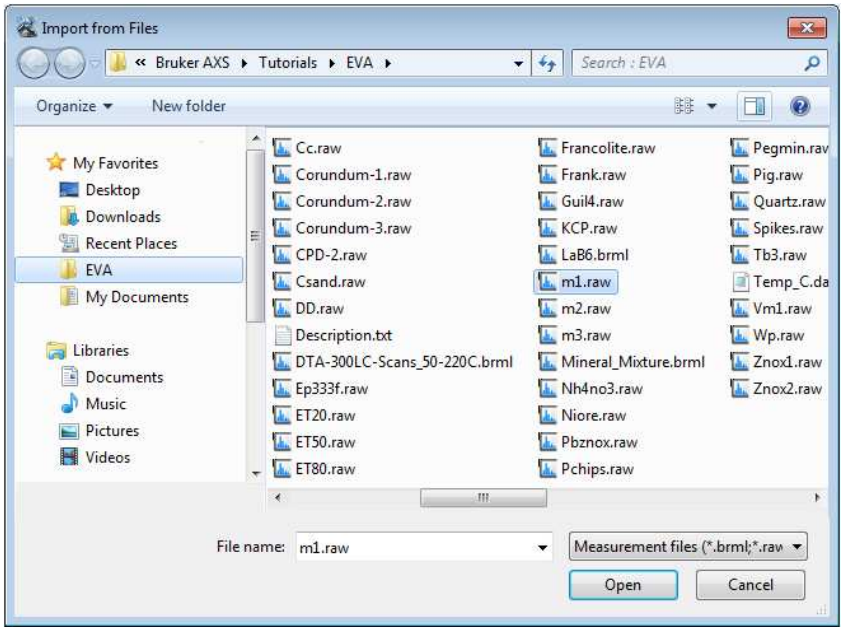


Figure 25.1: Importing the m1.RAW file

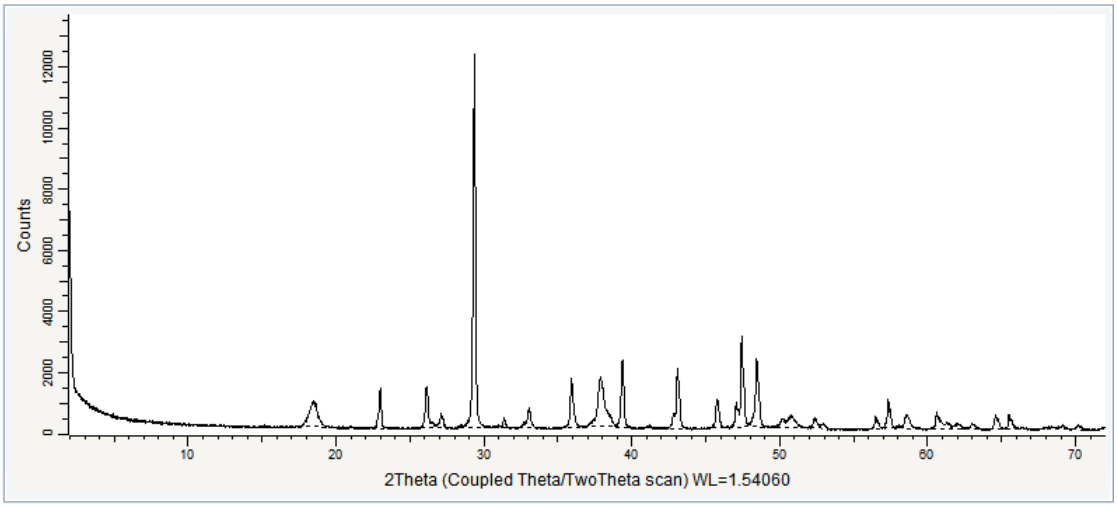


Figure 25.2: m1.RAW file imported in the Graphical view

25.2 Step 2: Creating and working with the PIP and VIP views.

Case #1: Creating a PIP view

1. Click the **PIP mode** button on the view toolbar
   — or —
   right-click anywhere in the graphical view to display the context menu. In the context menu, click the **PIP Mode** command.
   ➡ A **PIP** text box will be added below the pointer.
2. Select the zone around the peak between the 2θ angles 22° and 24°.
   ➡ A window corresponding to the selected zone is created.

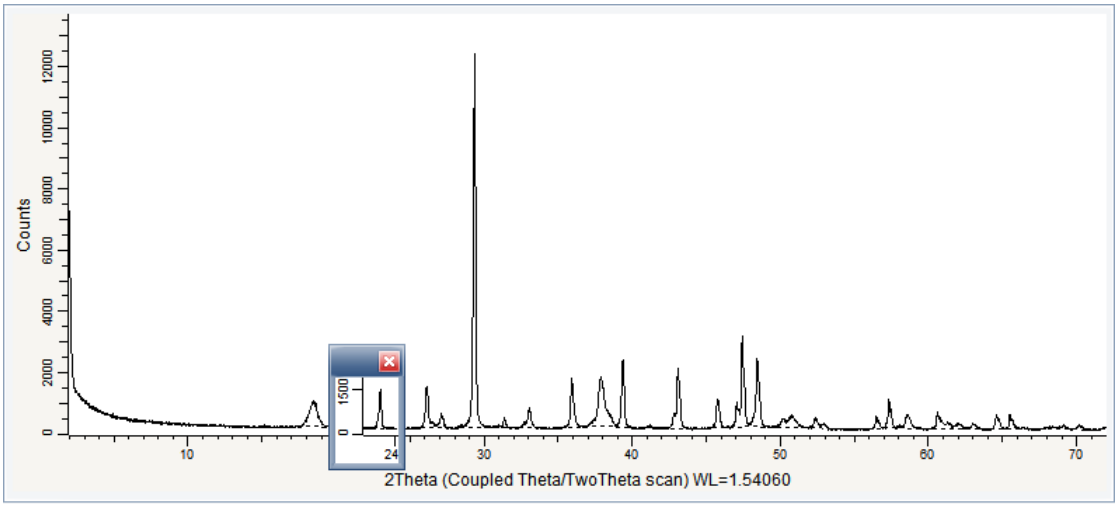


Figure 25.3: Creating a PIP view

3. Move and resize the window to have a better view of the peak.

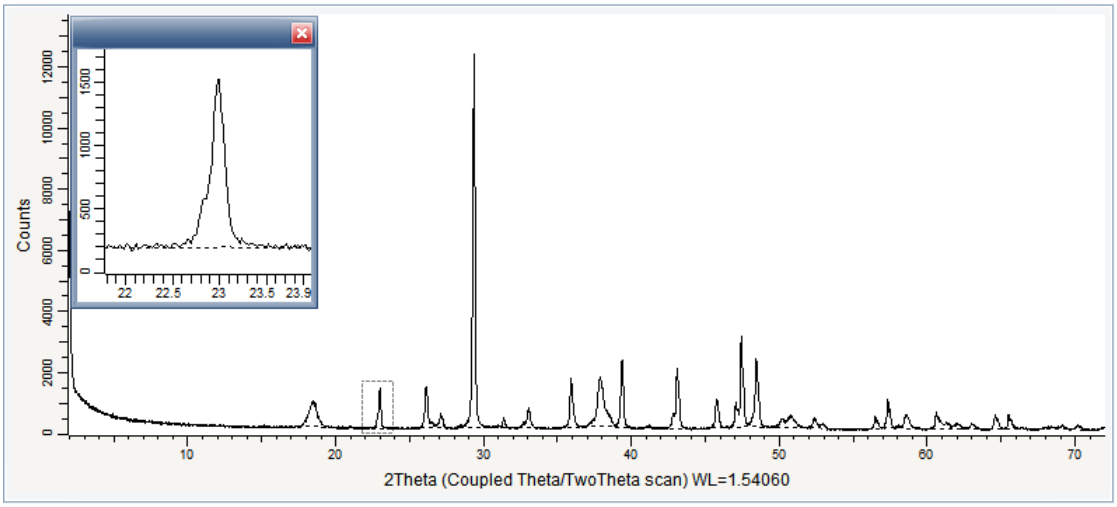


Figure 25.4: Moving and resizing the PIP view

4. Once you are satisfied with the PIP view, click anywhere in the graphical view.
   ➡ The PIP view is inserted in the graphical view and is linked to the corresponding zone in the scan.

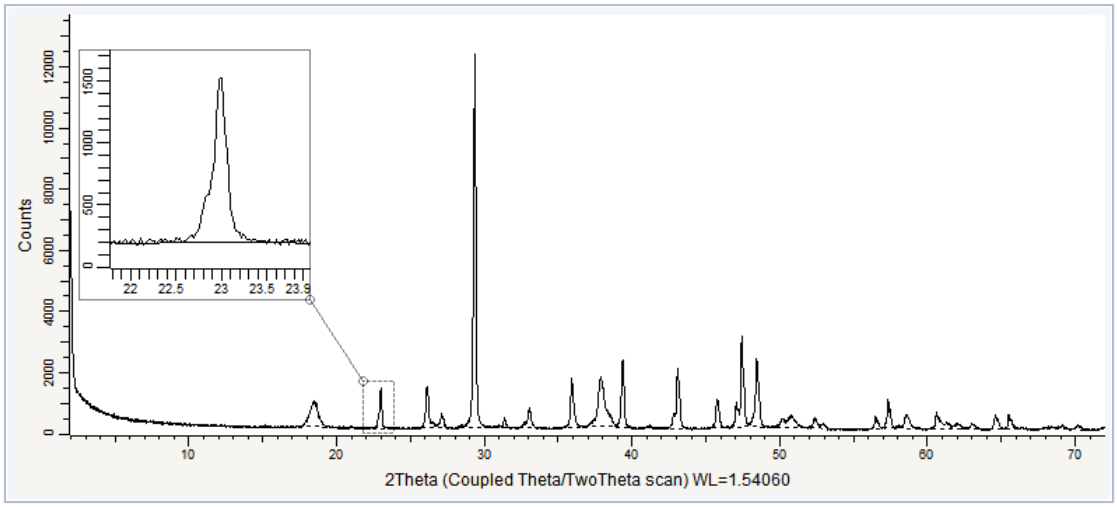


Figure 25.5: PIP view inserted and linked to the original zone

Case #2: Creating a VIP view

1. Zoom in on the zone between the 2θ angles 37° and 47°.
2. Click the **VIP mode** button on the view toolbar
   — or —
   right-click anywhere in the graphical view to display the context menu. In the context menu, click the **VIP Mode** command.
   ➡ A **VIP** text box will be added below the pointer.
3. Select the zone between the 2θ angles 40.5° and 41.5.°
   ➡ The VIP view editor is displayed.

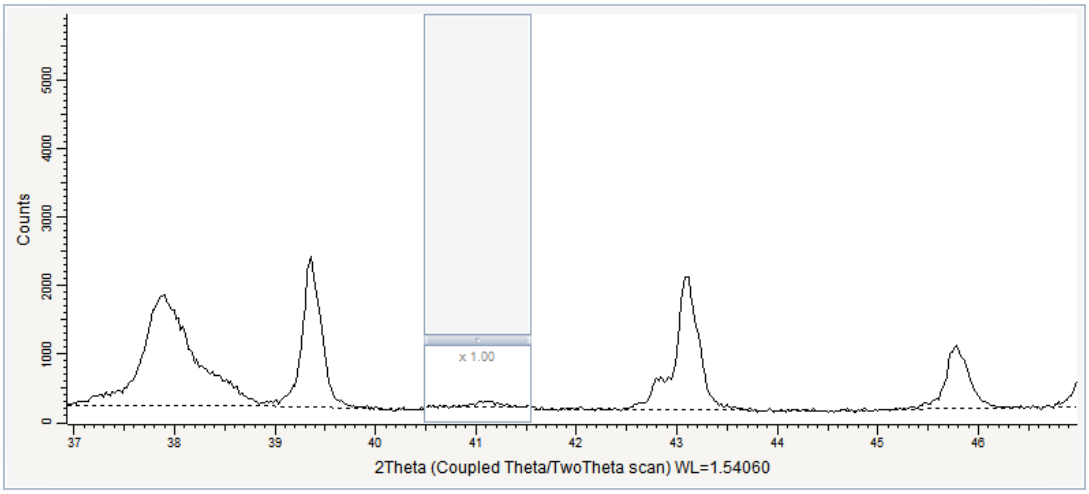


Figure 25.6: Creating a VIP view

4. Move the scale bar to increase the scale factor until 4.00 for example.

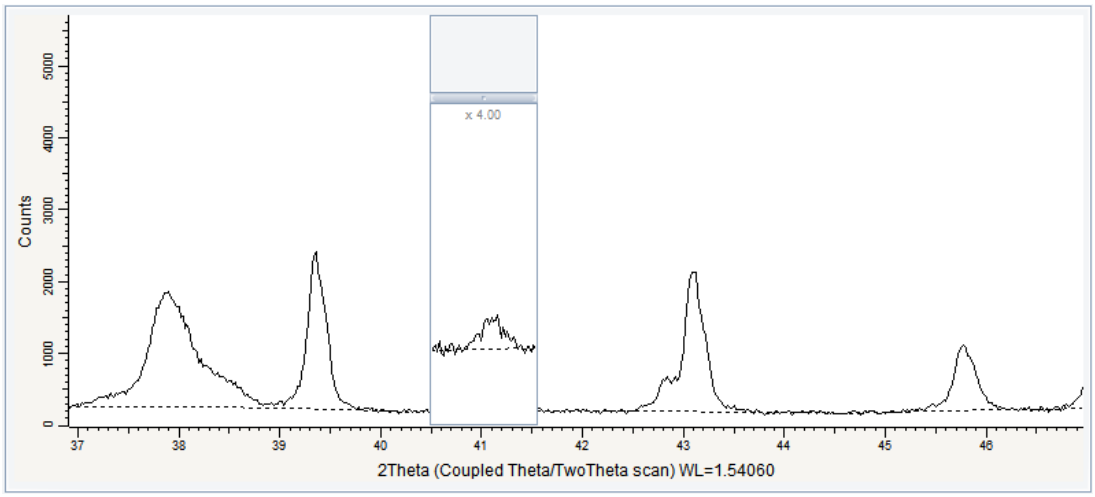


Figure 25.7: Changing the scale

5. To insert the VIP view in the document, click anywhere in the graphical view.

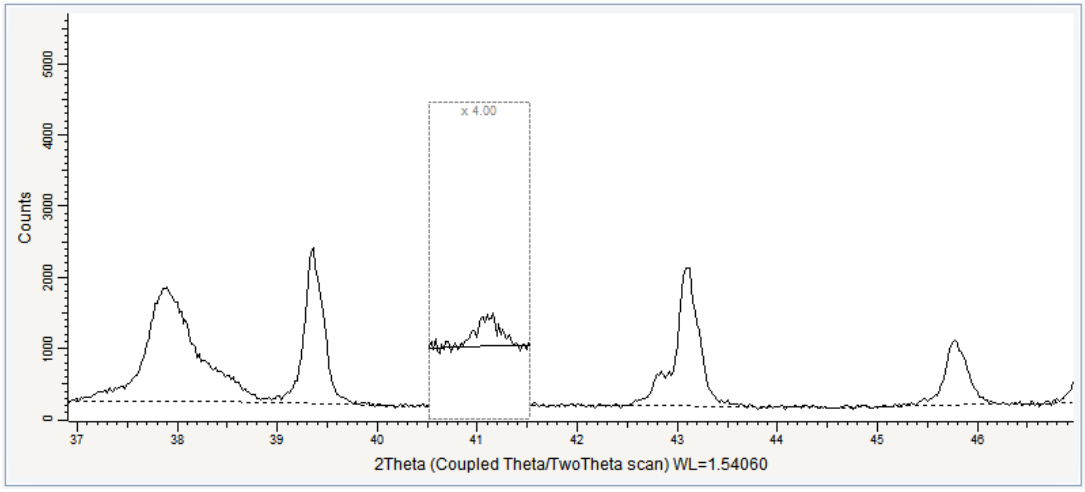


Figure 25.8: VIP view inserted in the graphical view

The VIP view can be modified by right-clicking anywhere in the graphical view and then clicking **VIP mode** on the context menu and then **Edit**.

26 Creating a Label from a Peak

Peaks can be used to create labels.

To do so:

1. Right-click a scan at the position you want to input a label (peak) to display the context menu.
2. Click **Create Peak at 2Th=…**
   ➨ The peak is displayed in the graphical view and added to the peak list in the data tree.

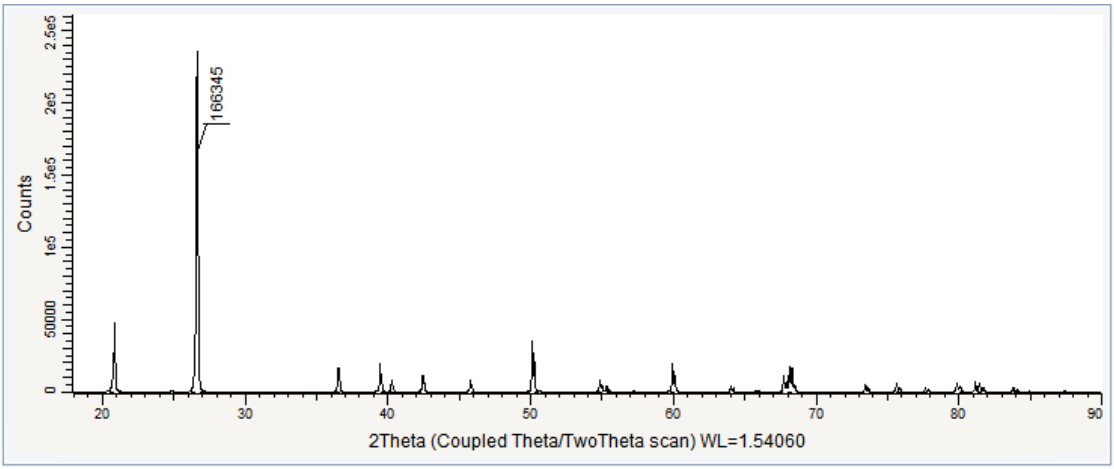


Figure 26.1: Peak inserted manually in the graphical view

3. Select the peak in the data tree if necessary.
4. In the Peak Property table, select the **Anchor lock** check box to be able to move the anchor and text position freely. Press the **Control** key and point to the scan to change the pointer into a hand. Move the hand to drag the anchor and the text. Clear the **Anchor lock** check box and proceed the same way to move the text position only.

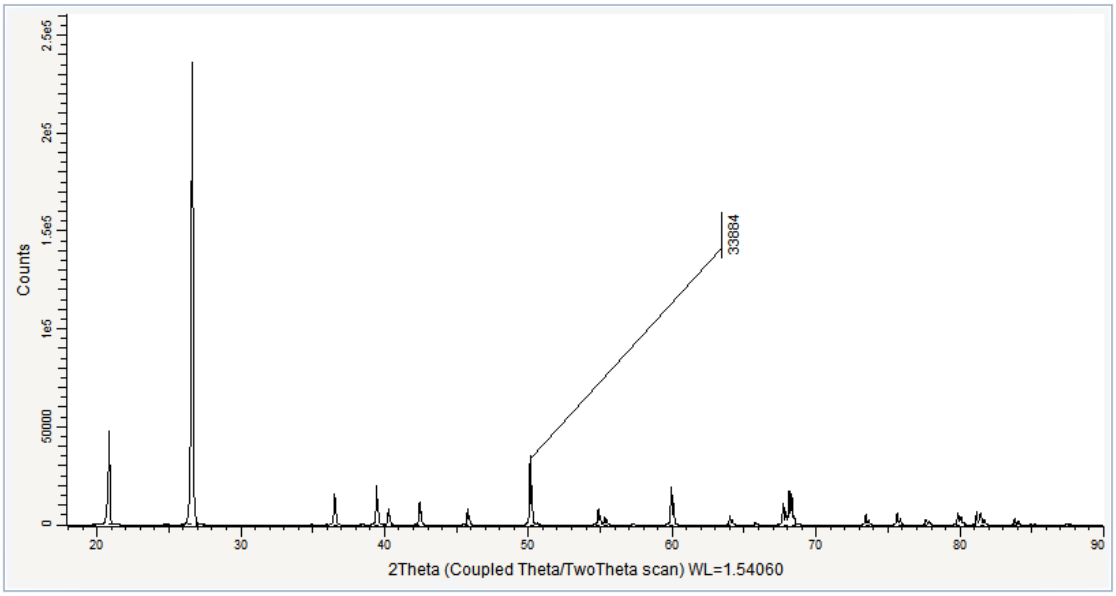


Figure 26.2: Anchor and text position changed

5. Clear the **Caption** text field and enter the desired text.

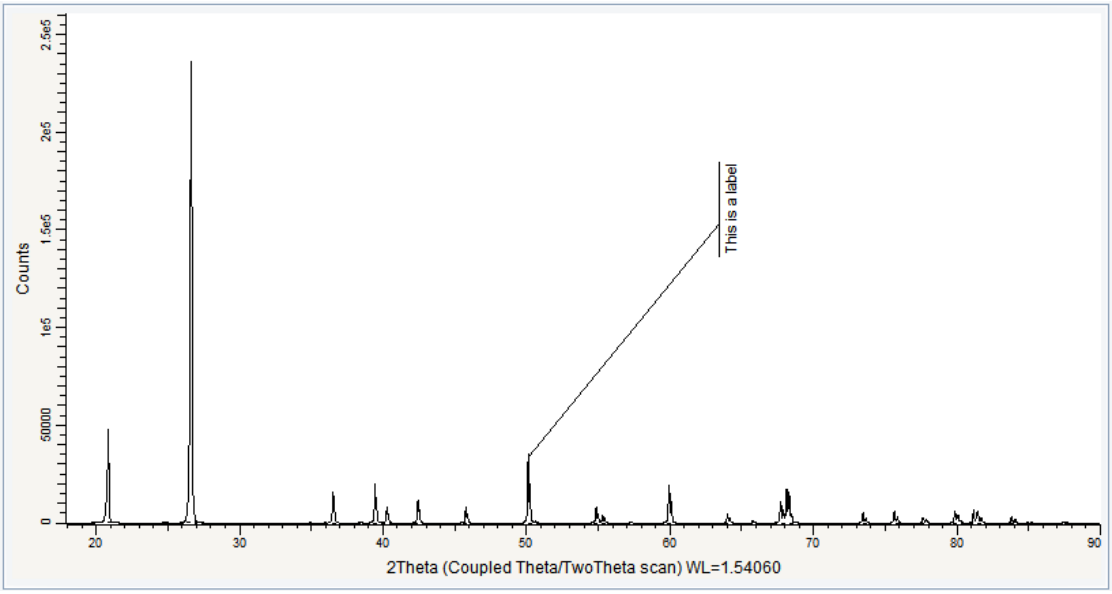


Figure 26.3: Anchor and text position changed

Customize the resulting “label” if necessary:

1. The peak color can be changed: in the Peak property table, select the desired color in the **Color** drop-down list. (Blue in the example).
2. The background and text color can be changed: in the Peak property table, select the desired color in the **Background Color and Text Color** drop-down lists (Light gray and Dark violet in the example).
3. The font size can be changed: in the Peak property table, enter the desired font size (in points) in the **Font Size** field (10 points in the example).
4. The text rotation can be changed: in the Peak property table, enter desired the angle value in degrees in the **Text rotation** field (0° in the example).
5. The text margin can be changed: in the Peak property table, enter the desired text margin (in points) in the **Text margin** field (2 points in the example).
6. The anchor can be removed or its style changed: in the Peak property table, select **None** or another anchor style in the **Anchor Style** drop-down list (Rectangle in the example).

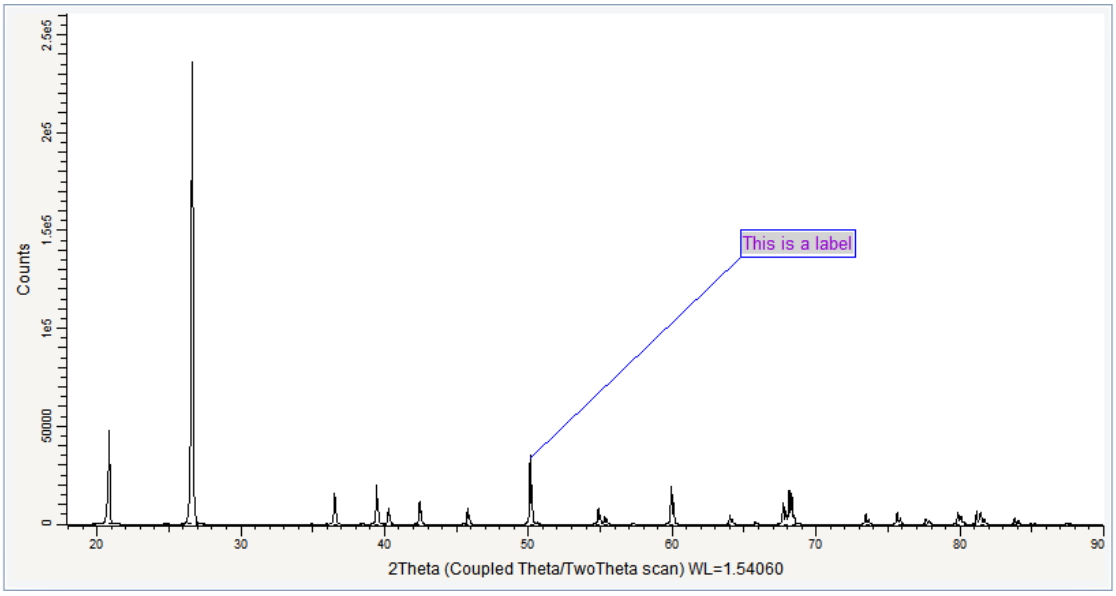


Figure 26.4: Label customized according to the procedure previously described

27 Loading and Integrating Mergeable 2D Frames

The following procedure describes how to create an integrated scan from a set of frames which have been measured with different 2-theta angles to form a diagram like a Debye-Scherrer image.

The measurement used is stored as a tutorial file, Cor standard.brml, found in the Tutorial\2D Frame Data directory.

Steps

1. Creating a new EVA document and importing Cor standard.brml.
2. Selecting the integration cursor and drawing the integration area.
3. Displaying the Cursors Preview tool and integrate.

27.1 Step 1: Creating a New EVA Document and Importing the 2D Frames

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   - ➨ The EVA document is empty.

2. Click the **Import from files** data command or the **Import from files** button.
   - ➨ The **Import From Files** dialog box will be displayed.
3. Search the Tutorials\EVA* directory and select the Cor standard.brml file in the 2D Frame Data sub-directory.
4. Click **Open**.
   - ➨ The frames which were measured will be displayed in the frame view of the EVA document. A **Mergeable Frame List** will appear in the tree.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

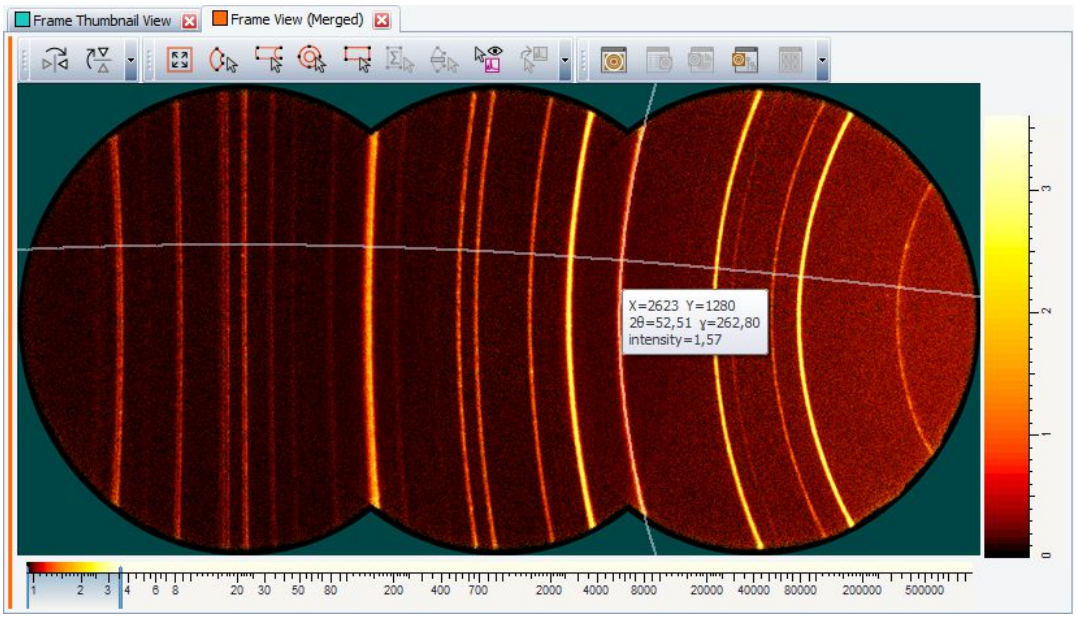


Figure 27.1: 2D Frame View after loading a measurement with three mergeable frames

27.2 Step 2: Selecting the Integration Cursor and Drawing the Integration Area

1. Click the **Slice Cursor** button on the Frame Integration toolbar.
2. Click with the left mouse button in the top left of the area which is to be integrated.
3. Drag the mouse to the bottom right until the desired integration area has been displayed. Release the left mouse button.
   - ➨ The cursor will be added as child to the frame list node in the tree.
4. If necessary, adjust the integration area by clicking and dragging the handles of the cursor.

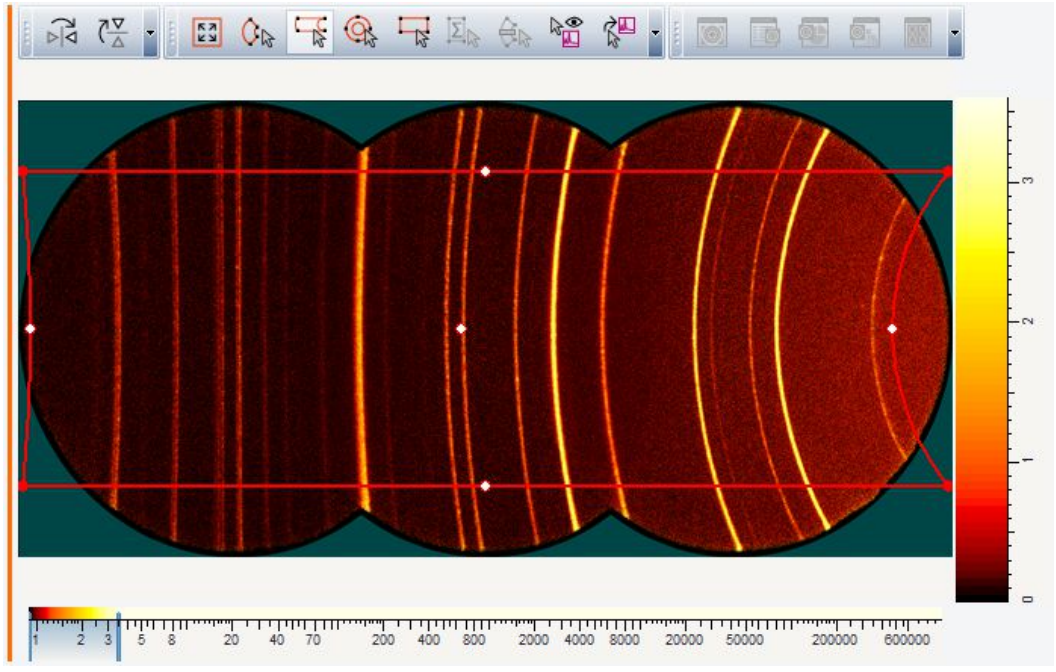
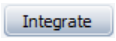


Figure 27.2: Slice Cursor prepared for the subsequent integration

27.3 Step 3: Displaying the Cursors Preview Tool and Integration

1. Click the **Cursors Preview** button on the Frame Integration toolbar
   — or —
   click the **Cursors Preview** command in the command bar or the context menu of the slice cursor.



2. IIf the preview is satisfactory, click on the **Integrate** button to create the final integrated scan.
   ➨ The scan is created in a separate scan list.

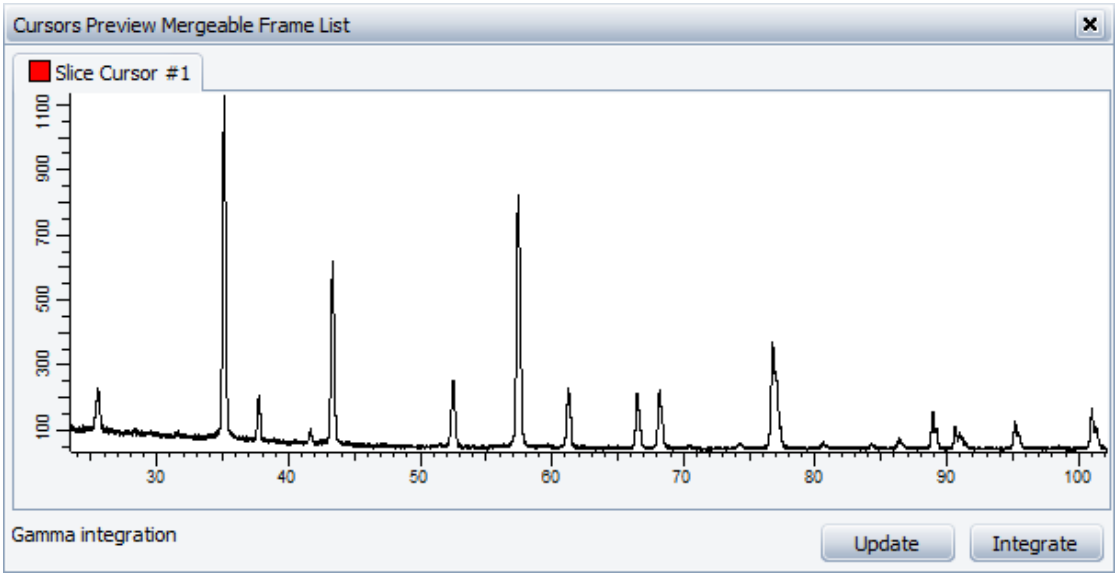


Figure 27.3: The Cursors Preview Tool with the preview of the integration result

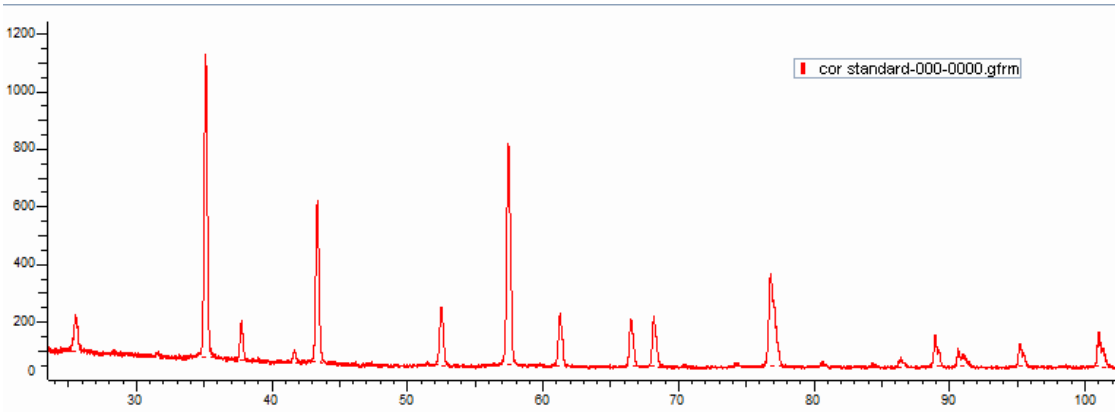


Figure 27.4: The resulting integrated scan

28 Loading and Integrating Stackable 2D Frames

The following procedure describes how to create an integrated scan from a set of frames which were measured with the same 2-theta angle and different theta angles to form a stackable frame list.

The measurement used is stored as a set of tutorial files, HTSR258*.gfrm, found in the Tutorial\2D Frame Data\HTSR258 directory.

Steps

1. Creating a new EVA document and importing the 2D frames.
2. Selecting the integration cursor and drawing the integration area.
3. Displaying the Cursors Preview tool and integrate.

28.1 Step 1: Creating a New EVA Document and Importing the 2D Frames

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   ➨ The EVA document is empty.

2. Click the **Import from files** data command or the **Import from files** button.
   ➨ The **Import From Files** dialog box will be displayed.
3. Search the Tutorials\EVA\2D Frame Data directory* and select all of the “HTSR258*.gfrm” files in the “HTSR258” sub-directory.
4. Click **Open**. The frames will be displayed in the frame view of the EVA document. A **Stackable Frame List** will appear in the tree.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

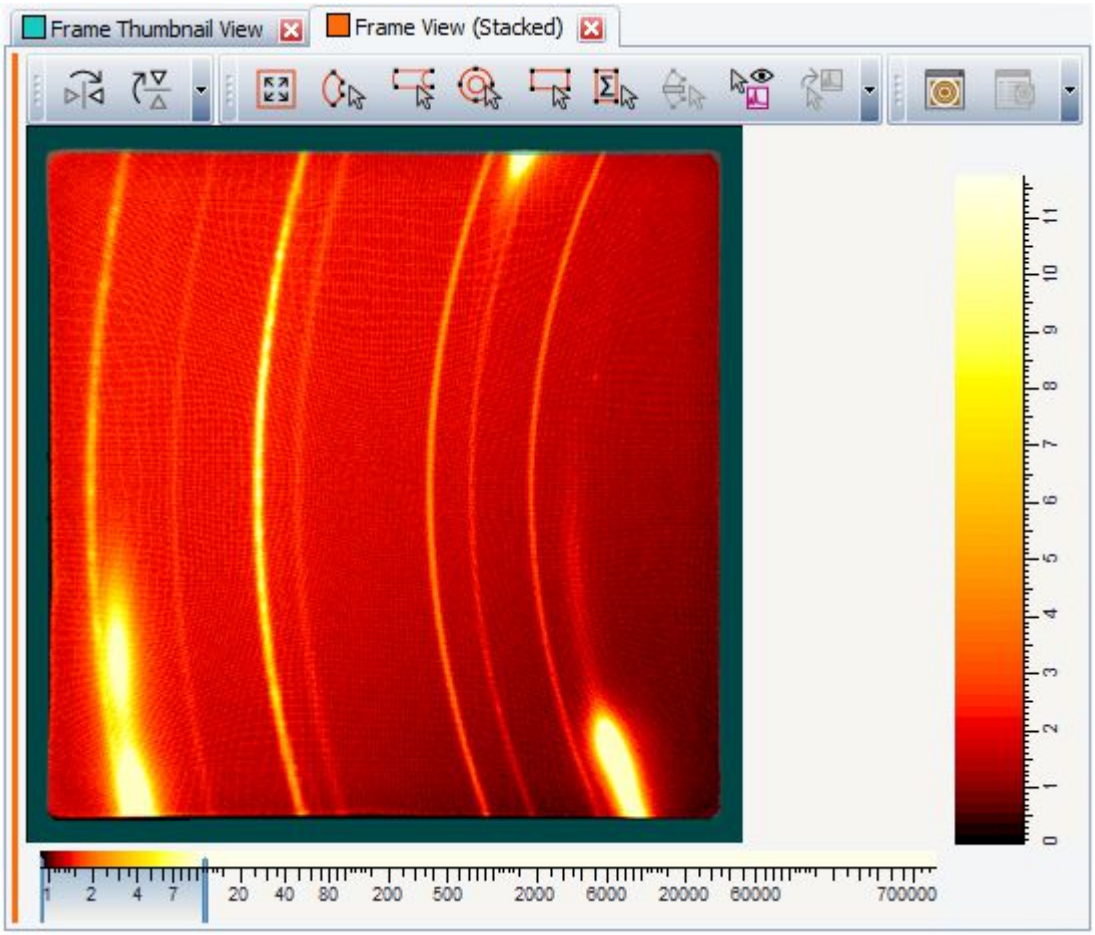


Figure 28.1: 2D Frame View after loading a measurement with stackable frames

28.2 Step 2: Selecting the Integration Cursor and Drawing the Integration Area

1. Click the **Ring Cursor** button on the Frame Integration toolbar.
2. Click with the left mouse button in the left of the area which is to be integrated.
3. Drag the mouse to the right until the desired integration area has been displayed. Release the left mouse button.
   - ➨ The cursor will be added as child to the frame list node in the tree.
4. If necessary, adjust the integration area by clicking and dragging the handles of the cursor.

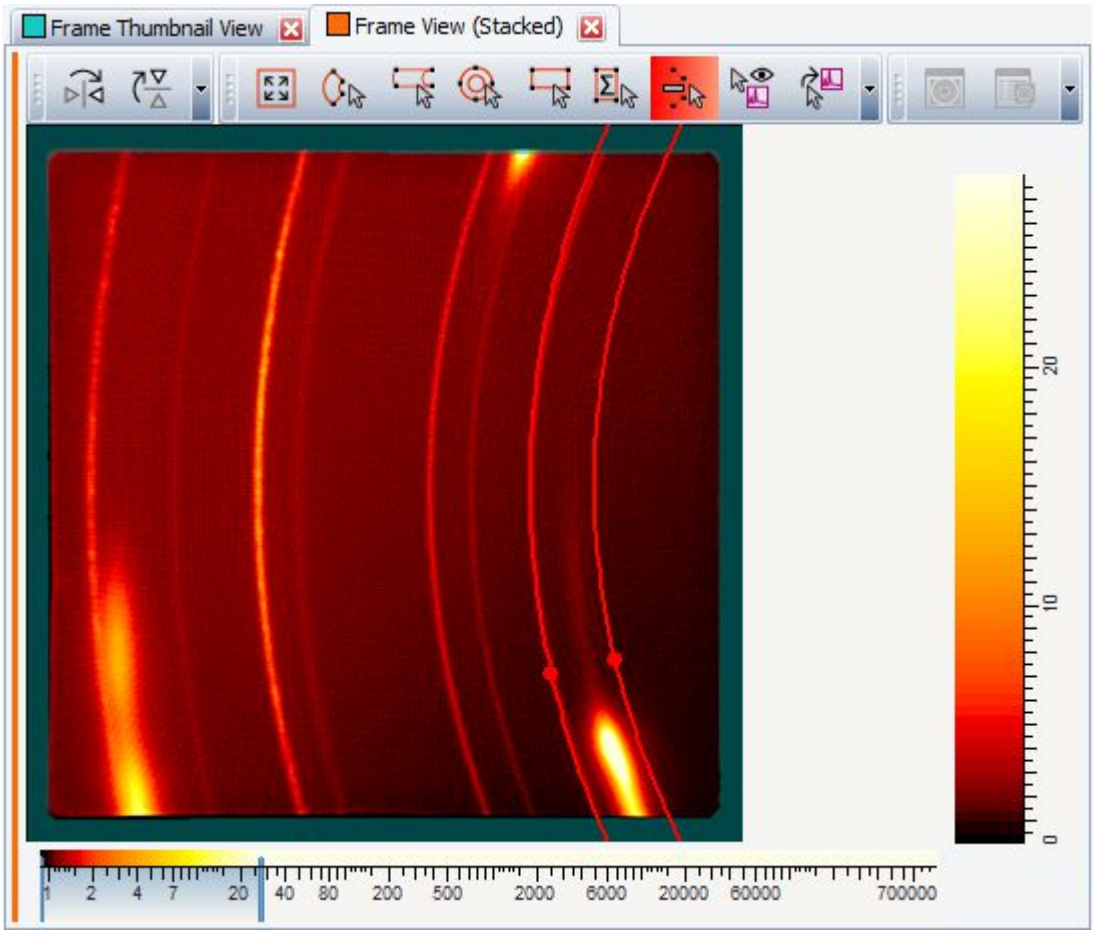
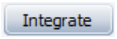


Figure 28.2: Ring Cursor prepared for the subsequent integration

28.3 Step 3: Displaying the Cursors Preview Tool and Integrate

1. Change the direction of the integration in the cursor's properties to **2-Theta integration**. Select **Merge as Single Scan**.

2. Click the **Cursors Preview** button on the Frame Integration toolbar
   — or —
   click on the **Cursors Preview** command in the command bar or the context menu of the cursor.



3. If the preview is satisfactory, click the **Integrate** button to create the final integrated scan. The scan will be created in a separate scan list.

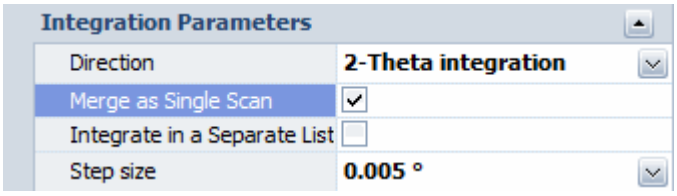


Figure 28.3: The integration parameters of the ring cursor

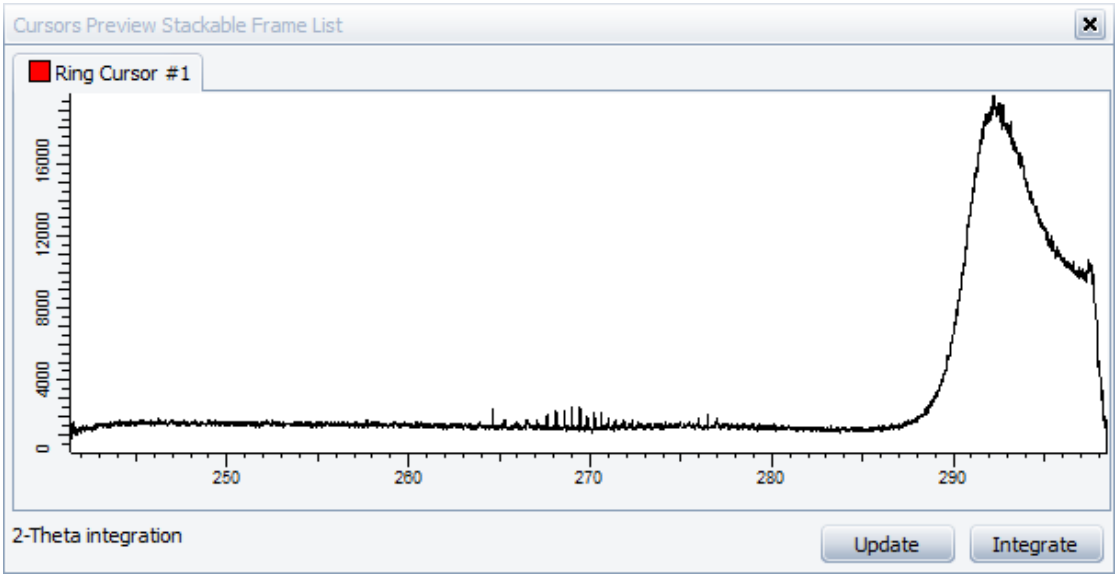


Figure 28.4: The Cursors Preview Tool with the preview of the integration result

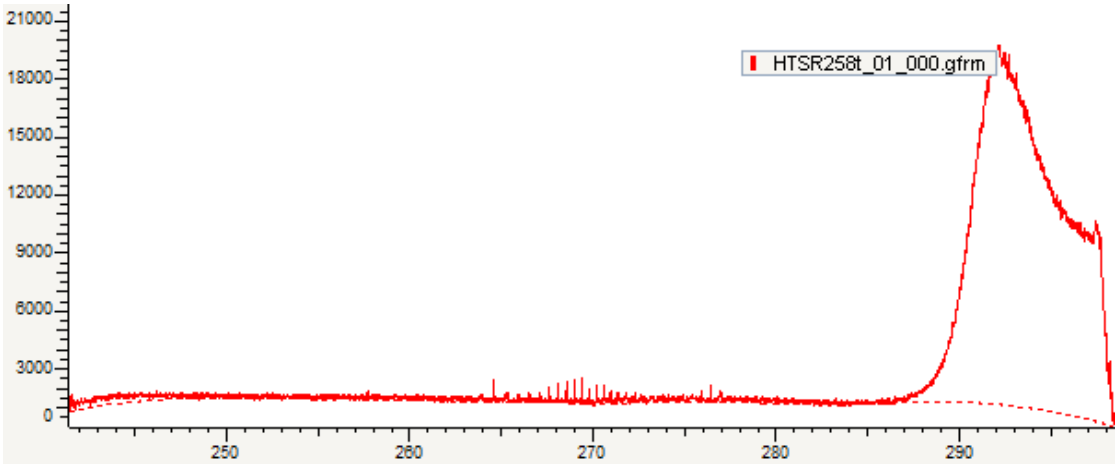


Figure 28.5: The resulting integrated scan

29 Rocking Curve Integration on Stackable 2D Frames

The following procedure describes how to create an integrated scan from a set of frames which have been measured with the same 2-theta angle and different theta angles to form a stackable frame list.

The measurement used is stored as a set of tutorial files, “GM_XRR.gfrm”, found in the Tutorial\2D Frame Data\GM_XRR.gfrm directory.

Steps

1. Creating a new EVA document and importing the 2D frames.
2. Selecting the integration cursor and drawing the integration area.
3. Displaying the Cursors Preview tool and integrate.

29.1 Step 1: Creating a New EVA Document and Importing the 2D Frames

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   ➨ The EVA document is empty.

2. Click the **Import from files** data command or the **Import from files** button.
   ➨ The **Import From Files** dialog box will be displayed.
3. Search the Tutorials\EVA\2D Frame Data directory* and select all of the “GM_XRR*.gfrm” files in the “GM_XRR” sub-directory.
4. Click **Open**.

⇨ The frames will be displayed in the frame view of the EVA document. A **Stackable Frame List** will appear in the tree.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

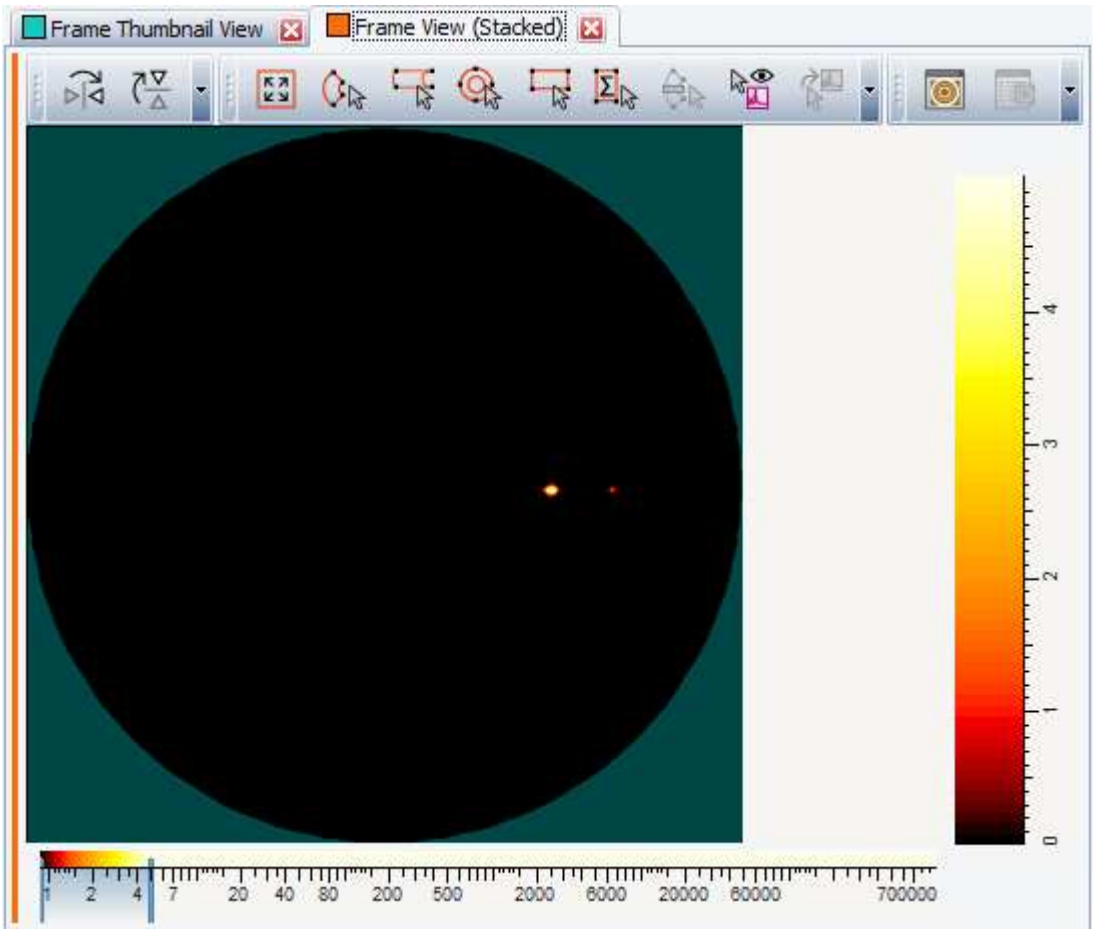


Figure 29.1: 2D Frame View after loading a measurement with stackable frames

29.2 Step 2: Selecting the Integration Cursor and Drawing the Integration Area

1. Zoom into the frame view by clicking and dragging the mouse to make the bright spots clearly visible.
2. Click the **Area Cursor** button on the Frame Integration toolbar.
3. Click with the left mouse button in the top left of the area which is to be integrated.
4. Drag the mouse to the bottom right until the desired integration area has been displayed. Release the left mouse button. The cursor will be added as child to the frame list node in the tree.
5. If necessary, adjust the integration area by clicking and dragging the handles of the cursor.

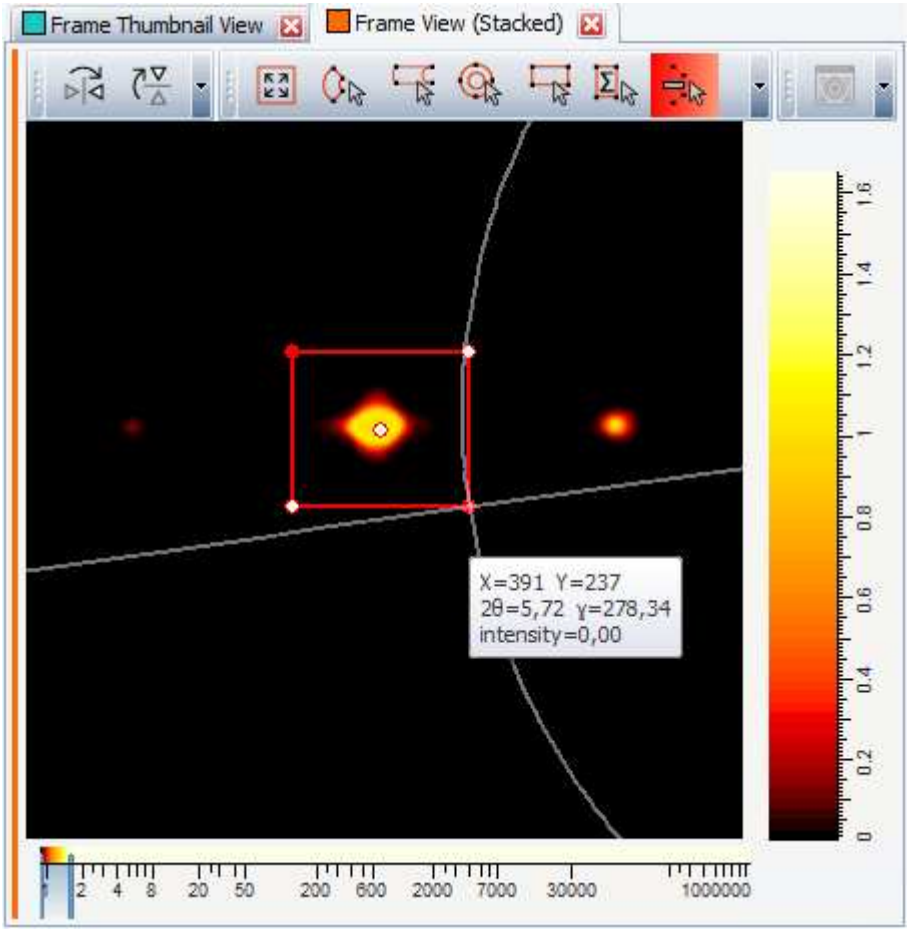
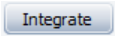


Figure 29.2: Area Cursor prepared for the subsequent integration

29.3 Step 3: Displaying the Cursors Preview Tool and Integrate

1. Change the X-axis of the integration in the cursor's properties to "Theta".

2. Click the **Cursors Preview** button on the Frame Integration toolbar
   — or —
   click the **Cursors Preview** command in the command bar or the context menu of the cursor.



3. If the preview is satisfactory, click the **Integrate** button to create the final integrated scan. The scan will be created in a separate scan list.

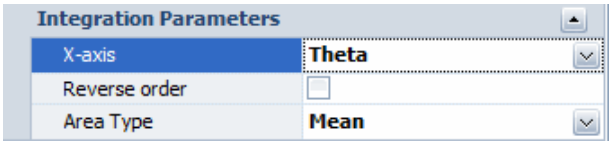


Figure 29.3: The integration parameters of the ring cursor

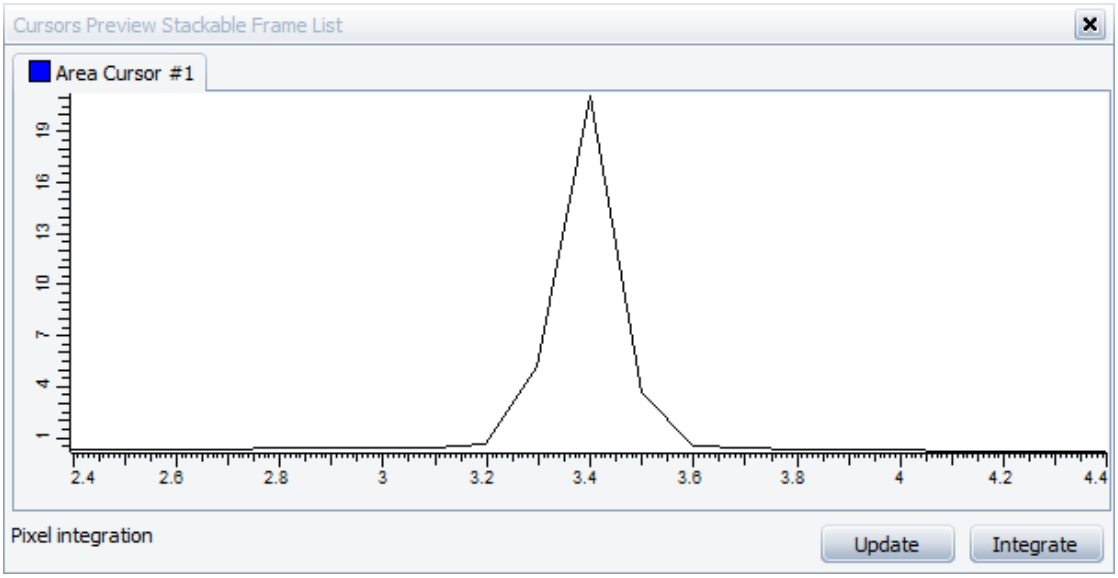


Figure 29.4: The Cursors Preview Tool with the preview of the integration result

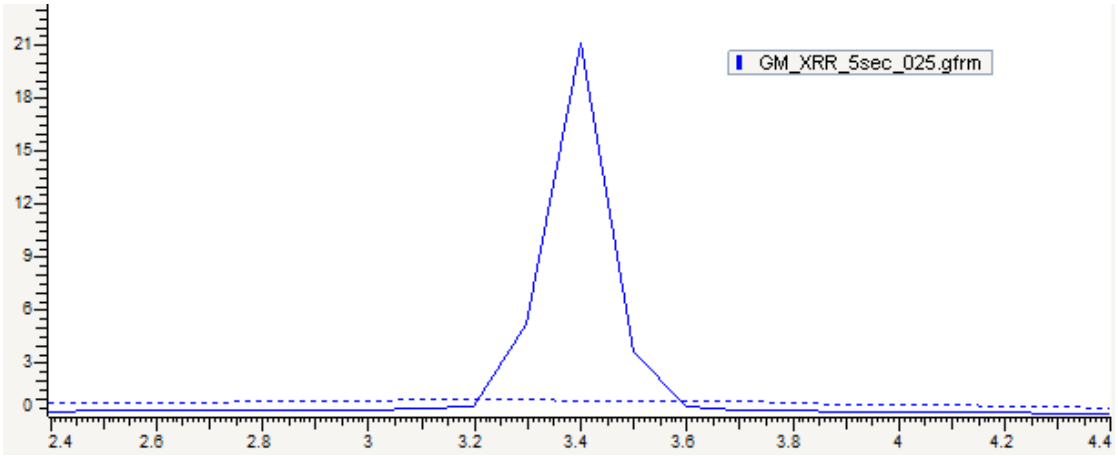


Figure 29.5: The resulting integrated scan

30 Adjusting the Default Mask of a 2D Frame

The following procedure describes how to adjust the default mask on a set of frames which have been measured with different 2-theta angles to form a diagram like a Debye-Scherrer image. Excluding the non-exposed area will lead to a more precise integration result.

The measurement used is stored as a tutorial file, “Cor standard.brml”, found in the “Tutorial\2D Frame Data” directory.

Steps

1. Creating a new EVA document and importing Cor standard.brml.
2. Check the integration with the Full Frame cursor.
3. Changing the default mask to exclude non-exposed areas.
4. Selecting the integration cursor and integrate.

30.1 Step 1: Creating a New EVA Document and Importing the 2D Frames

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   - ➨ The EVA document is empty.

2. Click the **Import from files** data command or the **Import from files** button.
   - ➨ The **Import From Files** dialog box will be displayed.
3. Search the Tutorials\EVA directory* and select the “Cor standard.brml” file in the 2D Frame Data sub-directory.
4. Click **Open**. The frames which have been measured will be displayed in the frame view of the EVA document.
   - ➨ A **Mergeable Frame List** will appear in the tree. The default masks which are part of the frame data will be drawn in green.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

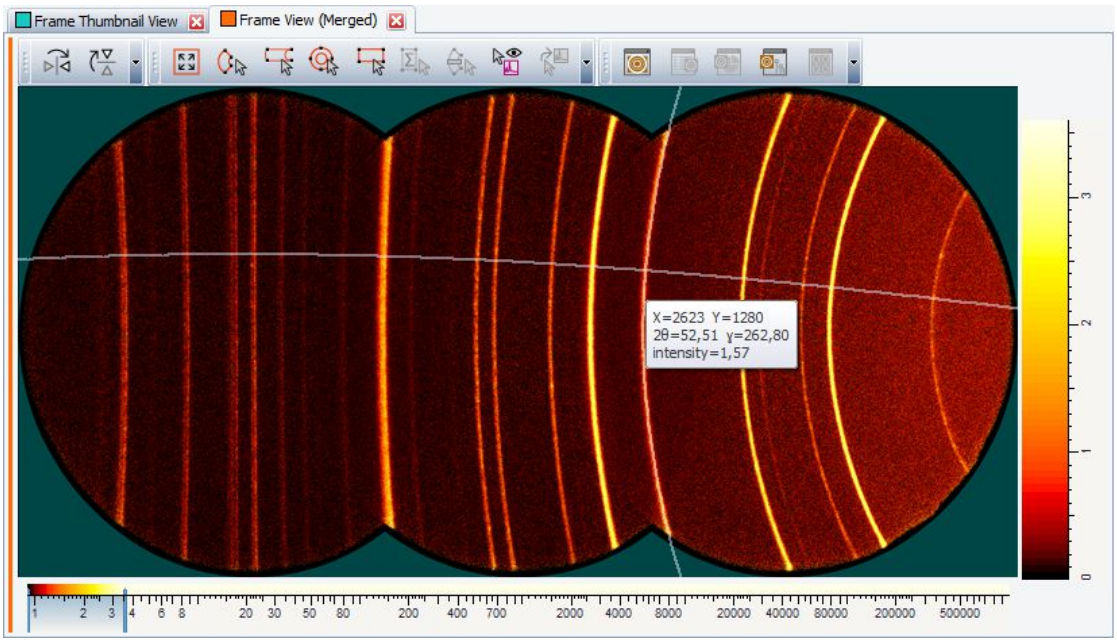


Figure 30.1: 2D Frame View exhibiting non-exposed areas around the frames

30.2 Step 2: Check the Integration with the Full Frame Cursor

1. Click the **Full Frame Cursor** button on the Frame Integration toolbar. The whole merged frame is marked for integration.

2. Click the **Integrate Cursor** button on the Frame Integration toolbar
   — or —
   click the **Integrate Cursor** command in the command bar or the context menu of the cursor.
   ➨ The scan will be created in a separate scan list. A problem is clearly visible at the beginning of the scan where the intensity drops.

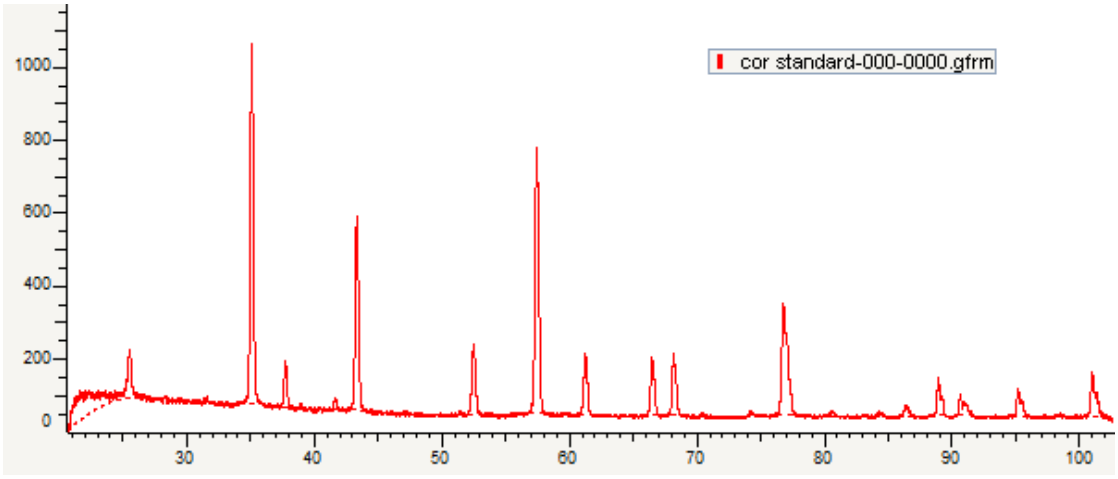
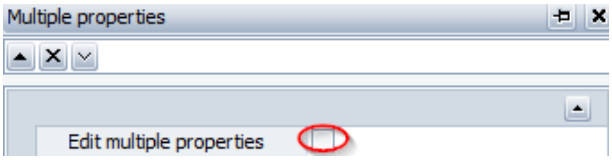


Figure 30.2: Integrated scan with intensity drop at low angles due to mask misalignment

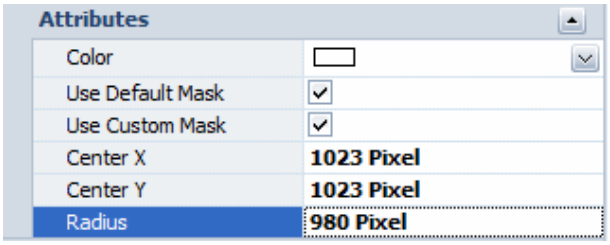
30.3 Step 3: Changing the Default Mask to Exclude Non-Exposed Areas

1. Select the **Edit Multiple Properties** check box to display the combined properties for all three frames.



2. Select the **Use Custom Mask** check box to display the mask properties.

3. Change the Radius to 980 pixel.



➨ The displayed masks change according to the chosen radius. No non-exposed areas remain visible.

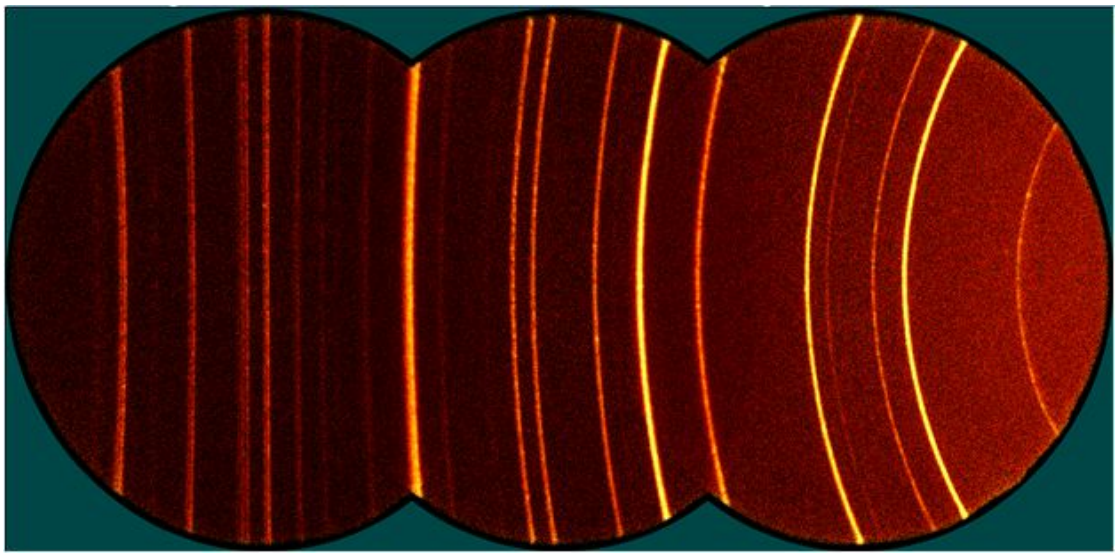


Figure 30.3: 2D Frame View with an adjusted default mask

30.4 Step 4: Selecting the Integration Cursor and Integration

1. Click the **Full Frame Cursor** button on the Frame Integration toolbar. The whole merged frame is marked for integration.

2. Click the **Integrate Cursor** button on the Frame Integration toolbar
   — or —
   click the **Integrate Cursor** command in the command bar or the context menu of the cursor.
   ➨ The scan is created in a separate scan list.

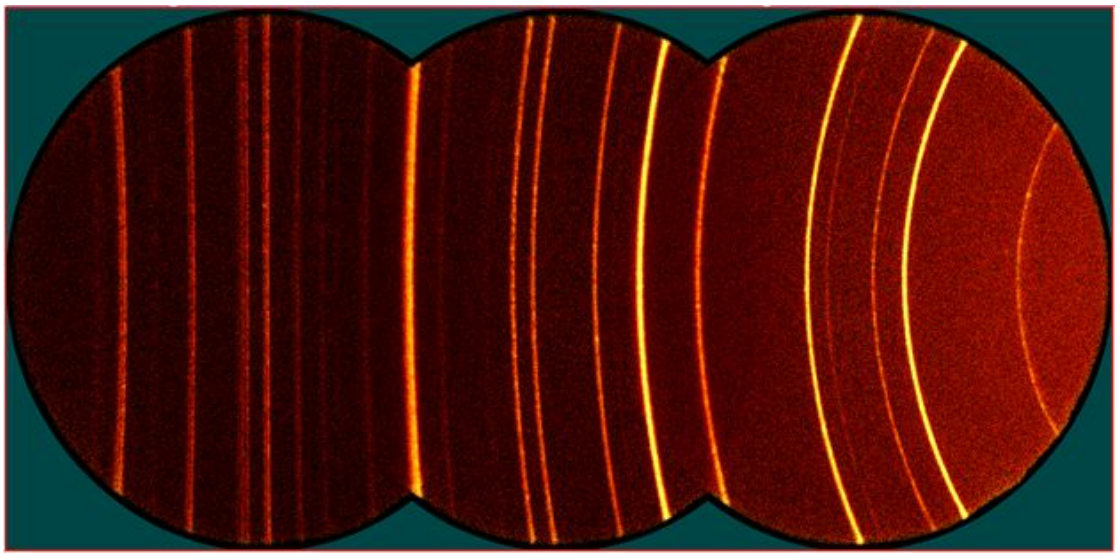


Figure 30.4: 2D Frame View with the full frame cursor drawn along its edges

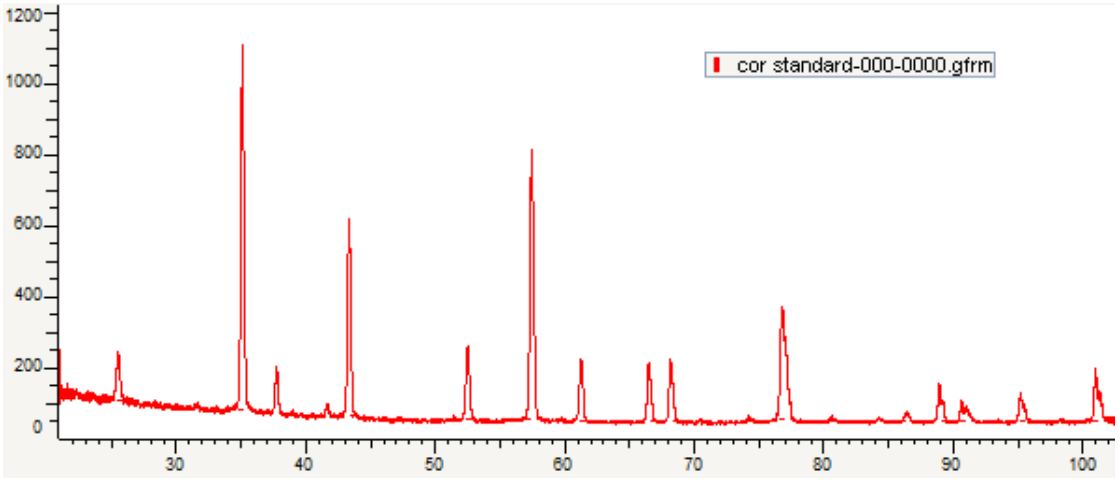


Figure 30.5: The resulting integrated scan

31 Using Printing Options

This chapter will describe how to use some printing options.

31.1 Vertical Table

Vertical Table is an option which allows “permuting” columns and rows. It proves useful when printing a column view with few objects but numerous properties.

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   - ➨ The EVA document is empty.

2. Click the **Import from files** data command or the **Import from files** button.
   - ➨ The **Import From Files** dialog box will be displayed.
3. Search the Tutorials/EVA* directory and select the ET20.RAW, ET50.RAW and ET80.RAW files.
4. Click **Open**.
5. The scans will be added to the Data Tree and displayed in the graphical view of the EVA document and added to the data tree.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

Figure 31.1: Importing the 3 scans

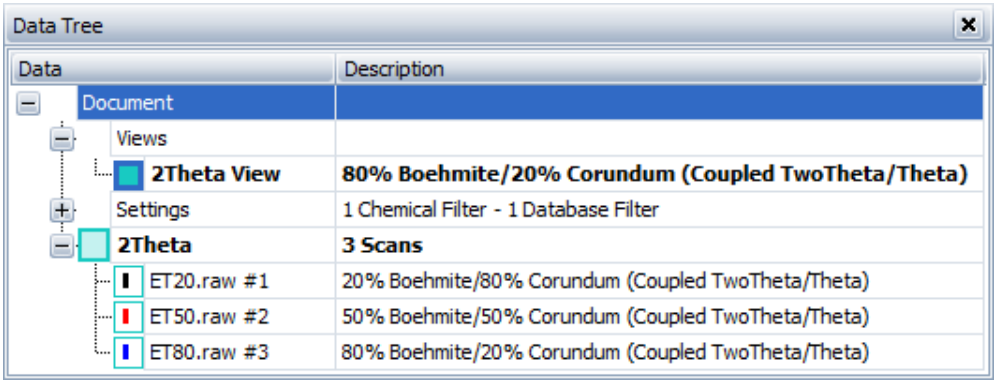
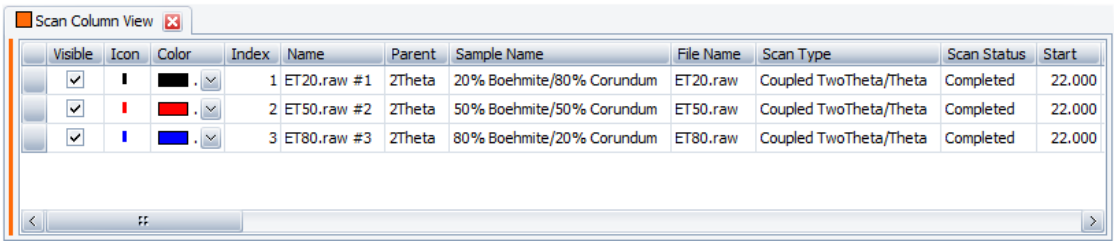
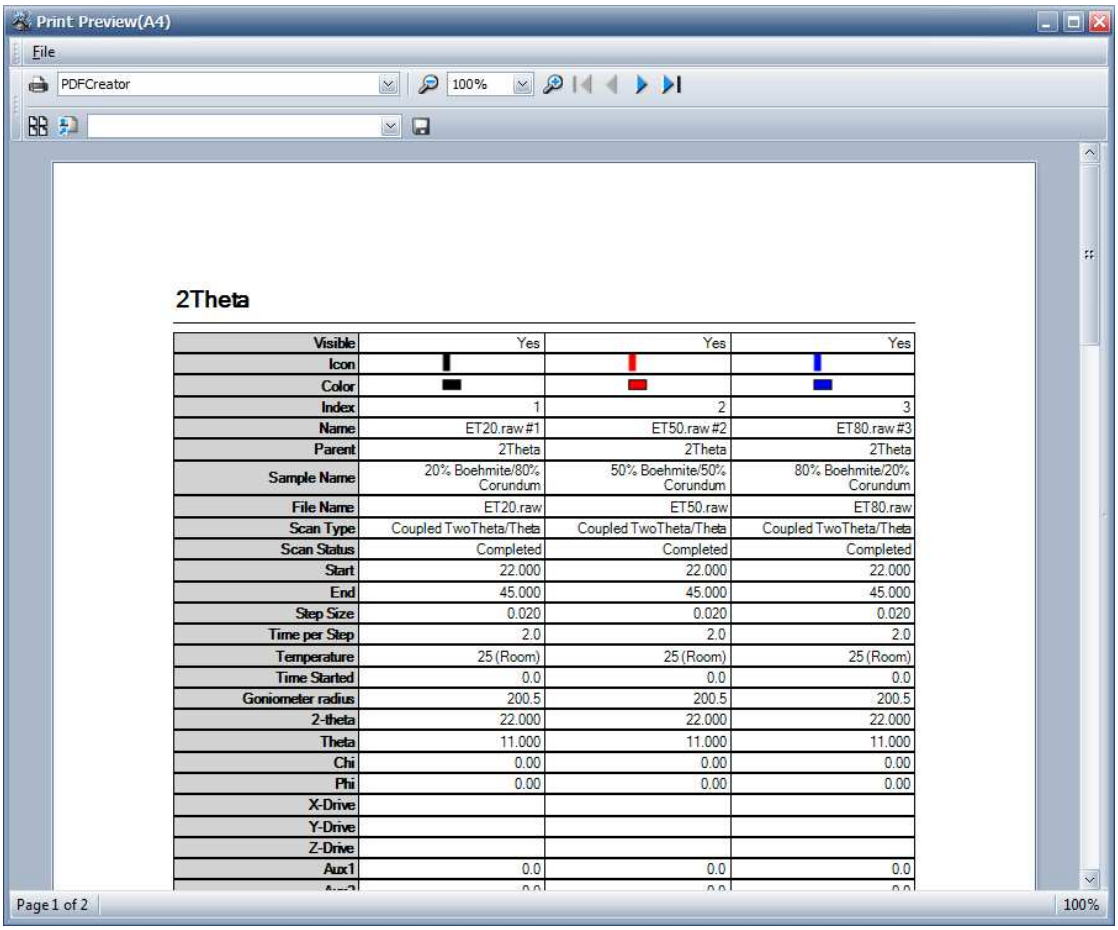


Figure 31.2: ET20.RAW, ET50.RAW and ET80.RAW added to the data tree

1. Select the scan list (2Theta list in the example).
2. Click **Scan Column View** in the Create list of the Data Command panel
   — or —
   click the **Scan Column View** button on the Create View toolbar
   — or —
   right-click the scan list in the data tree to display the context menu. Click **Create** and then **Scan Column View** on the related submenu.
   ➨ A Scan Column View will be created.



3. Configure the table columns if necessary. To do so, right-click a column header to display the context menu. You can also drag and drop the columns to changer their order.
4. In the Scan Column view Property table, select the **Vertical Table** check box.
   ➨ No change is visible in the scan column view. The resulting table will be visible in the Print preview.
5. Check the view is printable.
6. Click **Print Preview** in the View Data Command panel,
   — or —
   Right-click the scan column view in the data tree to display the context menu. Click **Print preview**.
   ➨ The print preview with the vertical table will be displayed.



Visible	Yes	Yes	Yes
Icon			
Color			
Index	1	2	3
Name	ET20.raw #1	ET50.raw #2	ET80.raw #3
Parent	2Theta	2Theta	2Theta
Sample Name	20% Boehmite/80% Corundum	50% Boehmite/50% Corundum	80% Boehmite/20% Corundum
File Name	ET20.raw	ET50.raw	ET80.raw
Scan Type	Coupled TwoTheta/Theta	Coupled TwoTheta/Theta	Coupled TwoTheta/Theta
Scan Status	Completed	Completed	Completed
Start	22.000	22.000	22.000
End	45.000	45.000	45.000
Step Size	0.020	0.020	0.020
Time per Step	2.0	2.0	2.0
Temperature	25 (Room)	25 (Room)	25 (Room)
Time Started	0.0	0.0	0.0
Goniometer radius	200.5	200.5	200.5
2-theta	22.000	22.000	22.000
Theta	11.000	11.000	11.000
Chi	0.00	0.00	0.00
Phi	0.00	0.00	0.00
X-Drive			
Y-Drive			
Z-Drive			
Aux1	0.0	0.0	0.0

Figure 31.3: Vertical table visible in the print preview

31.2 Repeat Columns

Repeat Columns is an option which allows repeating the N first columns of a column view on each “row”. It proves useful when printing a column view with numerous objects and properties.

The **Repeat Columns** feature is available up to version 3.1.

1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
   ➨ The EVA document is empty.
2. Click the **Import from files** data command or the **Import from files** button.
   ➨ The **Import From Files** dialog box will be displayed.
3. Search the Tutorials/EVA* directory and select the fifteen first .RAW files from Aa.raw to Corundum-3.Raw in this example.
4. Click **Open**. The scans will be displayed in the graphical view of the EVA document and added to the Data tree.

* The directory path to the EVA tutorial files is **C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials** under Windows XP and **C:\ProgramData\Bruker AXS\Tutorials** under Windows 7.

To access the folder with the **Explorer**, select **Display hidden files and folders** in the **Folders** options.

Figure 31.4: Importing Scans

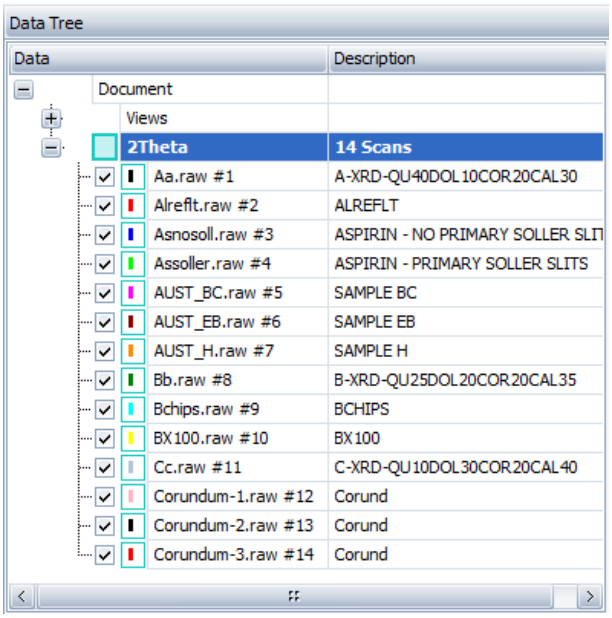


Figure 31.5: Scans added to the data tree

5. Select the scan list (2Theta list in the example).
6. Click **Scan Column View** in the Create list of the Data Command panel
   — or —
   click the **Scan Column View** button on the Create View toolbar.
   — or —
   right-click the scan list in the data tree to display the context menu. Click **Create** and then **Scan Column View** on the related submenu.
   ➨ A Scan Column View will be created.

Scan Column View

Visible	Icon	Color	Index	Name	Parent	Sample Name	File Name	Scan Type
☑		Red	1	Aa.raw #1	2Theta	A-XRD-QU40DOL10COR20CAL30	Aa.raw	Coupled TwoTheta/Theta
☑		Blue	2	Alrefit.raw #2	2Theta	ALREFLT	Alrefit.raw	Coupled TwoTheta/Theta
☑		Lime	3	Asnosoll.raw #3	2Theta	ASPIRIN - NO PRIMARY SOLLER SLIT	Asnosoll.raw	Coupled TwoTheta/Theta
☑		Magenta	4	Assoller.raw #4	2Theta	ASPIRIN - PRIMARY SOLLER SLITS	Assoller.raw	Coupled TwoTheta/Theta
☑		Black	5	AUST_BC.raw #5	2Theta	SAMPLE BC	AUST_BC.raw	Coupled TwoTheta/Theta
☑		DarkRed	6	AUST_EB.raw #6	2Theta	SAMPLE EB	AUST_EB.raw	Coupled TwoTheta/Theta
☑		DarkOr...	7	AUST_H.raw #7	2Theta	SAMPLE H	AUST_H.raw	Coupled TwoTheta/Theta
☑		Green	8	Bb.raw #8	2Theta	B-XRD-QU25DOL20COR20CAL35	Bb.raw	Coupled TwoTheta/Theta
☑		Cyan	9	Bchips.raw #9	2Theta	BCHIPS	Bchips.raw	Coupled TwoTheta/Theta
☑		Yellow	10	BX100.raw #10	2Theta	BX100	BX100.raw	Coupled TwoTheta/Theta
☑		LightSt...	11	Cc.raw #11	2Theta	C-XRD-QU10DOL30COR20CAL40	Cc.raw	Coupled TwoTheta/Theta
☑		LightPink	12	Corundum-1.raw #12	2Theta	Corund	Corundum-1.raw	Coupled TwoTheta/Theta
☑		Red	13	Corundum-2.raw #13	2Theta	Corund	Corundum-2.raw	Coupled TwoTheta/Theta
☑		Blue	14	Corundum-3.raw #14	2Theta	Corund	Corundum-3.raw	Coupled TwoTheta/Theta

Figure 31.6: Scan column view

7. In this example, it is interesting to configure the table columns differently. To do so, right-click a column header to display the context menu and access the configuration tools. You can also drag and drop the columns to changer their order.

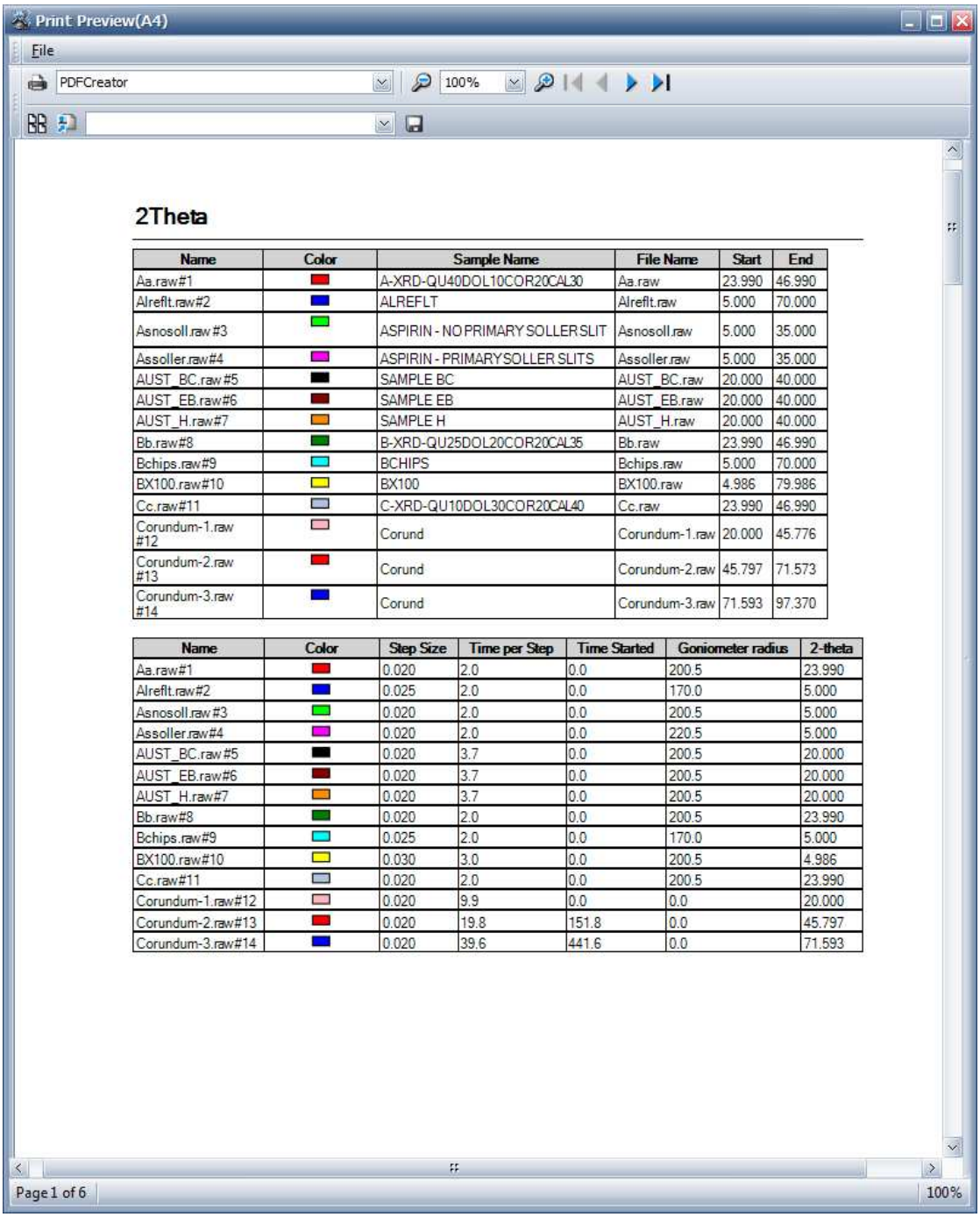
Scan Column View

Name	Color	Sample Name	File Name	Start	End	Step Size	Time per Step	Time Started	Goniometer radius
Aa.raw #1	Red	A-XRD-QU40DOL10COR20CAL30	Aa.raw	23.990	46.990	0.020	2.0	0.0	200.5
Alrefit.raw #2	Blue	ALREFLT	Alrefit.raw	5.000	70.000	0.025	2.0	0.0	170.0
Asnosoll.raw #3	Lime	ASPIRIN - NO PRIMARY SOLLER SLIT	Asnosoll.raw	5.000	35.000	0.020	2.0	0.0	200.5
Assoller.raw #4	Magenta	ASPIRIN - PRIMARY SOLLER SLITS	Assoller.raw	5.000	35.000	0.020	2.0	0.0	220.5
AUST_BC.raw #5	Black	SAMPLE BC	AUST_BC.raw	20.000	40.000	0.020	3.7	0.0	200.5
AUST_EB.raw #6	DarkRed	SAMPLE EB	AUST_EB.raw	20.000	40.000	0.020	3.7	0.0	200.5
AUST_H.raw #7	DarkOr...	SAMPLE H	AUST_H.raw	20.000	40.000	0.020	3.7	0.0	200.5
Bb.raw #8	Green	B-XRD-QU25DOL20COR20CAL35	Bb.raw	23.990	46.990	0.020	2.0	0.0	200.5
Bchips.raw #9	Cyan	BCHIPS	Bchips.raw	5.000	70.000	0.025	2.0	0.0	170.0
BX100.raw #10	Yellow	BX100	BX100.raw	4.986	79.986	0.030	3.0	0.0	200.5
Cc.raw #11	LightSt...	C-XRD-QU10DOL30COR20CAL40	Cc.raw	23.990	46.990	0.020	2.0	0.0	200.5
Corundum-1.raw #12	LightPink	Corund	Corundum-1.raw	20.000	45.776	0.020	9.9	0.0	0.0
Corundum-2.raw #13	Red	Corund	Corundum-2.raw	45.797	71.573	0.020	19.8	151.8	0.0
Corundum-3.raw #14	Blue	Corund	Corundum-3.raw	71.593	97.370	0.020	39.6	441.6	0.0

Figure 31.7: Scan column view with a new column configuration: file name and color in first

This table has many columns. Therefore it will not be possible to have all columns on each row when printing. It may be nice to keep, for example, the file name and its corresponding color at the beginning of each row.

1. In the Scan Column view Property table, enter 2 for the **Repeat Columns** value. It means the two first columns will be repeated on each row when printing.
   ➨ No change is visible in the scan column view. The resulting table will be visible in the Print preview.
2. Check the view is printable.
3. Click **Print Preview** in the View Data Command panel,
   — or —
   Right-click the scan column view in the data tree to display the context menu. Click **Print preview**.
   ➨ The print preview will be displayed.



2Theta

Name	Color	Sample Name	File Name	Start	End
Aa.raw#1		A-XRD-QU40DOL10COR20CAL30	Aa.raw	23.990	46.990
Alreflt.raw#2		ALREFLT	Alreflt.raw	5.000	70.000
Asnosoll.raw#3		ASPIRIN - NO PRIMARY SOLLER SLIT	Asnosoll.raw	5.000	35.000
Assoller.raw#4		ASPIRIN - PRIMARY SOLLER SLITS	Assoller.raw	5.000	35.000
AUST_BC.raw#5		SAMPLE BC	AUST_BC.raw	20.000	40.000
AUST_EB.raw#6		SAMPLE EB	AUST_EB.raw	20.000	40.000
AUST_H.raw#7		SAMPLE H	AUST_H.raw	20.000	40.000
Bb.raw#8		B-XRD-QU25DOL20COR20CAL35	Bb.raw	23.990	46.990
Bchips.raw#9		BCHIPS	Bchips.raw	5.000	70.000
BX100.raw#10		BX100	BX100.raw	4.986	79.986
Cc.raw#11		C-XRD-QU10DOL30COR20CAL40	Cc.raw	23.990	46.990
Corundum-1.raw #12		Corund	Corundum-1.raw	20.000	45.776
Corundum-2.raw #13		Corund	Corundum-2.raw	45.797	71.573
Corundum-3.raw #14		Corund	Corundum-3.raw	71.593	97.370

Name	Color	Step Size	Time per Step	Time Started	Goniometer radius	2-theta
Aa.raw#1		0.020	2.0	0.0	200.5	23.990
Alreflt.raw#2		0.025	2.0	0.0	170.0	5.000
Asnosoll.raw#3		0.020	2.0	0.0	200.5	5.000
Assoller.raw#4		0.020	2.0	0.0	220.5	5.000
AUST_BC.raw#5		0.020	3.7	0.0	200.5	20.000
AUST_EB.raw#6		0.020	3.7	0.0	200.5	20.000
AUST_H.raw#7		0.020	3.7	0.0	200.5	20.000
Bb.raw#8		0.020	2.0	0.0	200.5	23.990
Bchips.raw#9		0.025	2.0	0.0	170.0	5.000
BX100.raw#10		0.030	3.0	0.0	200.5	4.986
Cc.raw#11		0.020	2.0	0.0	200.5	23.990
Corundum-1.raw#12		0.020	9.9	0.0	0.0	20.000
Corundum-2.raw#13		0.020	19.8	151.8	0.0	45.797
Corundum-3.raw#14		0.020	39.6	441.6	0.0	71.593

Figure 31.8: The two first columns “Name” and “Color” are repeated in the print preview

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