DIFFRAC.SUITE

Tutorial

DIFFRAC.EVALUATION PACKAGE
DIFFRAC.EVA

Original Instructions

XRD

Innovation with Integrity

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Bruker AXS GmbH
Östliche Rheinbrückenstr. 49
76187 Karlsruhe, Germany
Tel. +49 721 50997-0
Fax +49 721 50997-5654
info@bruker-axs.de
www.bruker.com

DIFFRAC.EVA Tutorial

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EVA Tutorial

Performing a Search/Match Operation

NOTE

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

This tutorial was prepared using PDF 4+ 2009 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 (pattern 00-036-0426), Calcite (01-89-1304) and Quartz (01-075-8322)
4. Preparing the residual scan.
5. Performing a subsequent search on the residual scan.
6. Matching procedure

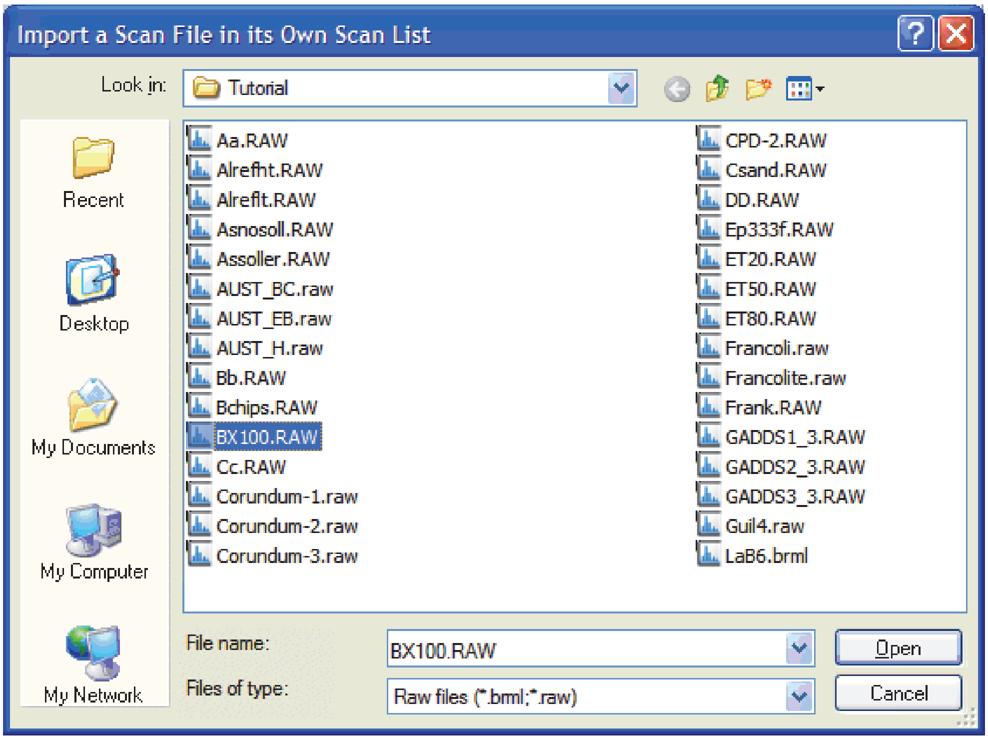
   Identification of Clinochlore (01-083-1365)
7. Saving the EVA document containing the scan.

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

New button

Import from file button

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 file** data command or the **Import from file** button. The Import a Scan File dialog box will be displayed.
3. Search the Tutorials/EVA[1] directory and select the Bchips.RAW file.
4. Click **Open**. The scan Bchips will be displayed in the graphical view of the EVA document.



Look in: Tutorial

File name: BX100.RAW

Files of type: Raw files (*.brml;*.raw)

Fig. 1: Importing the Bchips.Raw file

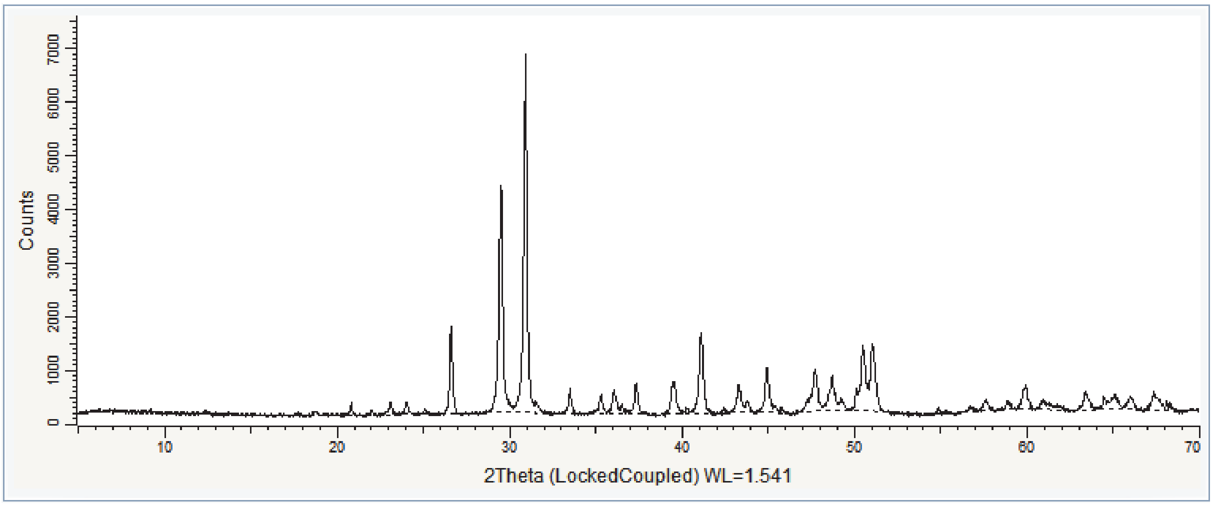


Fig. 2: Bchips.RAW file imported in the graphical view

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[1] 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.

Step 2: Setting the Search Parameters

1. Make certain the scan is selected; if not, select it either in the Data tree or in the graphical view.
2. Click **Search / Match (scan)** in the Data Command panel
   — or —
   Right-click the scan, click **Tool** on the context menu and then **Search / Match (scan)** on the related submenu.

   The **Search / Match (scan)** dialog box will be displayed.

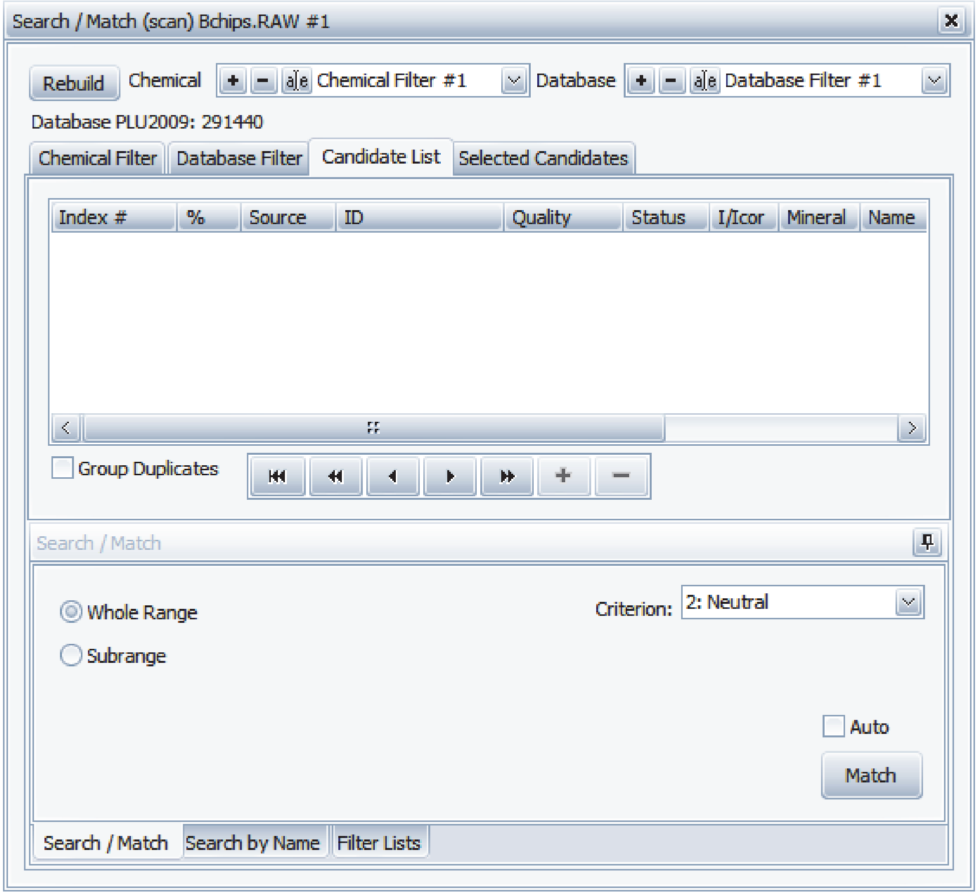


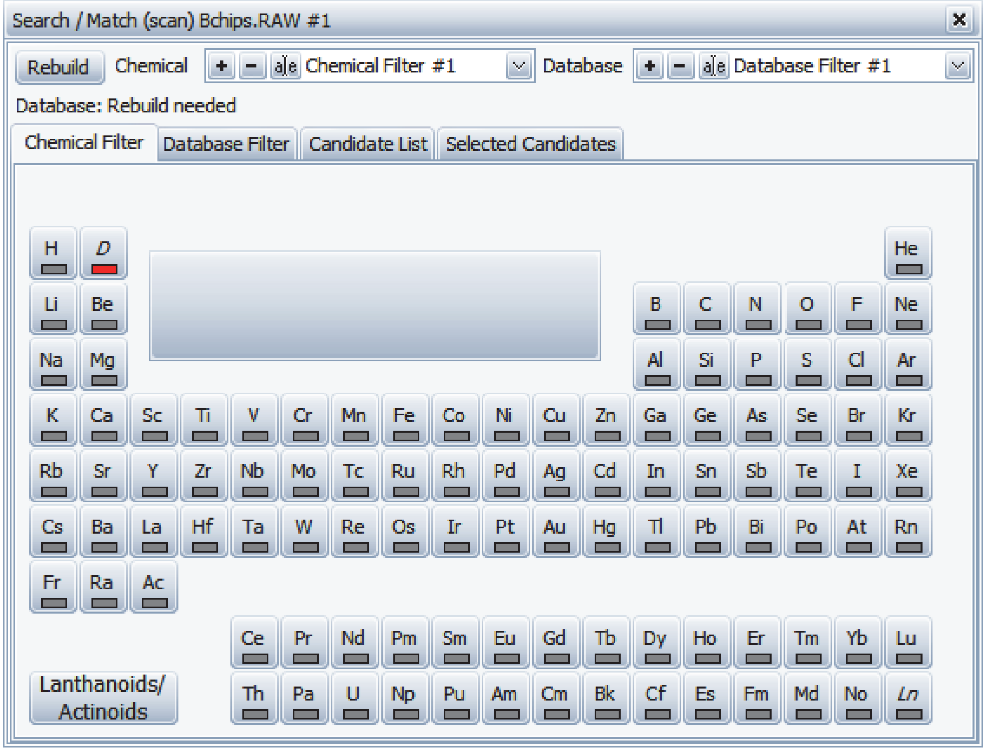
Fig. 3: Search/match dialog box

3. Keep the default parameters:
   ⇒ In the Candidate List tab:
   - ☐ Group duplicates
   - Criterion = **2** (**Neutral**)
   - **Whole Range** selected
   - ☐ Auto

NOTE

The Group duplicates option is not used in this example but this is a practical option which can be used without any risk.

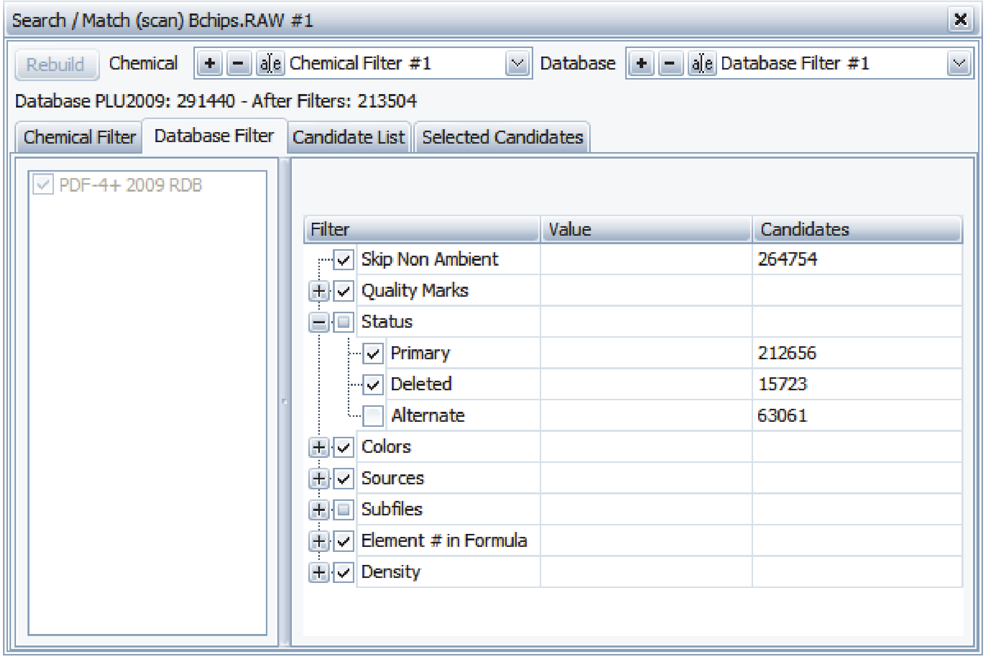
⇒ In the Chemical Filter tab:



Database: Rebuild needed

No chemical filter, except D (deuterium) is Discarded (red)

⇒ In the Database Filter tab:



Database PLU2009: 291440 - After Filters: 213504

☑ PDF-4+ 2009 RDB

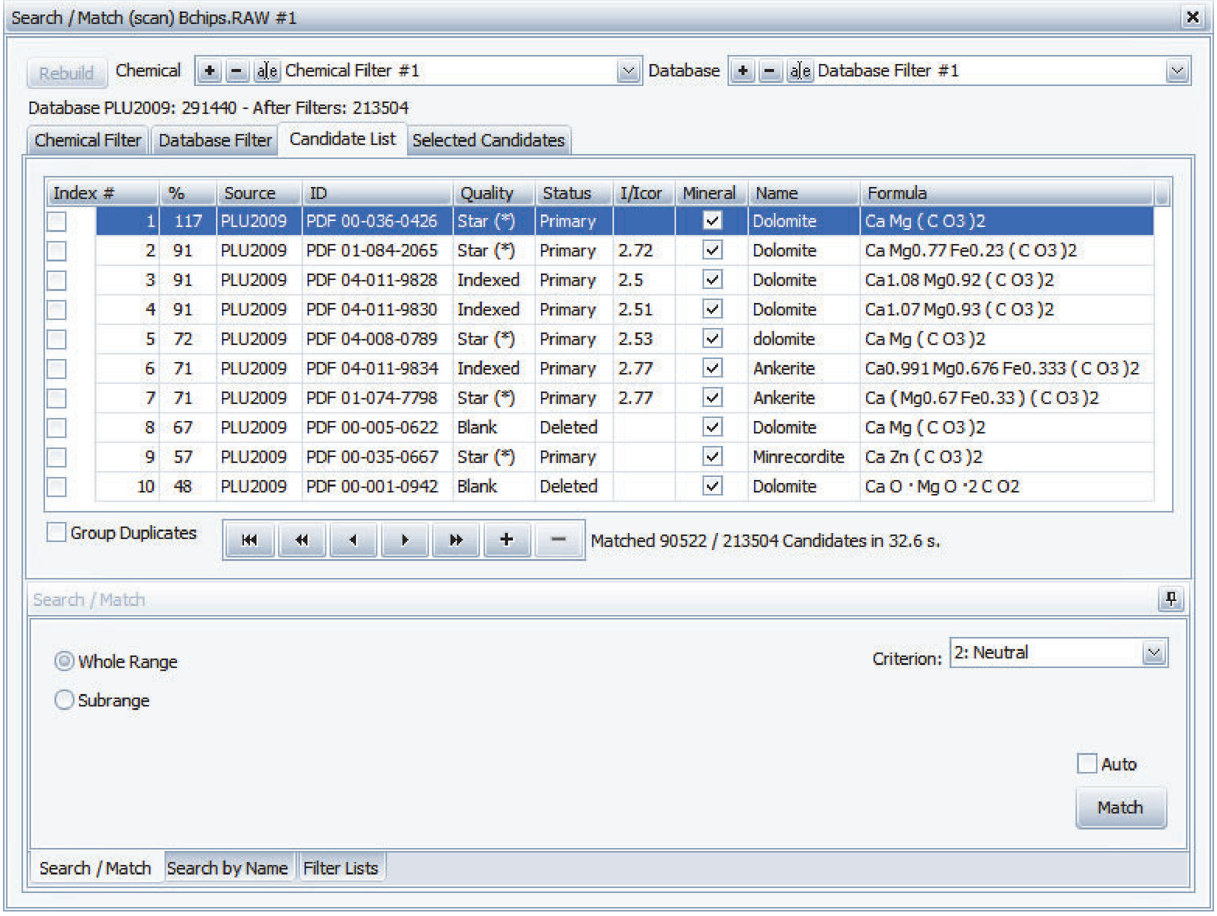
Filter	Value	Candidates
☑ Skip Non Ambient		264754
☑ Quality Marks		
☐ Status		
☑ Primary		212656
☑ Deleted		15723
☐ Alternate		63061
☑ Colors		
☑ Sources		
☐ Subfiles		
☑ Element # in Formula		
☑ Density		

- ☑ all Subfiles are selected
- ☑ all Quality Marks are selected
- ☑ all Status are selected except ☐ **A** (alternative) that is cleared

4. Click the **Match** button. The candidates are listed in the Candidate List tab.

Step 3: Matching Procedure

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.



Search / Match (scan) Bchips.RAW #1

Database PLU2009: 291440 - After Filters: 213504

	Index #	%	Source	ID	Quality	Status	I/Icor	Mineral	Name	Formula
☐	1	117	PLU2009	PDF 00-036-0426	Star (*)	Primary		☑	Dolomite	Ca Mg (C O3)2
☐	2	91	PLU2009	PDF 01-084-2065	Star (*)	Primary	2.72	☑	Dolomite	Ca Mg0.77 Fe0.23 (C O3)2
☐	3	91	PLU2009	PDF 04-011-9828	Indexed	Primary	2.5	☑	Dolomite	Ca1.08 Mg0.92 (C O3)2
☐	4	91	PLU2009	PDF 04-011-9830	Indexed	Primary	2.51	☑	Dolomite	Ca1.07 Mg0.93 (C O3)2
☐	5	72	PLU2009	PDF 04-008-0789	Star (*)	Primary	2.53	☑	dolomite	Ca Mg (C O3)2
☐	6	71	PLU2009	PDF 04-011-9834	Indexed	Primary	2.77	☑	Ankerite	Ca0.991 Mg0.676 Fe0.333 (C O3)2
☐	7	71	PLU2009	PDF 01-074-7798	Star (*)	Primary	2.77	☑	Ankerite	Ca (Mg0.67 Fe0.33) (C O3)2
☐	8	67	PLU2009	PDF 00-005-0622	Blank	Deleted		☑	Dolomite	Ca Mg (C O3)2
☐	9	57	PLU2009	PDF 00-035-0667	Star (*)	Primary		☑	Minrecordite	Ca Zn (C O3)2
☐	10	48	PLU2009	PDF 00-001-0942	Blank	Deleted		☑	Dolomite	Ca O · Mg O ·2 C O2

☐ Group Duplicates

Matched 90522 / 213504 Candidates in 32.6 s.

● Whole Range
○ Subrange

Criterion: 2: Neutral

☐ Auto

Fig. 4: Candidate List with the first pattern selected

1. In the Candidate List tab, the first pattern in the list is selected: 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 00-036-0426 matches a part of the peaks of the scan.
3. Mark this pattern by selecting the corresponding check box (or by clicking the **Check** button below the table). The pattern is associated to a color and the image of its stick patterns remains when it is no longer selected (highlighted) in the Candidate List.
4. Go down in the list using the arrow buttons below the table. Compare the stick patterns to the scan peaks. The Calcite and Quartz patterns (01-089-1304 and 01-075-8322) appear to match the scan. Select the corresponding check boxes: the images of their stick patterns remain when they are no longer selected.
5. Leave the non-matching stick patterns unchecked.

+
Check button
☑ 🟥

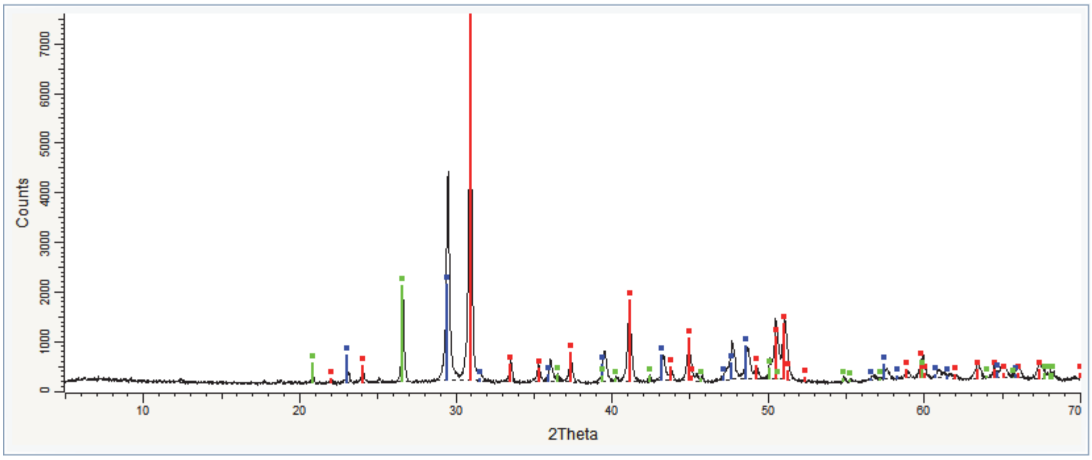


Fig. 5: Bchips scan displayed in the graphical view with the three patterns 00-036-0426, 01-89-1304 and 01-075-8322

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.

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. In the Selected Candidates tab of the Search/Match (scan) dialog box, click **Residue**.
2. Click the first selected pattern in the Selection list: the areas to be removed are displayed as ghosts in the graphical view. Adjust the width of the zone to exclude around the pattern sticks with the slider if necessary.
3. Click the **Apply** button.
4. Proceed the same way for the other selected patterns. The removed zones are displayed using the ghost color.

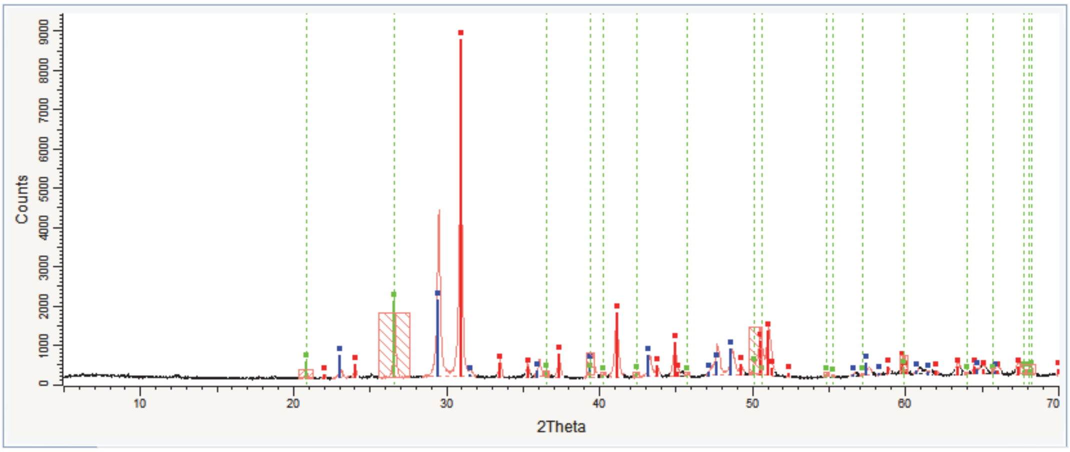


Fig. 6: Scan with the removed zones in red (ghost color)

Step 5: Performing a Subsequent Search on the Residual Scan

1. In the graphical view, zoom in on the first half of the diagram (5° to about 36° 2θ). Working on relatively low angles for the identification of clay materials is highly recommended.
2. Keep the default parameters:
   - ☐ Group duplicates
   - Criterion = **2** (**Neutral**)
   - **Whole Range** selected
   - ☐ Auto
   - No chemical filter, except D (deuterium) is Discarded (red)
   - ☑ all Subfiles are selected
   - ☑ all Quality Marks are selected
   - ☑ all Status are selected except ☐ **A** (alternative) that is cleared
3. In the Candidate List tab, click the **Match** button. The candidates will be listed.

NOTE

The Group duplicates option is not used in this example but this is a practical option which can be used without any risk.

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)

➕
Check button

2. In the Candidate List tab, the first pattern in the list is selected: it is Gadolinium Zirconium Selenium (pattern PDF 04-003-8951). The corresponding ghost stick pattern is displayed in the graphical view.

☑ 🟥

3. Compare the stick patterns to the current scan peaks. Identify the Clinochlore (pattern PDF 01-083-1365) which ranks 5. It ranks 2 selecting the Mineral database only.
4. Mark this pattern by selecting the corresponding check box (by clicking the **Check** button below the table). The pattern is associated to a color. The image of its stick patterns remains when it is no longer selected in the Candidate List.
5. Leave the non-matched stick patterns unchecked.

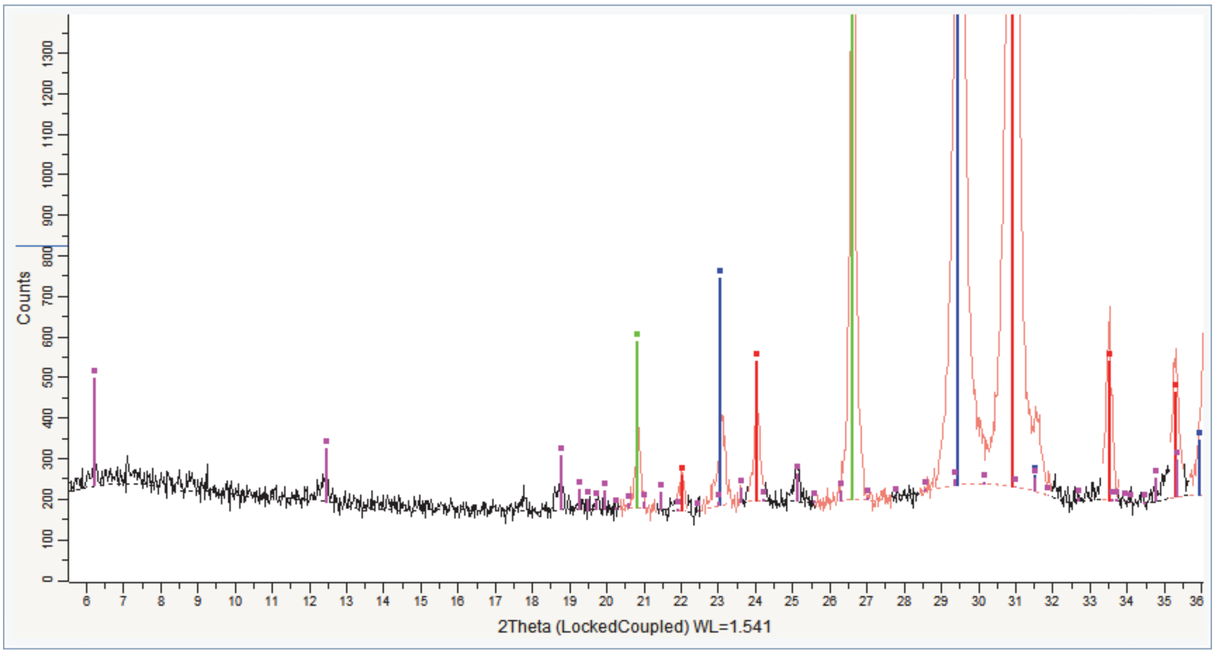
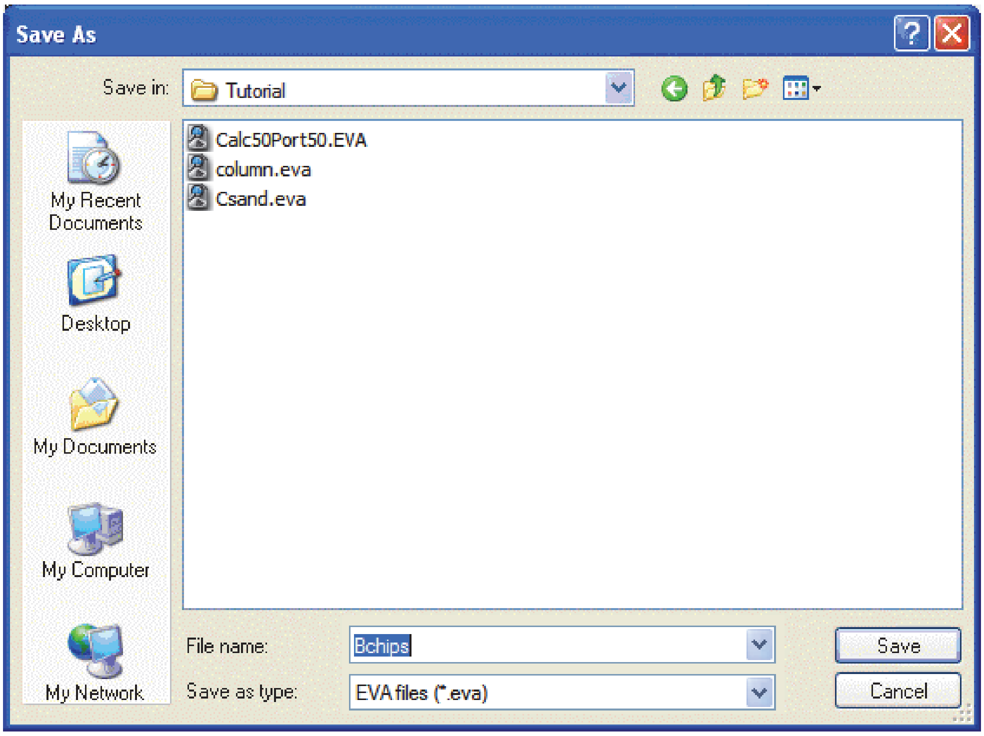


Fig. 7: Zoom on the first half of the diagram with the Clinochlore phase identified

Step 7: Saving

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



Save in: Tutorial

Calc50Port50.EVA
column.eva
Csand.eva

File name: Bchips

Save as type: EVA files (*.eva)

Fig. 8: Bchips.EVA document

Performing an Automatic Search/Match Operation

NOTE

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

This tutorial was prepared using PDF 4+ 2009 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.

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

On the contrary, the interactive Search/Match is quite insensitive to line overlaps, to relative intensity mismatches, whereas line broadening is not a major issue, which makes the identification of phases possible in complex scans, even with relatively strong preferred orientations.

One has to be very careful using the automatic search. It is great when the three conditions are fulfilled, but this can hardly be guessed before trying. In praxis, one will often have to keep on searching with the interactive Search/Match after a trial with the Automatic Search.

The scans used are held as tutorial files, m1.RAW, CPD-2.RAW and Mineral_Mixture.BRML found in the Tutorial 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.

Case #1: m1.RAW

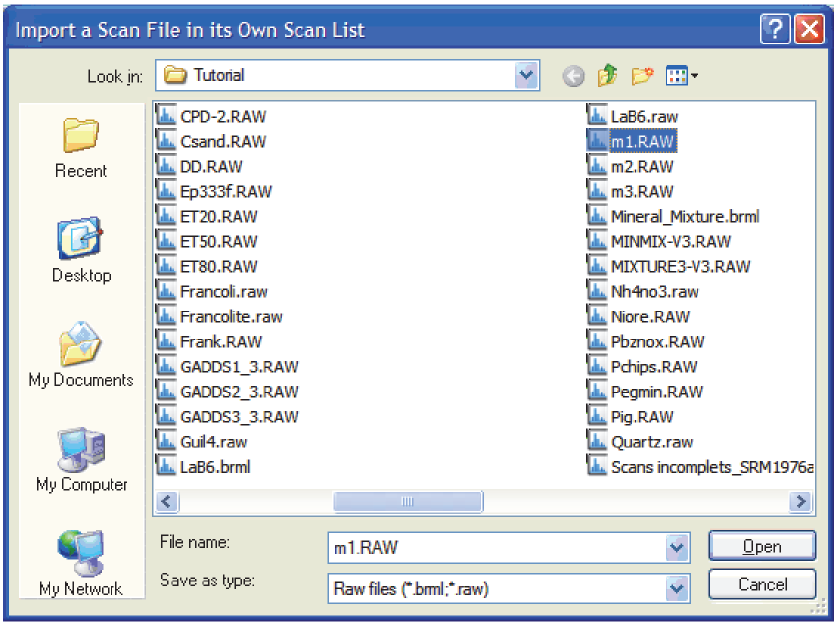
M1 is a mixture of Calcite, Aragonite and Brucite.

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

New button

Import from file button

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 file** data command or the **Import from file** button. The Import a Scan File dialog box will be displayed.
3. Search the Tutorials/EVA[1] directory and select the m1.RAW file.
4. Click **Open**. The scan m1 will be displayed in the graphical view of the EVA document.



Look in: Tutorial

File name: m1.RAW

Save as type: Raw files (*.brml;*.raw)

Fig. 9: Importing the m1.RAW file

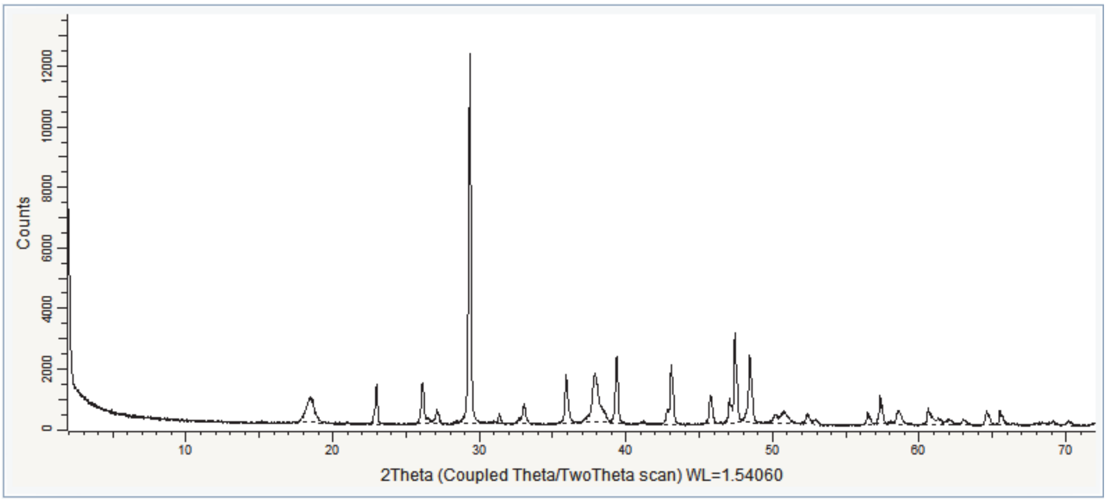


Fig. 10: m1.RAW file imported in the graphical view

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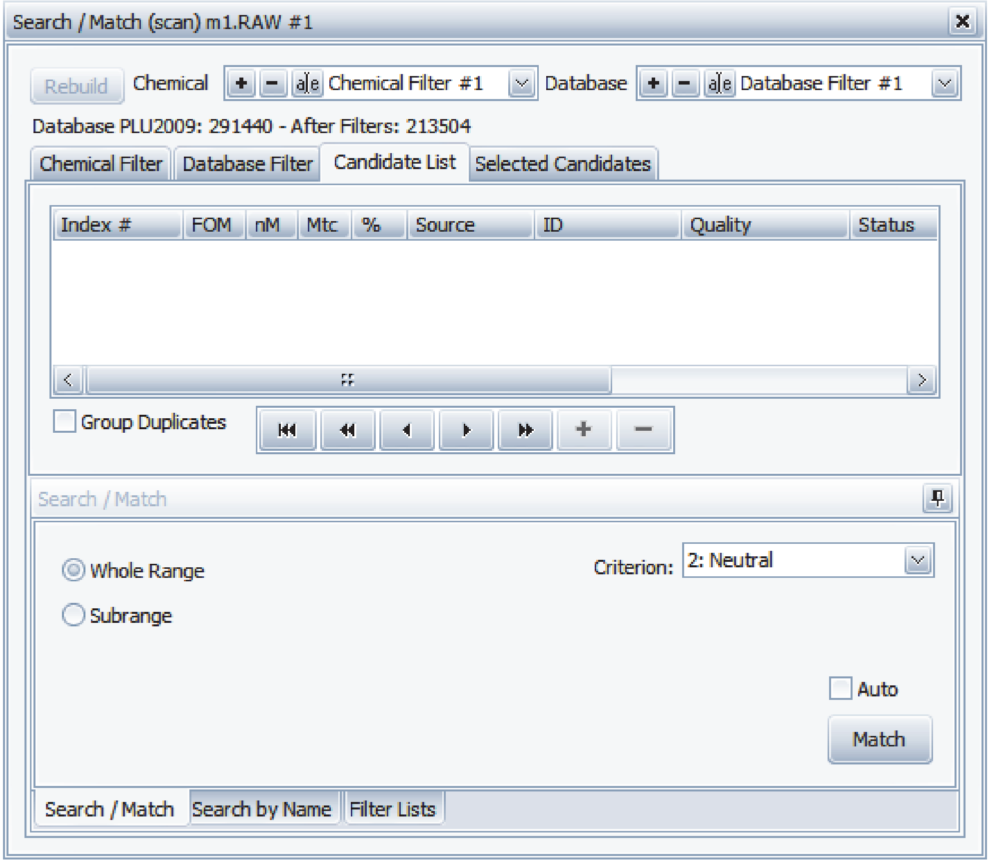
[1] The directory path to the EVA tutorial files is "C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials" under Windows XP and "C:\ProgramData\Bruker AXS\Tutorials" under Windows 7.
To access the folder with the explorer, select "Display hidden files and folders" in the Folders options.

Step 2: Setting the Search Parameters

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

2. Click **Search / Match (scan)** in the Data Command panel
— or —
Right-click the scan, click **Tool** on the context menu and then **Search / Match (scan)** on the related submenu.

The **Search / Match (scan)** dialog box will be displayed.



Database PLU2009: 291440 - After Filters: 213504

☐ Group Duplicates

● Whole Range

○ Subrange

Criterion: 2: Neutral

☐ Auto

Fig. 11: Search/match dialog box

3. Select the **Auto** check box.

4. Set the parameters to use for the Search/Match:

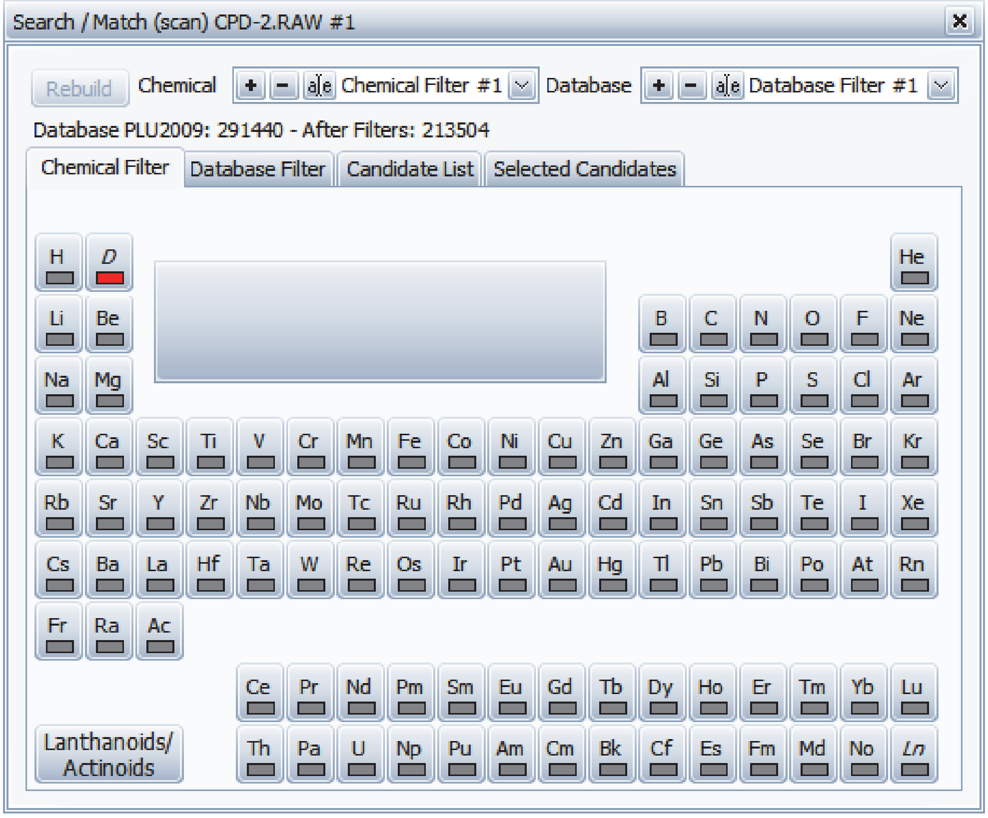
⇒ In the Candidate List tab:

- ☐ Group duplicates
- Criterion = **2** (**Neutral**)
- **Whole Range** selected

NOTE

The Group duplicates option is not used in this example but this is a practical option which can be used without any risk.

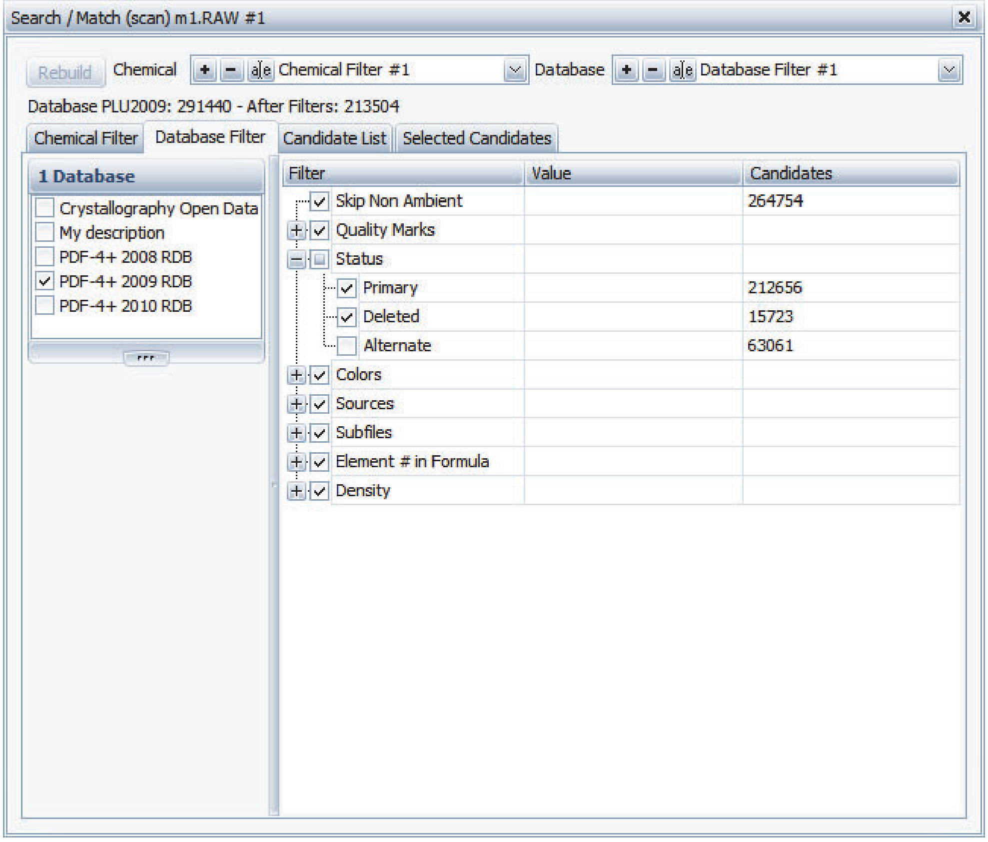
⇒ In the Chemical Filter tab:



Database PLU2009: 291440 - After Filters: 213504

No chemical filter, except D (deuterium) is Discarded (red)

⇒ In the Database Filter tab:



Database PLU2009: 291440 - After Filters: 213504

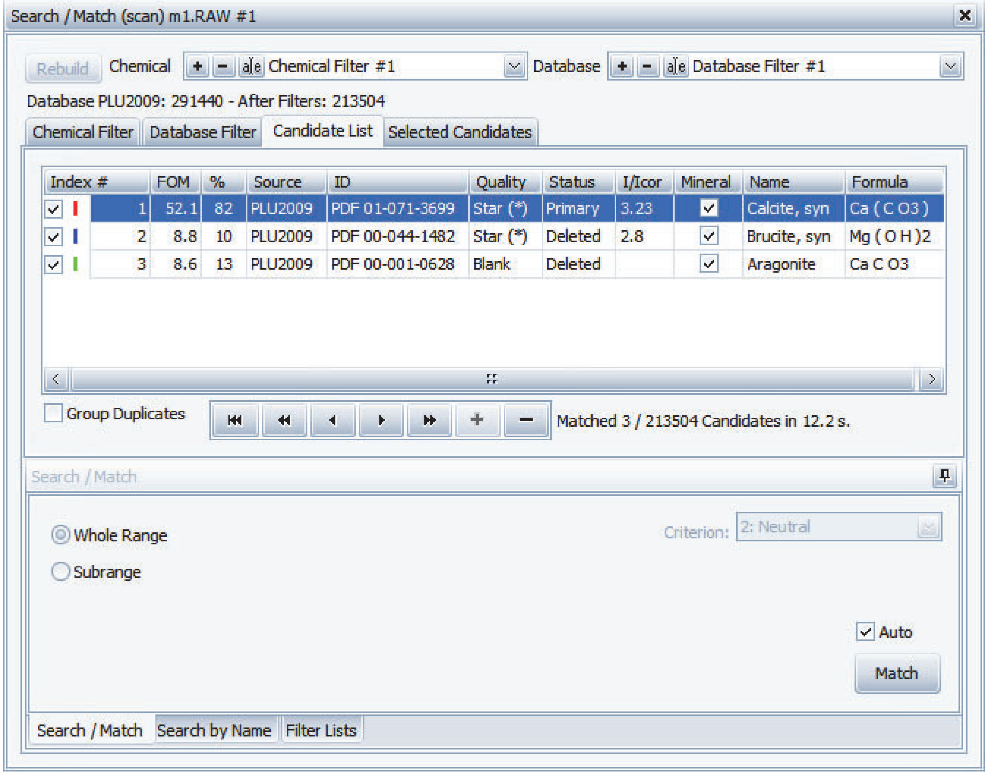
☐ Crystallography Open Data
☐ My description
☐ PDF-4+ 2008 RDB
☑ PDF-4+ 2009 RDB
☐ PDF-4+ 2010 RDB

Filter	Value	Candidates
☑ Skip Non Ambient		264754
☑ Quality Marks		
☐ Status		
☑ Primary		212656
☑ Deleted		15723
☐ Alternate		63061
☑ Colors		
☑ Sources		
☑ Subfiles		
☑ Element # in Formula		
☑ Density		

- ☑ all Subfiles are selected
- ☑ all Quality Marks are selected
- ☑ all Status are selected except ☐ **A** (alternative) that is cleared

5. Click the **Match** button. The candidates are listed in the Candidate List tab.

Step 3: Automatic Matching Procedure



Search / Match (scan) m1.RAW #1

Rebuild Chemical Chemical Filter #1 Database Database Filter #1

Database PLU2009: 291440 - After Filters: 213504

Chemical Filter | Database Filter | Candidate List | Selected Candidates

Index #	FOM	%	Source	ID	Quality	Status	I/Icor	Mineral	Name	Formula
☑ 🟥 1	52.1	82	PLU2009	PDF 01-071-3699	Star (*)	Primary	3.23	☑	Calcite, syn	Ca (C O3)
☑ 🟦 2	8.8	10	PLU2009	PDF 00-044-1482	Star (*)	Deleted	2.8	☑	Brucite, syn	Mg (O H)2
☑ 🟩 3	8.6	13	PLU2009	PDF 00-001-0628	Blank	Deleted		☑	Aragonite	Ca C O3

☐ Group Duplicates Matched 3 / 213504 Candidates in 12.2 s.

Search / Match

● Whole Range

○ Subrange

Criterion: 2: Neutral

☑ Auto

Match

Search / Match | Search by Name | Filter Lists

Fig. 12: Candidate List with the identified patterns selected

☑ 🟥

Pattern checked

The results of the Automatic Search/Match are displayed in the candidate list. The three patterns identified are automatically checked and therefore added to the data tree and to the graphical view.

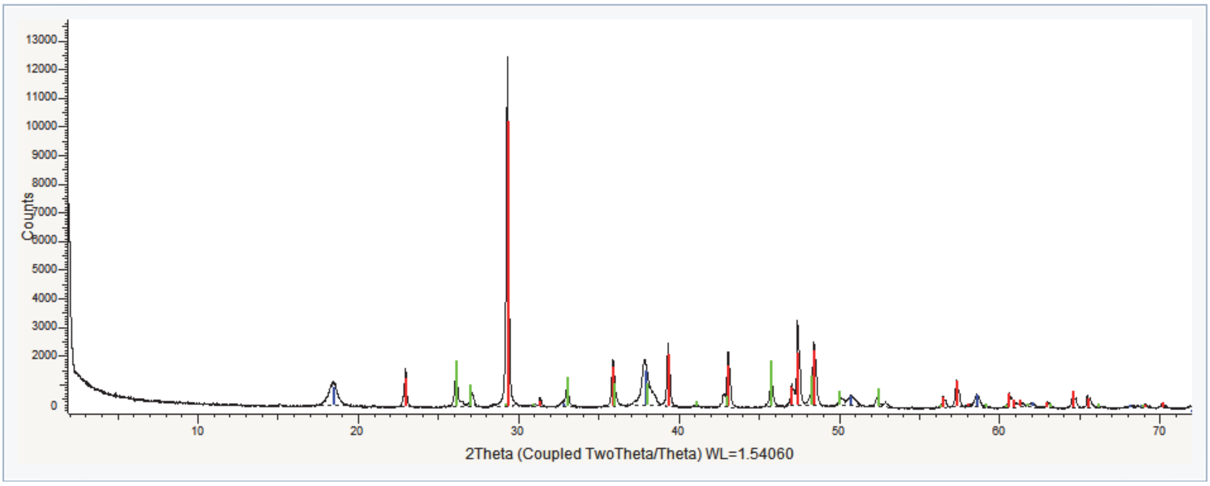


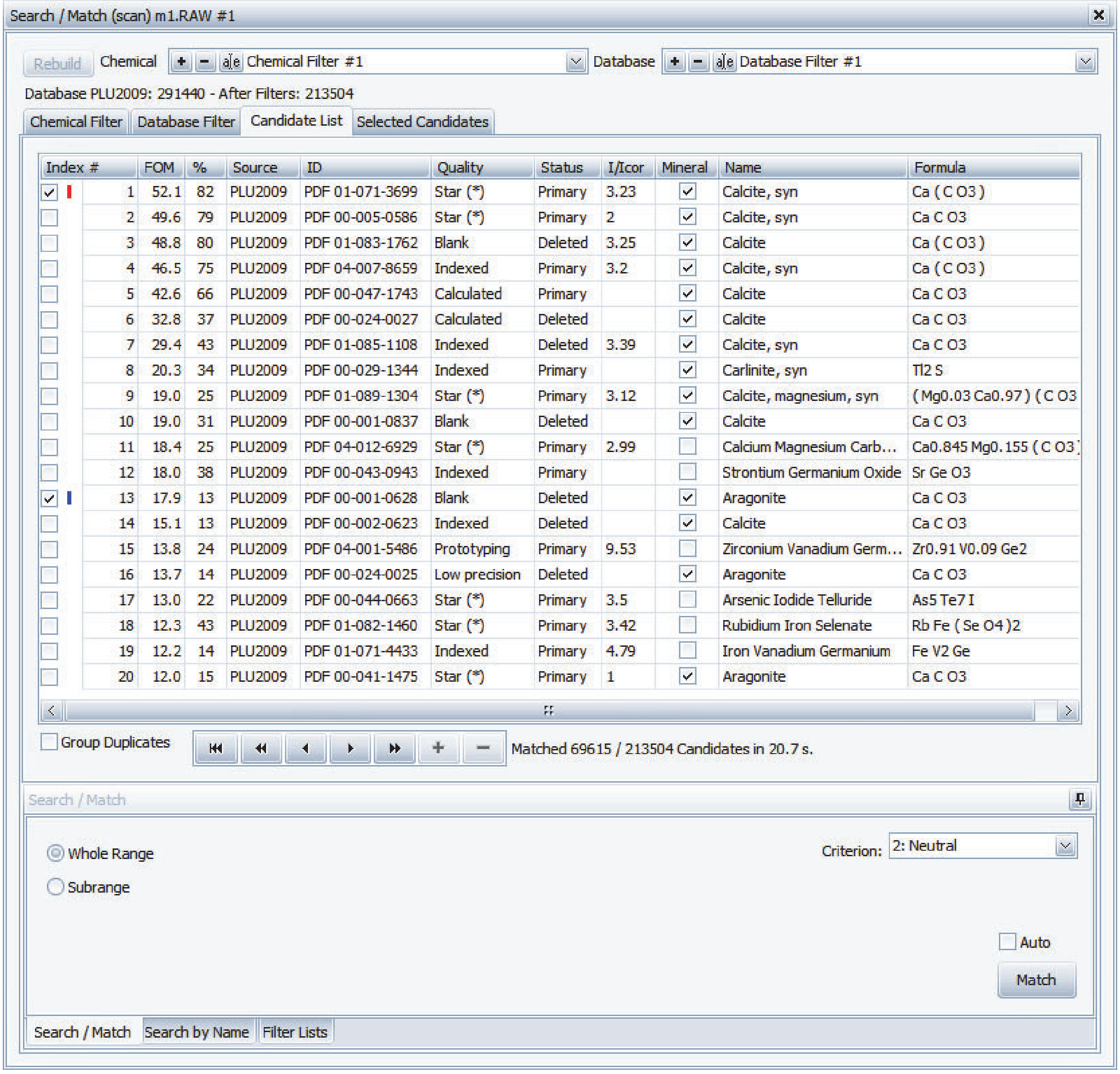
Fig. 13: m1 scan displayed in the graphical view with the three patterns 01-071-3699, 00-044-1482 and 00-001-0628

Results

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

“Normal” matching procedure

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



Search / Match (scan) m1.RAW #1

Database PLU2009: 291440 - After Filters: 213504

Index #	FOM	%	Source	ID	Quality	Status	I/Icor	Mineral	Name	Formula
☑ 🟥 1	52.1	82	PLU2009	PDF 01-071-3699	Star (*)	Primary	3.23	☑	Calcite, syn	Ca (C O3)
☐ 2	49.6	79	PLU2009	PDF 00-005-0586	Star (*)	Primary	2	☑	Calcite, syn	Ca C O3
☐ 3	48.8	80	PLU2009	PDF 01-083-1762	Blank	Deleted	3.25	☑	Calcite	Ca (C O3)
☐ 4	46.5	75	PLU2009	PDF 04-007-8659	Indexed	Primary	3.2	☑	Calcite, syn	Ca (C O3)
☐ 5	42.6	66	PLU2009	PDF 00-047-1743	Calculated	Primary		☑	Calcite	Ca C O3
☐ 6	32.8	37	PLU2009	PDF 00-024-0027	Calculated	Deleted		☑	Calcite	Ca C O3
☐ 7	29.4	43	PLU2009	PDF 01-085-1108	Indexed	Deleted	3.39	☑	Calcite, syn	Ca C O3
☐ 8	20.3	34	PLU2009	PDF 00-029-1344	Indexed	Primary		☑	Carlinite, syn	Tl2 S
☐ 9	19.0	25	PLU2009	PDF 01-089-1304	Star (*)	Primary	3.12	☑	Calcite, magnesium, syn	(Mg0.03 Ca0.97) (C O3
☐ 10	19.0	31	PLU2009	PDF 00-001-0837	Blank	Deleted		☑	Calcite	Ca C O3
☐ 11	18.4	25	PLU2009	PDF 04-012-6929	Star (*)	Primary	2.99	☐	Calcium Magnesium Carb...	Ca0.845 Mg0.155 (C O3
☐ 12	18.0	38	PLU2009	PDF 00-043-0943	Indexed	Primary		☐	Strontium Germanium Oxide	Sr Ge O3
☑ 🟦 13	17.9	13	PLU2009	PDF 00-001-0628	Blank	Deleted		☑	Aragonite	Ca C O3
☐ 14	15.1	13	PLU2009	PDF 00-002-0623	Indexed	Deleted		☑	Calcite	Ca C O3
☐ 15	13.8	24	PLU2009	PDF 04-001-5486	Prototyping	Primary	9.53	☐	Zirconium Vanadium Germ...	Zr0.91 V0.09 Ge2
☐ 16	13.7	14	PLU2009	PDF 00-024-0025	Low precision	Deleted		☑	Aragonite	Ca C O3
☐ 17	13.0	22	PLU2009	PDF 00-044-0663	Star (*)	Primary	3.5	☐	Arsenic Iodide Telluride	As5 Te7 I
☐ 18	12.3	43	PLU2009	PDF 01-082-1460	Star (*)	Primary	3.42	☐	Rubidium Iron Selenate	Rb Fe (Se O4)2
☐ 19	12.2	14	PLU2009	PDF 01-071-4433	Indexed	Primary	4.79	☐	Iron Vanadium Germanium	Fe V2 Ge
☐ 20	12.0	15	PLU2009	PDF 00-041-1475	Star (*)	Primary	1	☑	Aragonite	Ca C O3

☐ Group Duplicates

Matched 69615 / 213504 Candidates in 20.7 s.

● Whole Range
○ Subrange

Criterion: 2: Neutral

☐ Auto

Fig. 14: Candidate List with the first two patterns identified

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.

1. In the Candidate List tab, the first pattern in the list is selected: it is Calcite. 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 01-071-3699 matches a part of the peaks of the scan.
3. Mark this pattern by selecting the corresponding check box (or by clicking the **Check** button below the table). The pattern is associated to a color and the image of its stick patterns remains when it is no longer selected (highlighted) in the Candidate List.

+

Check button

☑ 🟥

4. Go down in the list using the arrow buttons below the table. Compare the stick patterns to the scan peaks. The Aragonite and Brucite patterns (00-001-0628 and 04-011-5938) appear to match the scan. Select the corresponding check boxes: the images of their stick patterns remain when they are no longer selected.
5. Leave the non-matching stick patterns unchecked.

Results

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

Case #2: CPD-2.RAW

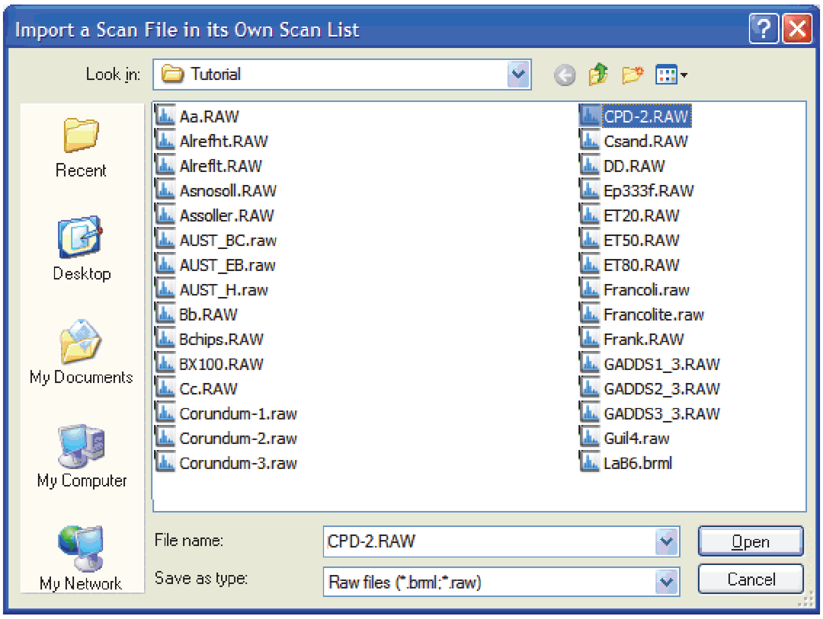
CPD-2 is a mixture of Zincite, Fluorite, Al203 and Brucite from the Rietveld quant round-robin.

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

New button

Import from file button

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 file** data command or the **Import from file** button. The Import a Scan File dialog box will be displayed.
3. Search the Tutorials/EVA[1] 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.



File name: CPD-2.RAW

Save as type: Raw files (*.brml;*.raw)

Fig. 15: Importing the CPD-2.RAW file

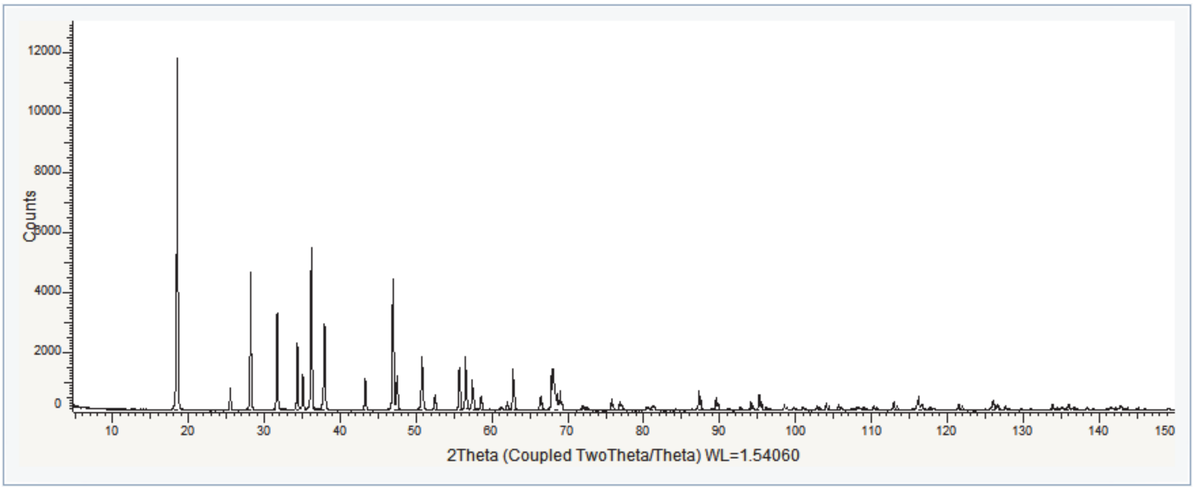


Fig. 16: CPD-2.RAW file imported in the graphical view

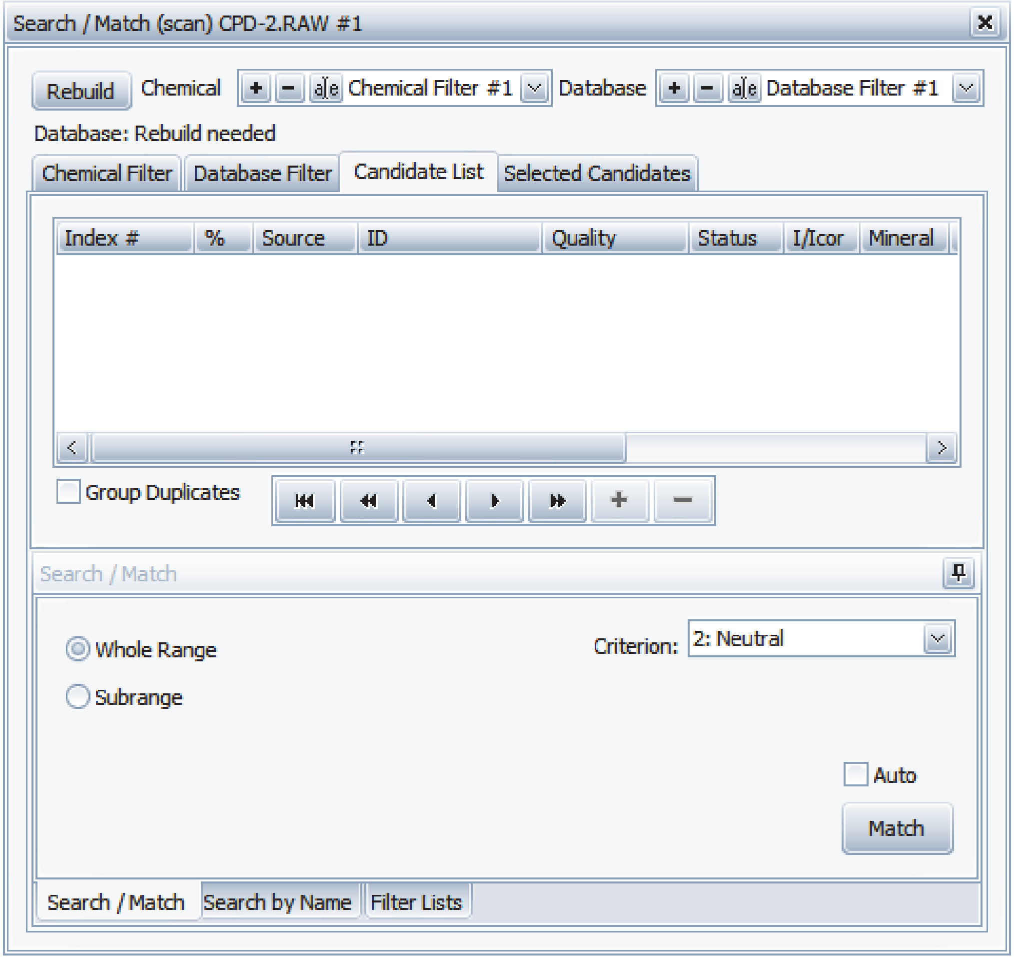
---

[1] 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.

Step 2: Setting the Search Parameters

1. Make certain the scan is selected; if not, select it either in the Data tree or in the graphical view.
2. Click **Search / Match (scan)** in the Data Command panel
— or —
Right-click the scan, click **Tool** on the context menu and then **Search / Match (scan)** on the related submenu.

The **Search / Match (scan)** dialog box will be displayed.



Database: Rebuild needed

☐ Group Duplicates

● Whole Range
○ Subrange

Criterion: 2: Neutral

☐ Auto

Fig. 17: Search/match dialog box

3. Select the **Auto** check box.
4. Set the parameters to use for the Search/Match:

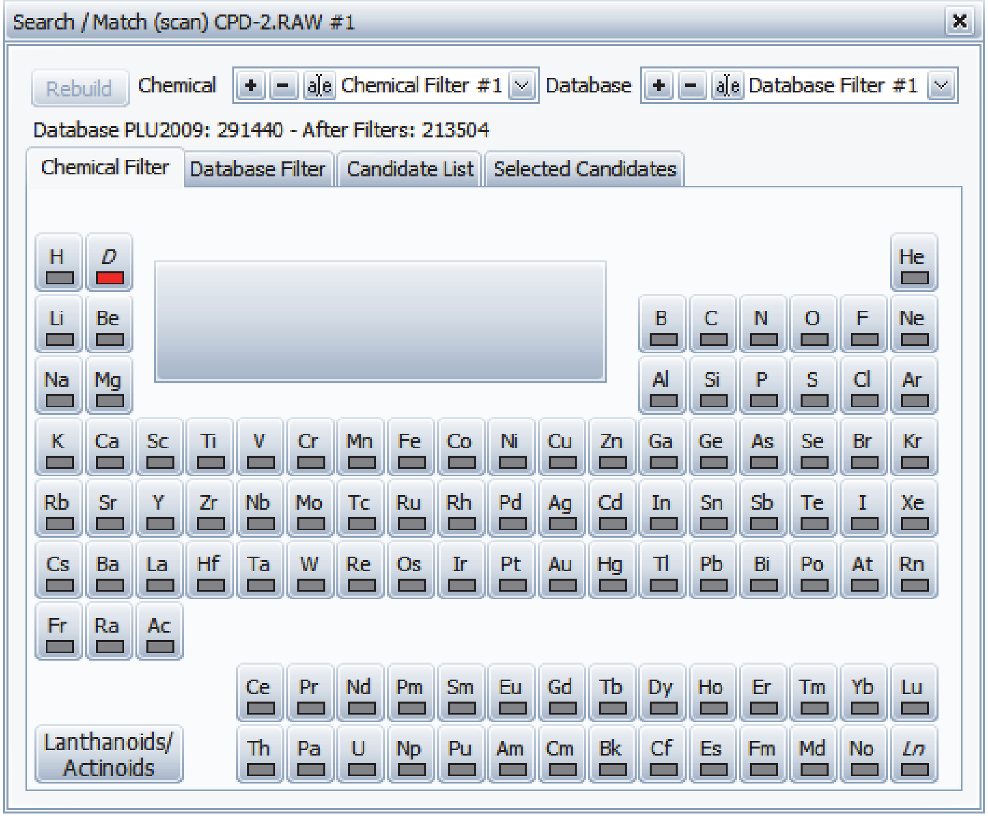
⇒ In the Candidate List tab:

- ☐ Group duplicates
- Criterion = **2** (**Neutral**)
- **Whole Range** selected

NOTE

The Group duplicates option is not used in this example but this is a practical option which can be used without any risk.

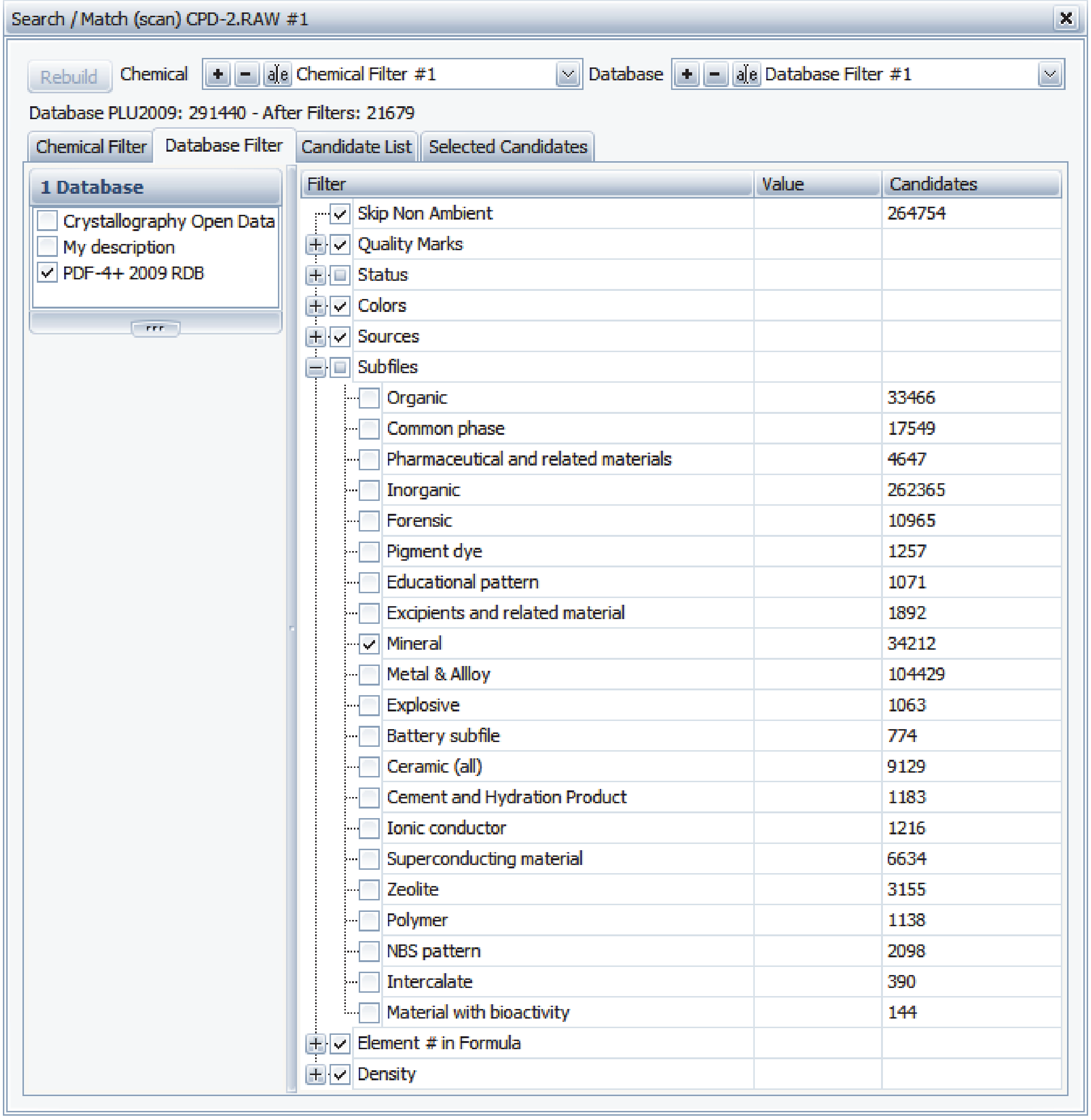
⇒ In the Chemical Filter tab:



Database PLU2009: 291440 - After Filters: 213504

No chemical filter, except D (deuterium) is Discarded (red)

⇒ In the Database Filter tab:



Database PLU2009: 291440 - After Filters: 21679

1 Database

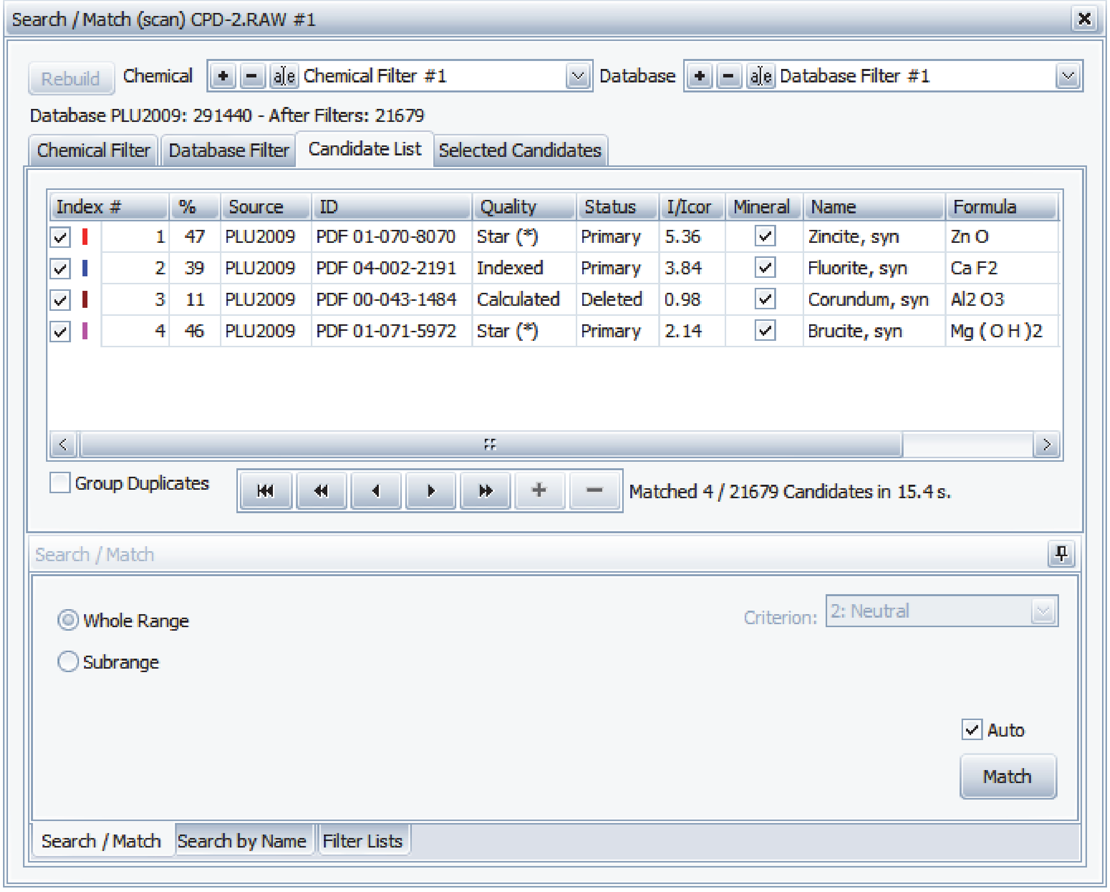
☐ Crystallography Open Data
☐ My description
☑ PDF-4+ 2009 RDB

Filter	Value	Candidates
☑ Skip Non Ambient		264754
☑ Quality Marks		
☐ Status		
☑ Colors		
☑ Sources		
☐ Subfiles		
☐ Organic		33466
☐ Common phase		17549
☐ Pharmaceutical and related materials		4647
☐ Inorganic		262365
☐ Forensic		10965
☐ Pigment dye		1257
☐ Educational pattern		1071
☐ Excipients and related material		1892
☑ Mineral		34212
☐ Metal & Allloy		104429
☐ Explosive		1063
☐ Battery subfile		774
☐ Ceramic (all)		9129
☐ Cement and Hydration Product		1183
☐ Ionic conductor		1216
☐ Superconducting material		6634
☐ Zeolite		3155
☐ Polymer		1138
☐ NBS pattern		2098
☐ Intercalate		390
☐ Material with bioactivity		144
☑ Element # in Formula		
☑ Density		

- ☑ only the Mineral subfile is selected
- ☑ all Quality Marks are selected
- ☑ all Status are selected except ☐ **A** (alternative) that is cleared

5. Click the **Match** button. The candidates are listed in the Candidate List tab.

Step 3: Automatic Matching Procedure



Search / Match (scan) CPD-2.RAW #1

Database PLU2009: 291440 - After Filters: 21679

Index #		%	Source	ID	Quality	Status	I/Icor	Mineral	Name	Formula
☑ 🟥	1	47	PLU2009	PDF 01-070-8070	Star (*)	Primary	5.36	☑	Zincite, syn	Zn O
☑ 🟦	2	39	PLU2009	PDF 04-002-2191	Indexed	Primary	3.84	☑	Fluorite, syn	Ca F2
☑ 🟥	3	11	PLU2009	PDF 00-043-1484	Calculated	Deleted	0.98	☑	Corundum, syn	Al2 O3
☑ 🟪	4	46	PLU2009	PDF 01-071-5972	Star (*)	Primary	2.14	☑	Brucite, syn	Mg (O H)2

☐ Group Duplicates

Matched 4 / 21679 Candidates in 15.4 s.

● Whole Range
○ Subrange

Criterion: 2: Neutral

☑ Auto

Fig. 18: Candidate List with the identified patterns selected

☑ 🟥

Pattern checked

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

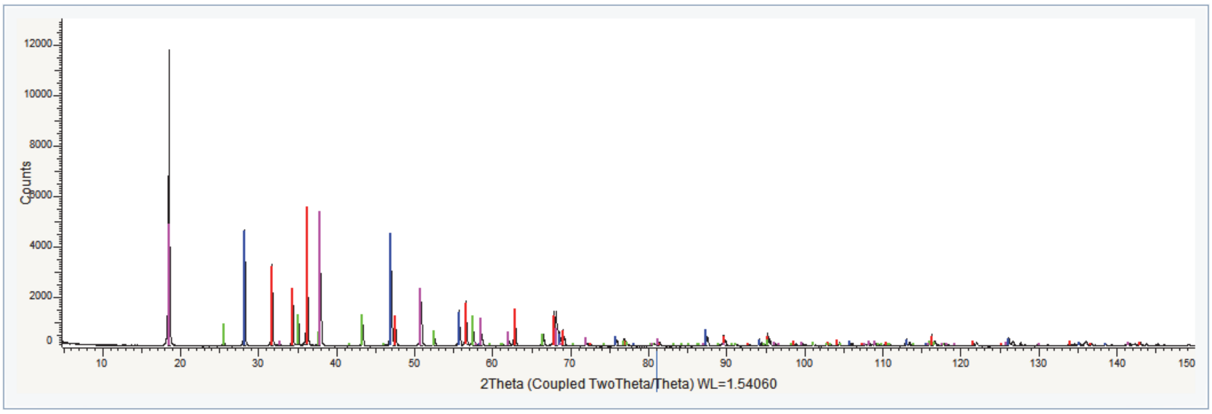


Fig. 19: CPD-2 scan displayed in the graphical view with the four patterns 01-070-8070, 04-002-2191, 00-043-1484 and 01-071-5972

Results

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

Case #3: Mineral mixture

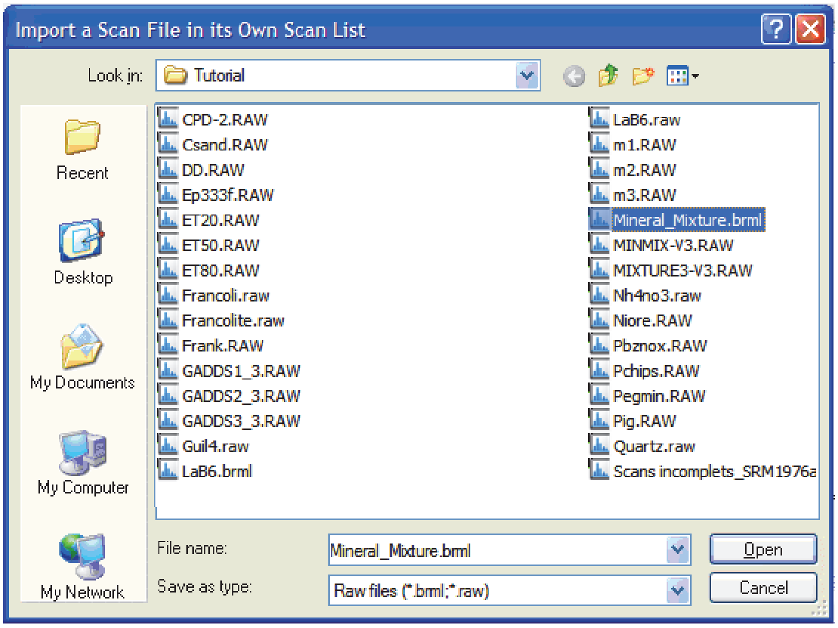
Mineral mixture is a mixture of Zincite, Quartz, Calcite, Galena, Fluorite, Corundum and Rutil.

Step 1: Creating a New EVA Document and Importing Mineral_mixture.brml

New button

Import from file button

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 file** data command or the **Import from file** button. The Import a Scan File dialog box will be displayed.
3. Search the Tutorials/EVA[1] directory and select the Mineral_mixture.brml file.
4. Click **Open**. The scan Mineral mixture will be displayed in the graphical view of the EVA document.



File name: Mineral_Mixture.brml

Save as type: Raw files (*.brml;*.raw)

Fig. 20: Importing the Mineral_mixture.brml file

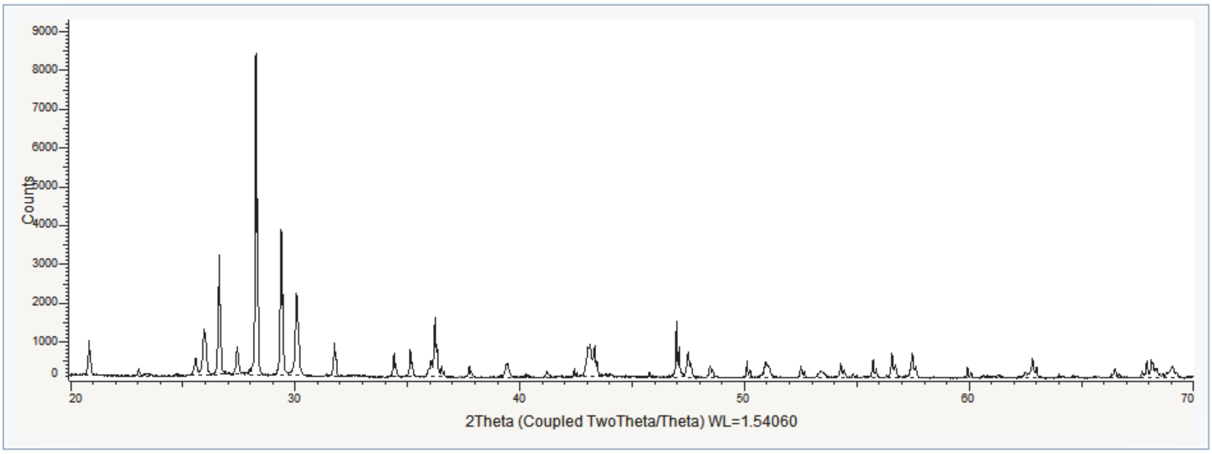


Fig. 21: Mineral_mixture.brml file imported in the graphical view

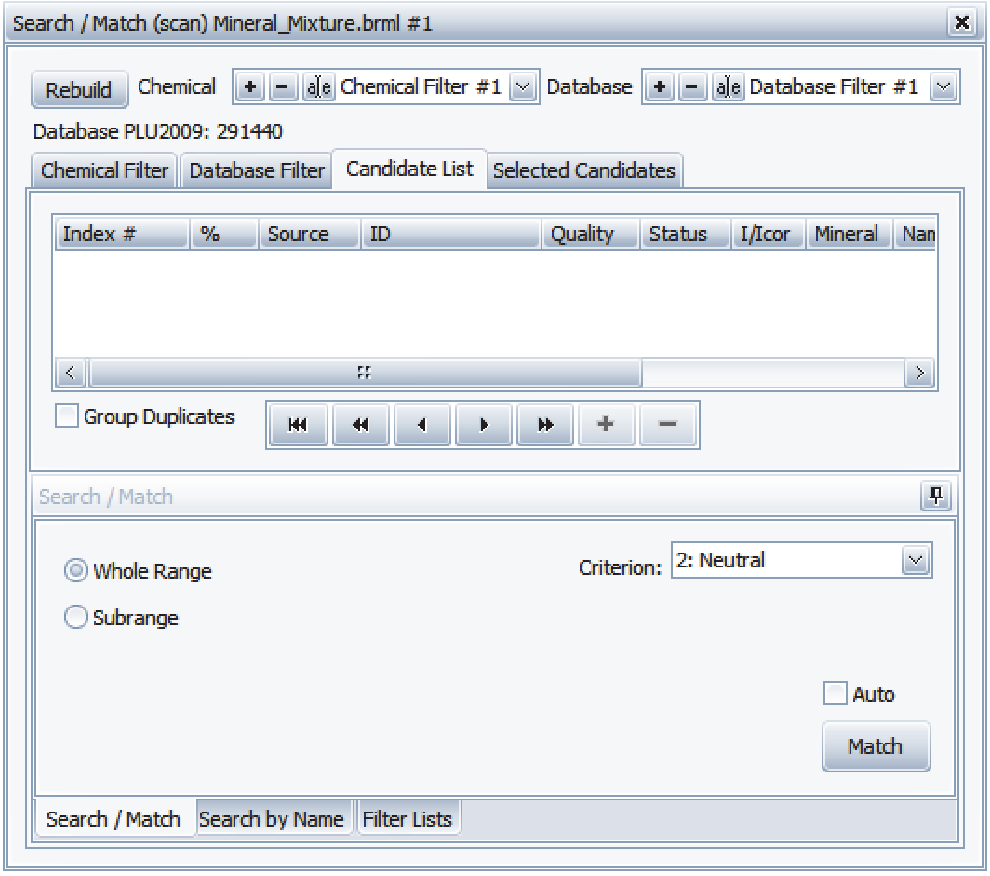
---

[1] 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.

Step 2: Setting the Search Parameters

1. Make certain the scan is selected; if not, select it either in the Data tree or in the graphical view.
2. Click **Search / Match (scan)** in the Data Command panel
   — or —
   Right-click the scan, click **Tool** on the context menu and then **Search / Match (scan)** on the related submenu.

   The **Search / Match (scan)** dialog box will be displayed.



Search / Match (scan) Mineral_Mixture.brml #1

Chemical Filter #1

Database Filter #1

Database PLU2009: 291440

☐ Group Duplicates

● Whole Range

○ Subrange

Criterion: 2: Neutral

☐ Auto

Fig. 22: Search/match dialog box

3. Select the **Auto** check box.
4. Set the parameters to use for the Search/Match:

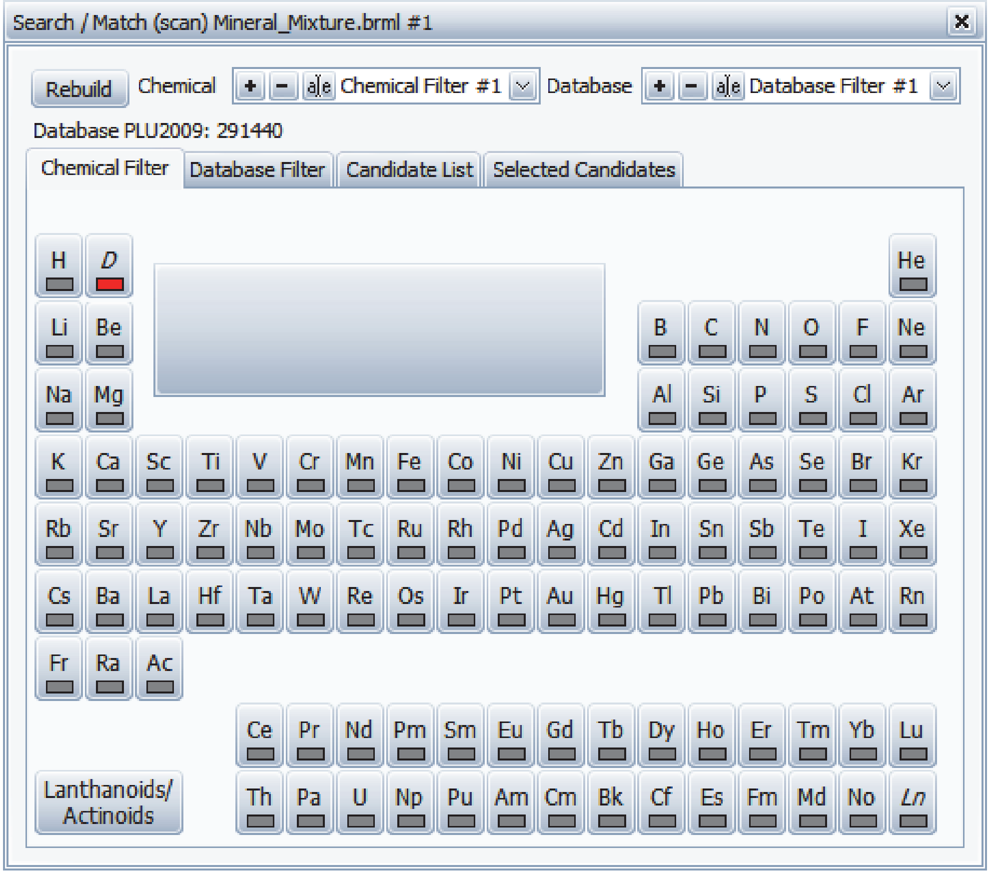
   ⇒ In the Candidate List tab:

   - ☐ Group duplicates
   - Criterion = **2** (**Neutral**)
   - **Whole Range** selected

NOTE

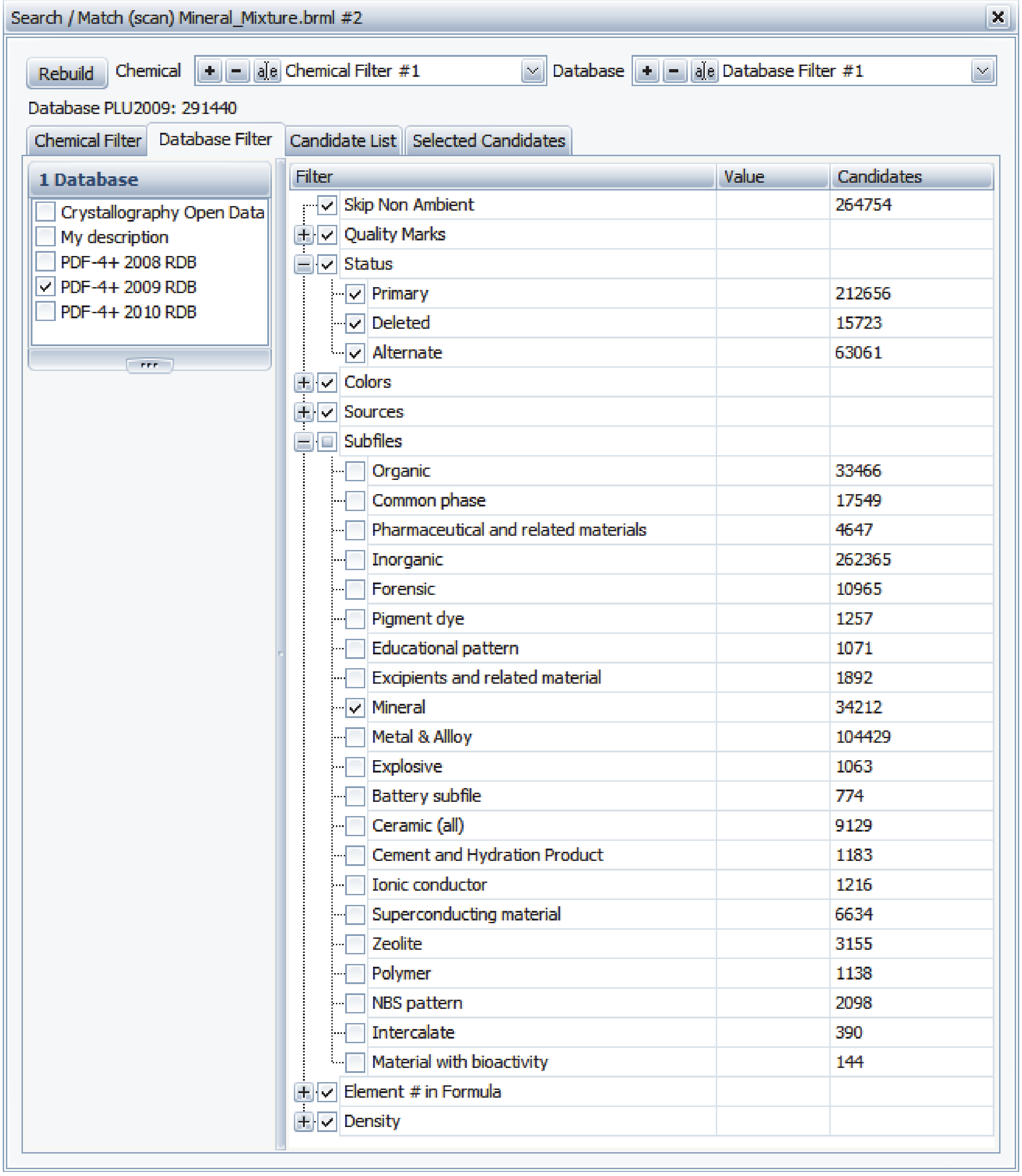
The Group duplicates option is not used in this example but this is a practical option which can be used without any risk.

⇒ In the Chemical Filter tab:



No chemical filter, except D (deuterium) is Discarded (red).

⇒ In the Database Filter tab:



Chemical: Chemical Filter #1
Database: Database Filter #1

Database PLU2009: 291440

1 Database

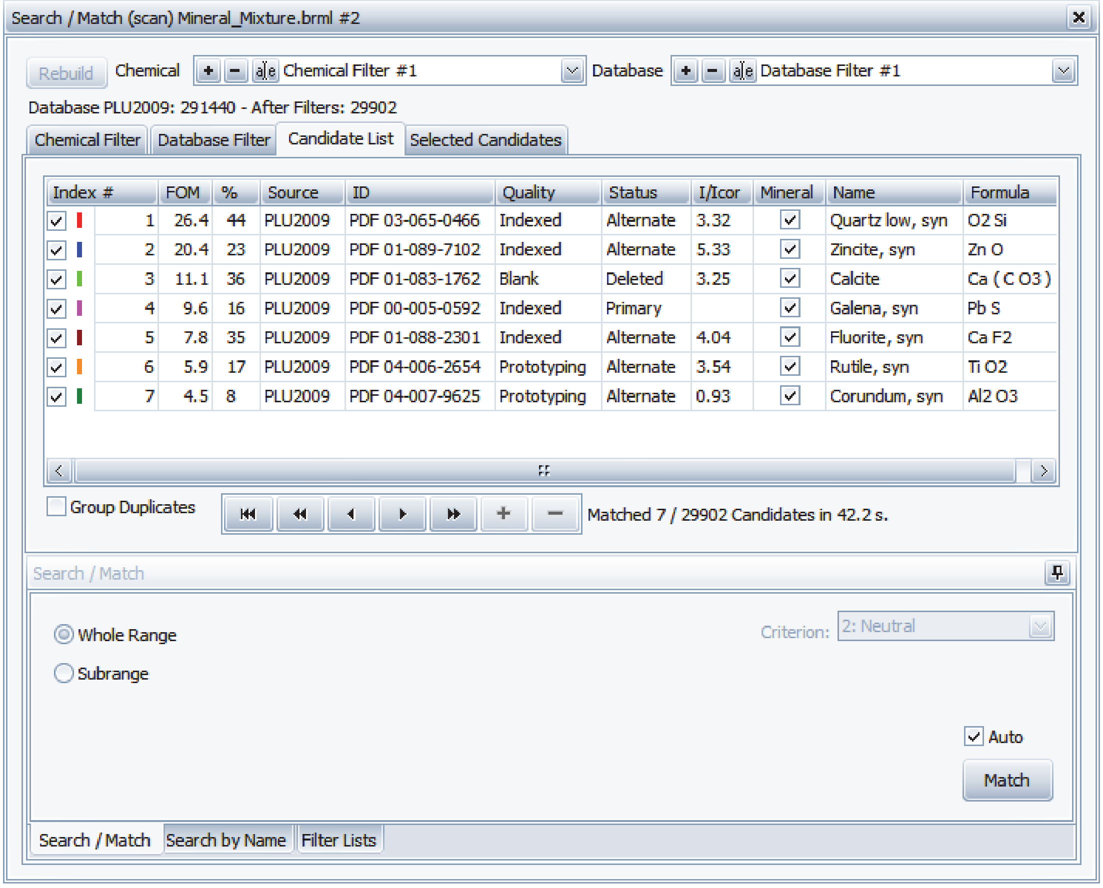
☐ Crystallography Open Data
☐ My description
☐ PDF-4+ 2008 RDB
☑ PDF-4+ 2009 RDB
☐ PDF-4+ 2010 RDB

Filter	Value	Candidates
☑ Skip Non Ambient		264754
☑ Quality Marks		
☑ Status		
☑ Primary		212656
☑ Deleted		15723
☑ Alternate		63061
☑ Colors		
☑ Sources		
☐ Subfiles		
☐ Organic		33466
☐ Common phase		17549
☐ Pharmaceutical and related materials		4647
☐ Inorganic		262365
☐ Forensic		10965
☐ Pigment dye		1257
☐ Educational pattern		1071
☐ Excipients and related material		1892
☑ Mineral		34212
☐ Metal & Allloy		104429
☐ Explosive		1063
☐ Battery subfile		774
☐ Ceramic (all)		9129
☐ Cement and Hydration Product		1183
☐ Ionic conductor		1216
☐ Superconducting material		6634
☐ Zeolite		3155
☐ Polymer		1138
☐ NBS pattern		2098
☐ Intercalate		390
☐ Material with bioactivity		144
☑ Element # in Formula		
☑ Density		

- ☑ only the **Mineral** subfile is selected
- ☑ all Quality Marks are selected
- ☑ all Status are selected

5. Click the **Match** button. The candidates are listed in the Candidate List tab.

Step 3: Automatic Matching Procedure



Search / Match (scan) Mineral_Mixture.brml #2

Database PLU2009: 291440 - After Filters: 29902

Index #	FOM	%	Source	ID	Quality	Status	I/Icor	Mineral	Name	Formula
☑ 🟥 1	26.4	44	PLU2009	PDF 03-065-0466	Indexed	Alternate	3.32	☑	Quartz low, syn	O2 Si
☑ 🟦 2	20.4	23	PLU2009	PDF 01-089-7102	Indexed	Alternate	5.33	☑	Zincite, syn	Zn O
☑ 🟩 3	11.1	36	PLU2009	PDF 01-083-1762	Blank	Deleted	3.25	☑	Calcite	Ca (C O3)
☑ 🟪 4	9.6	16	PLU2009	PDF 00-005-0592	Indexed	Primary		☑	Galena, syn	Pb S
☑ 🟥 5	7.8	35	PLU2009	PDF 01-088-2301	Indexed	Alternate	4.04	☑	Fluorite, syn	Ca F2
☑ 🟧 6	5.9	17	PLU2009	PDF 04-006-2654	Prototyping	Alternate	3.54	☑	Rutile, syn	Ti O2
☑ 🟩 7	4.5	8	PLU2009	PDF 04-007-9625	Prototyping	Alternate	0.93	☑	Corundum, syn	Al2 O3

☐ Group Duplicates

Matched 7 / 29902 Candidates in 42.2 s.

● Whole Range
○ Subrange

Criterion: 2: Neutral

☑ Auto

Fig. 23: Candidate List with the found patterns checked

☑ 🟥

Pattern checked

The results of the Automatic Search/Match are displayed in the candidate list. The seven patterns identified are automatically checked and therefore added to the data tree and to the graphical view.

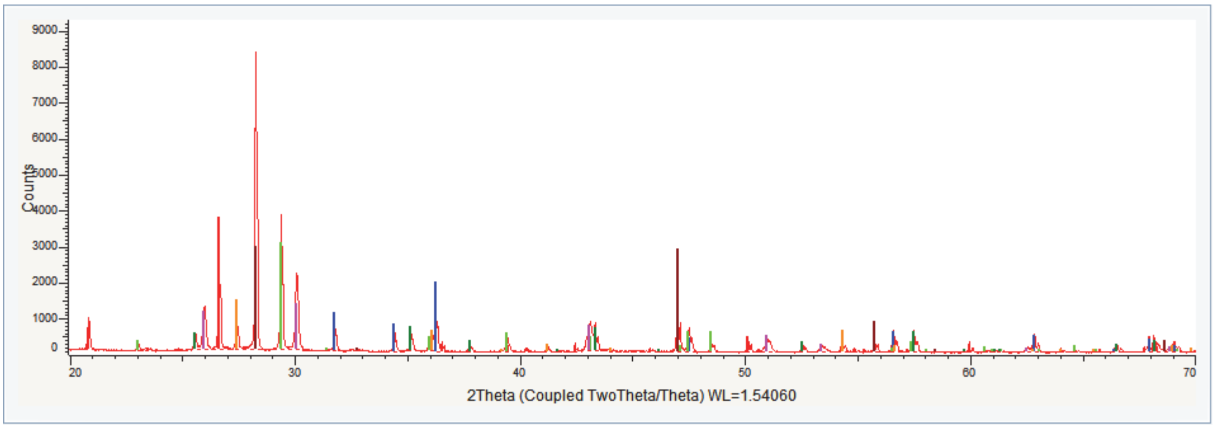


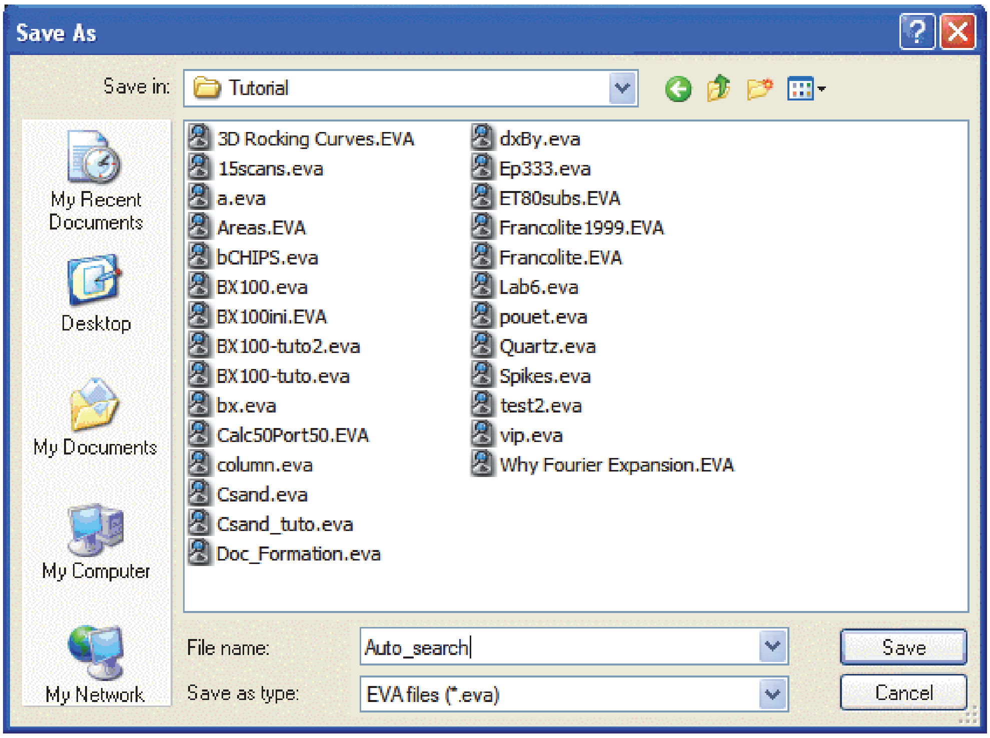
Fig. 24: Mineral_mixture scan displayed in the graphical view with the seven patterns 03-065-0466, 01-089-7102, 01-083-1762, 00-005-0592, 01-088-2301, 04-006-2654 and 04-007-9625

Results

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

Step 4: Saving

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



Save in: Tutorial

File name: Auto_search

Save as type: EVA files (*.eva)

Fig. 25: Auto_search.EVA document

Creating and Using Filter Lists

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

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. Creating a filter list.
3. Using a filter list.

NOTE

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

This tutorial was prepared using PDF 4+ 2009 as a reference database. You may have another reference database.

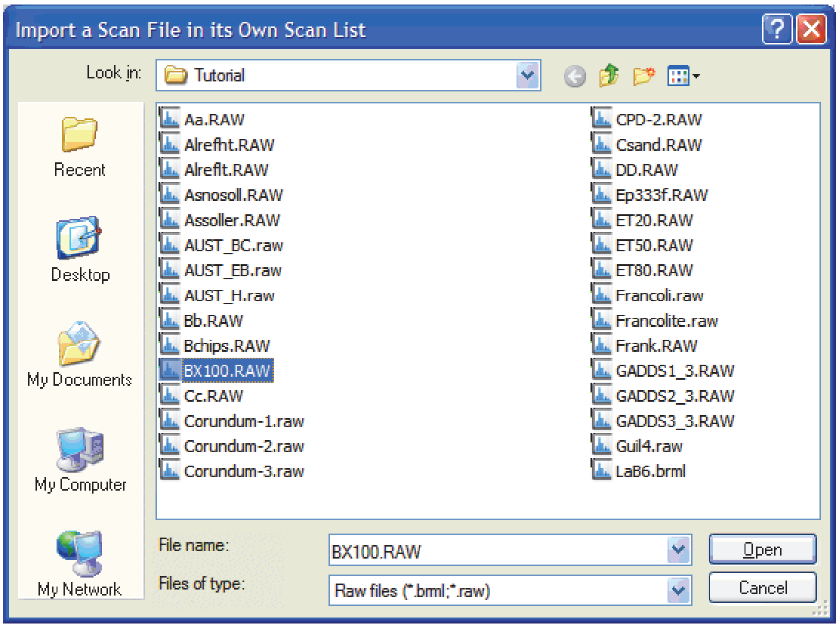
If you have no database, you cannot perform this part of the tutorial using the Search/Match.

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

New button

Import from file button

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 file** data command or the **Import from file** button. The Import from files dialog box will be displayed. Search the Tutorials/EVA[1] directory and select the BX100.RAW file.
3. Click **Open**. The scan BX100 will be displayed in the graphical view of the EVA document.



Import a Scan File in its Own Scan List

Look in: Tutorial

Aa.RAW
Alrefht.RAW
Alrefit.RAW
Asnosoll.RAW
Assoller.RAW
AUST_BC.raw
AUST_EB.raw
AUST_H.raw
Bb.RAW
Bchips.RAW
BX100.RAW
Cc.RAW
Corundum-1.raw
Corundum-2.raw
Corundum-3.raw
CPD-2.RAW
Csand.RAW
DD.RAW
Ep333f.RAW
ET20.RAW
ET50.RAW
ET80.RAW
Francoli.raw
Francolite.raw
Frank.RAW
GADDS1_3.RAW
GADDS2_3.RAW
GADDS3_3.RAW
Guil4.raw
LaB6.brml

File name: BX100.RAW

Files of type: Raw files (*.brml;*.raw)

Fig. 26: Import a Scan File dialog box

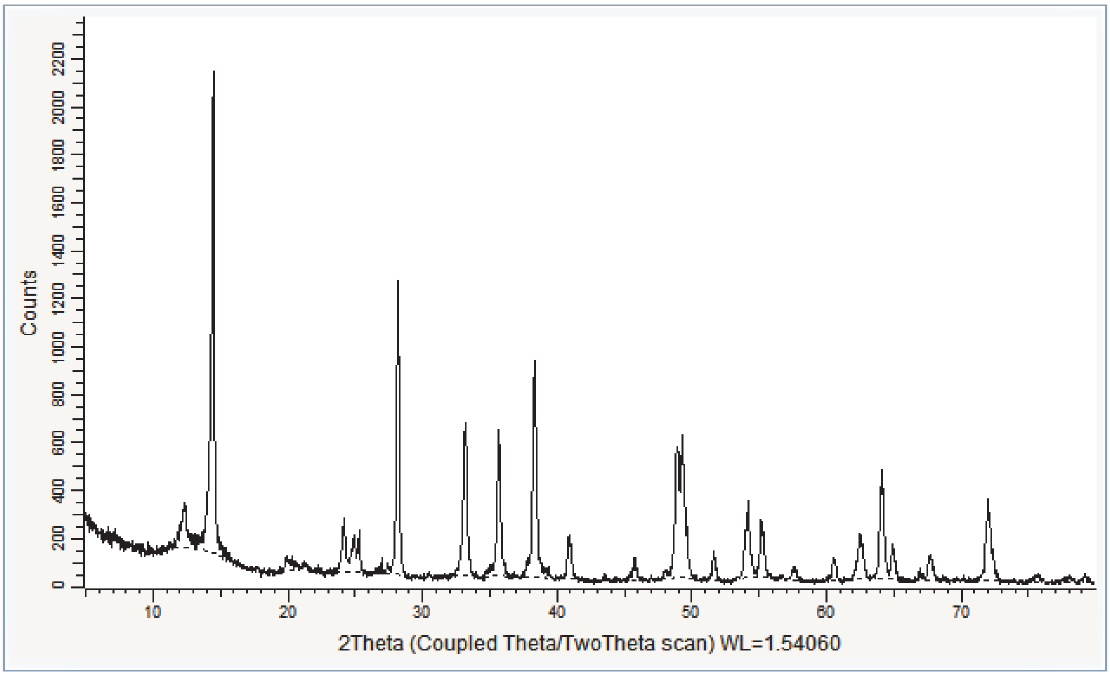


Fig. 27: BX100.RAW imported in the graphical view

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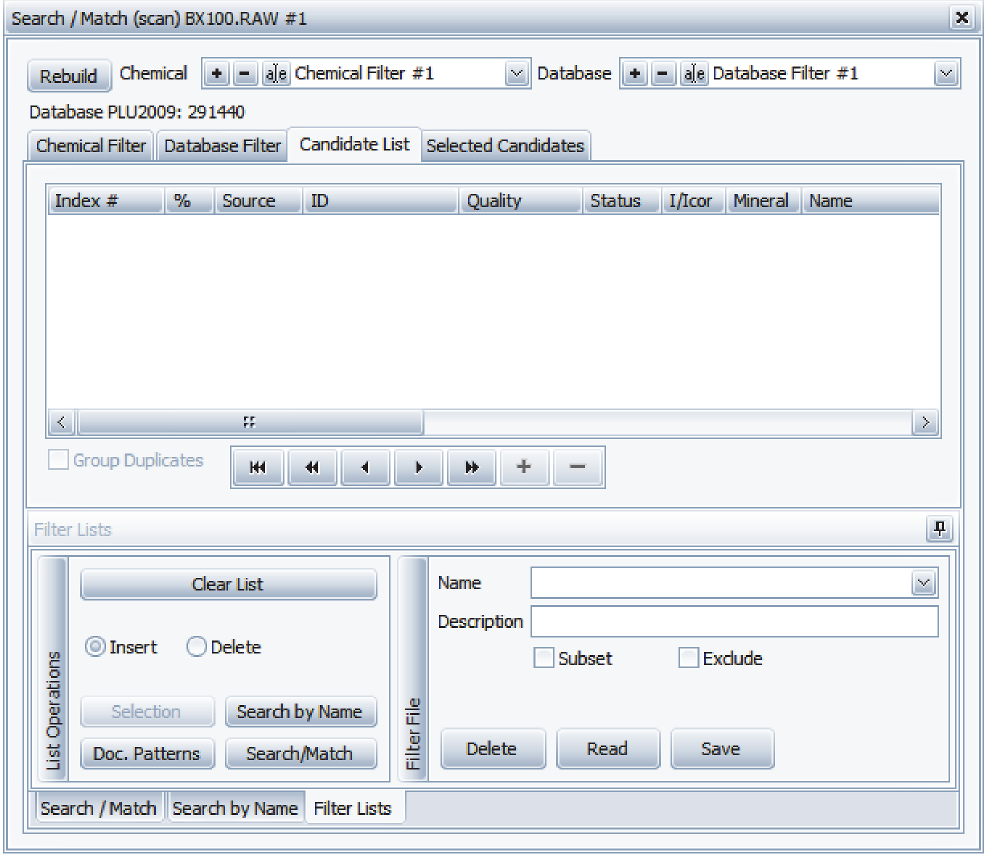
[1] The directory path to the EVA tutorial files is ″C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials″ under Windows XP and ″C:\ProgramData\Bruker AXS\Tutorials″ under Windows 7.
To access the folder with the explorer, select “Display hidden files and folders” in the Folders options.

Step 2: Creating a Filter List

When creating a filter list, there are three ways to add pattern to this list. Each way will be illustrated here.

Adding the document patterns:

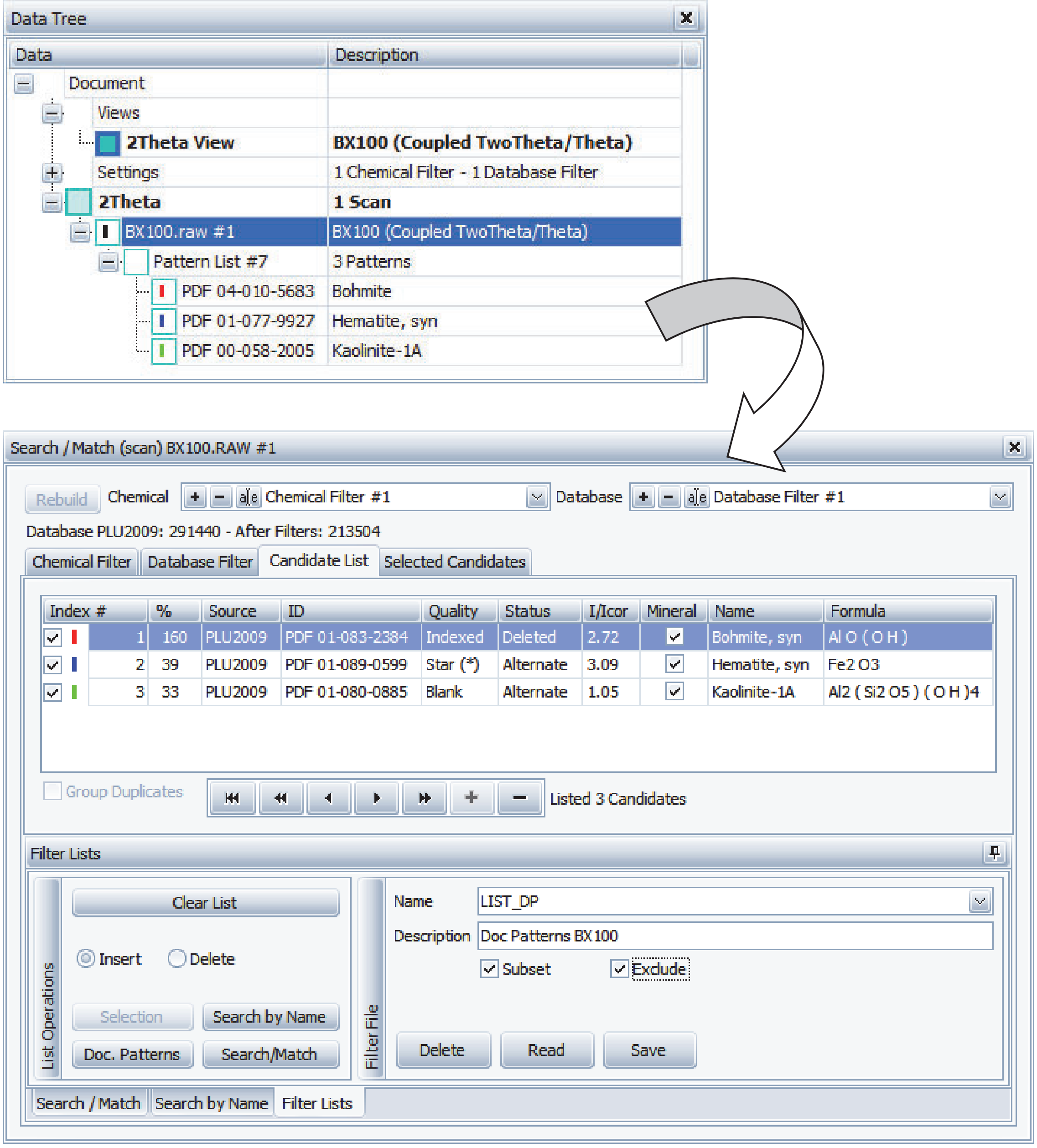
1. Proceed as described in the tutorial chapter “Performing the Semi-Quantitative Phase-Analysis and Comparing” on page 98 until the first Search/match step: Boehmite, Iron Oxide and Kaolinite-1A patterns identified.
2. Close the Search/Match dialog box. The three patterns are listed in the Data tree and displayed in the graphical view.
3. Select the BX100.RAW scan in the Data tree.
4. Click **Search / Match (scan)** in the Data Command panel
   — or —
   Right-click the scan, click **Tool** on the context menu and then **Search / Match (scan)** on the related submenu.
   The **Search / Match (scan)** dialog box will be displayed.
5. Go to the **Filter Lists** tab.



6. Click the **Doc. Patterns** button: the patterns from the current document are added to the Filter list.
7. Enter a name in the **Name** field (limited to 13 characters, spaces are replaced by “_”): *LIST_DP* (for list doc patterns).
8. Enter a description in the **Description** field (optional): *Doc Patterns BX100*.

NOTE

If no description is entered, the name will be used as the list name. If a description is entered, the description will be used as the list name in DIFFRAC.EVA (Database tab of the Settings dialog box, Database filter tab of the Search/match dialog box…).



Data	Description
Document	
Views	
2Theta View	BX100 (Coupled TwoTheta/Theta)
Settings	1 Chemical Filter - 1 Database Filter
2Theta	1 Scan
BX100.raw #1	BX100 (Coupled TwoTheta/Theta)
Pattern List #7	3 Patterns
PDF 04-010-5683	Bohmite
PDF 01-077-9927	Hematite, syn
PDF 00-058-2005	Kaolinite-1A

Database PLU2009: 291440 - After Filters: 213504

	Index #	%	Source	ID	Quality	Status	I/Icor	Mineral	Name	Formula
☑	1	160	PLU2009	PDF 01-083-2384	Indexed	Deleted	2.72	☑	Bohmite, syn	Al O (O H)
☑	2	39	PLU2009	PDF 01-089-0599	Star (*)	Alternate	3.09	☑	Hematite, syn	Fe2 O3
☑	3	33	PLU2009	PDF 01-080-0885	Blank	Alternate	1.05	☑	Kaolinite-1A	Al2 (Si2 O5) (O H)4

Name LIST_DP

Description Doc Patterns BX100

☑ Subset ☑ Exclude

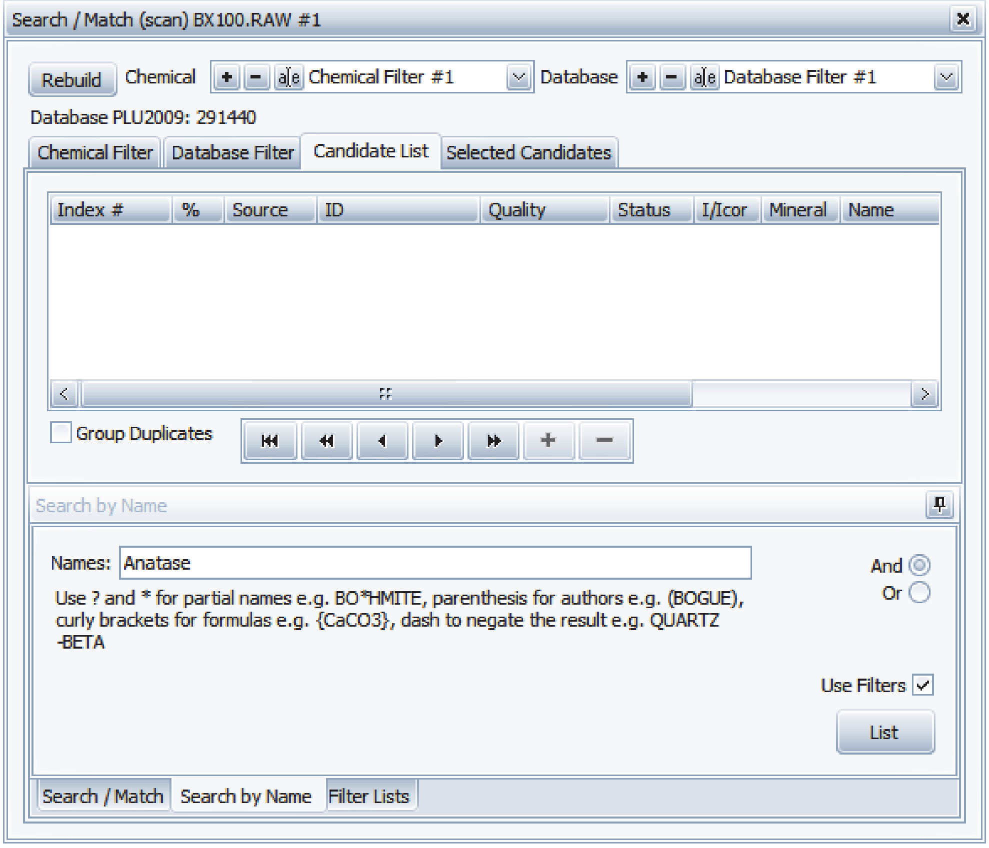
Fig. 28: Adding the document patterns to the filter list

9. Define the list type. It is recommended to select both types. Select the **Subset** and **Exclude** check boxes.

10. Click the **Save** button to save the filter list.

Adding the Search by Name results:

1. Select the BX100.RAW scan in the Data tree.
2. Click **Search / Match (scan)** in the Data Command panel
   — or —
   Right-click the scan, click **Tool** on the context menu and then **Search / Match (scan)** on the related submenu.
   The **Search / Match (scan)** dialog box will be displayed.
3. Go to the **Search by Name** tab.
4. In the **Names** field, enter Anatase.



Names: Anatase

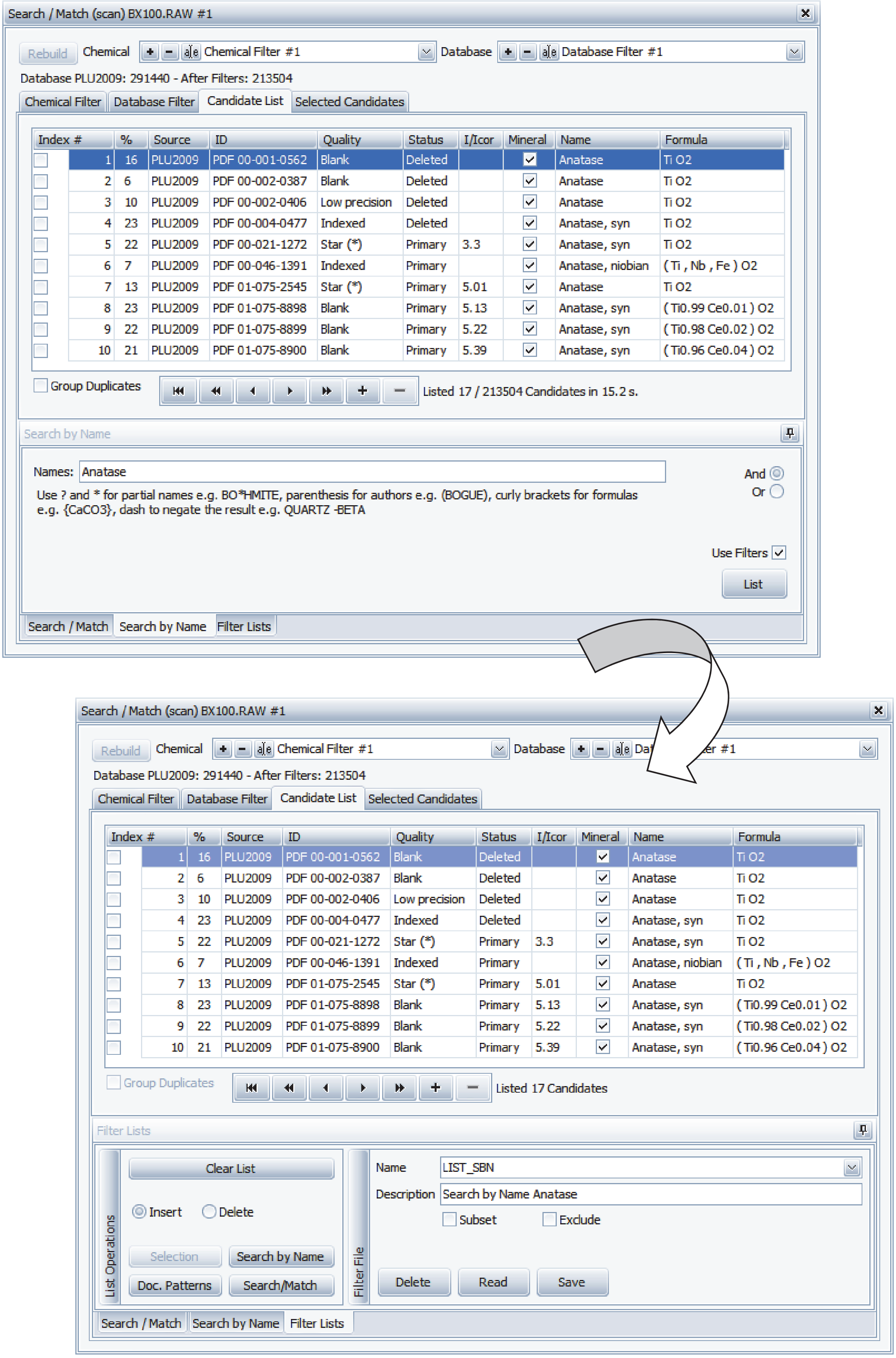
Use ? and * for partial names e.g. BO*HMITE, parenthesis for authors e.g. (BOGUE), curly brackets for formulas e.g. {CaCO3}, dash to negate the result e.g. QUARTZ -BETA

5. Click the **List** button to run the search: 17 candidates are found.
6. Once the search is completed, go to the **Filter Lists** tab. Click the **Search by Name** button: the patterns from the current Search by Name results are added to the Filter list.
7. Enter a name in the **Name** field (limited to 13 characters, spaces are replaced by "_"): *LIST_SBN* (for list Search by Name).
8. Enter a description in the **Description** field (optional): *Search by Name Anatase*.

NOTE

If no description is entered, the name will be used as the list name. If a description is entered, the description will be used as the list name in DIFFRAC.EVA (Database tab of the Settings dialog box, Database filter tab of the Search/match dialog box…).

9. Define the list type. It is recommended to select both types. Select the **Subset** and **Exclude** check boxes.
10. Click the **Save** button to save the filter list.



Database PLU2009: 291440 - After Filters: 213504

	Index #	%	Source	ID	Quality	Status	I/Icor	Mineral	Name	Formula
☐	1	16	PLU2009	PDF 00-001-0562	Blank	Deleted		☑	Anatase	Ti O2
☐	2	6	PLU2009	PDF 00-002-0387	Blank	Deleted		☑	Anatase	Ti O2
☐	3	10	PLU2009	PDF 00-002-0406	Low precision	Deleted		☑	Anatase	Ti O2
☐	4	23	PLU2009	PDF 00-004-0477	Indexed	Deleted		☑	Anatase, syn	Ti O2
☐	5	22	PLU2009	PDF 00-021-1272	Star (*)	Primary	3.3	☑	Anatase, syn	Ti O2
☐	6	7	PLU2009	PDF 00-046-1391	Indexed	Primary		☑	Anatase, niobian	(Ti , Nb , Fe) O2
☐	7	13	PLU2009	PDF 01-075-2545	Star (*)	Primary	5.01	☑	Anatase	Ti O2
☐	8	23	PLU2009	PDF 01-075-8898	Blank	Primary	5.13	☑	Anatase, syn	(Ti0.99 Ce0.01) O2
☐	9	22	PLU2009	PDF 01-075-8899	Blank	Primary	5.22	☑	Anatase, syn	(Ti0.98 Ce0.02) O2
☐	10	21	PLU2009	PDF 01-075-8900	Blank	Primary	5.39	☑	Anatase, syn	(Ti0.96 Ce0.04) O2

☐ Group Duplicates

Listed 17 / 213504 Candidates in 15.2 s.

Search by Name

Names: Anatase

Use ? and * for partial names e.g. BO*HMITE, parenthesis for authors e.g. (BOGUE), curly brackets for formulas e.g. {CaCO3}, dash to negate the result e.g. QUARTZ -BETA

And ●
Or ○

Use Filters ☑

List

Search / Match (scan) BX100.RAW #1

Database PLU2009: 291440 - After Filters: 213504

	Index #	%	Source	ID	Quality	Status	I/Icor	Mineral	Name	Formula
☐	1	16	PLU2009	PDF 00-001-0562	Blank	Deleted		☑	Anatase	Ti O2
☐	2	6	PLU2009	PDF 00-002-0387	Blank	Deleted		☑	Anatase	Ti O2
☐	3	10	PLU2009	PDF 00-002-0406	Low precision	Deleted		☑	Anatase	Ti O2
☐	4	23	PLU2009	PDF 00-004-0477	Indexed	Deleted		☑	Anatase, syn	Ti O2
☐	5	22	PLU2009	PDF 00-021-1272	Star (*)	Primary	3.3	☑	Anatase, syn	Ti O2
☐	6	7	PLU2009	PDF 00-046-1391	Indexed	Primary		☑	Anatase, niobian	(Ti , Nb , Fe) O2
☐	7	13	PLU2009	PDF 01-075-2545	Star (*)	Primary	5.01	☑	Anatase	Ti O2
☐	8	23	PLU2009	PDF 01-075-8898	Blank	Primary	5.13	☑	Anatase, syn	(Ti0.99 Ce0.01) O2
☐	9	22	PLU2009	PDF 01-075-8899	Blank	Primary	5.22	☑	Anatase, syn	(Ti0.98 Ce0.02) O2
☐	10	21	PLU2009	PDF 01-075-8900	Blank	Primary	5.39	☑	Anatase, syn	(Ti0.96 Ce0.04) O2

☐ Group Duplicates

Listed 17 Candidates

Filter Lists

● Insert ○ Delete

Name: LIST_SBN

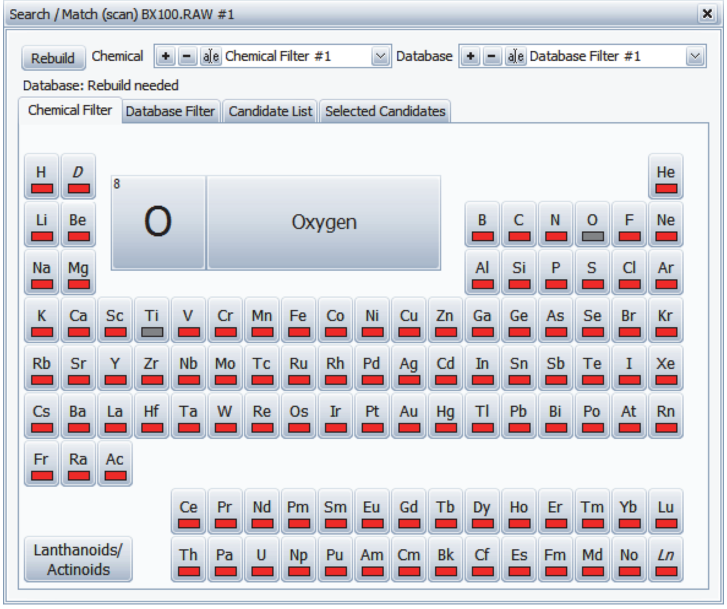
Description: Search by Name Anatase

☐ Subset ☐ Exclude

Fig. 29: Adding the Search by Name results to the filter list

Adding the Search/Match results:

1. Select the BX100.RAW scan in the Data tree.
2. Click **Search / Match (scan)** in the Data Command panel
   — or —
   Right-click the scan, click **Tool** on the context menu and then **Search / Match (scan)** on the related submenu.
   The **Search / Match (scan)** dialog box will be displayed.
3. In the **Chemical Filter** tab, set all the elements except Ti and O (grey) to discarded (red).

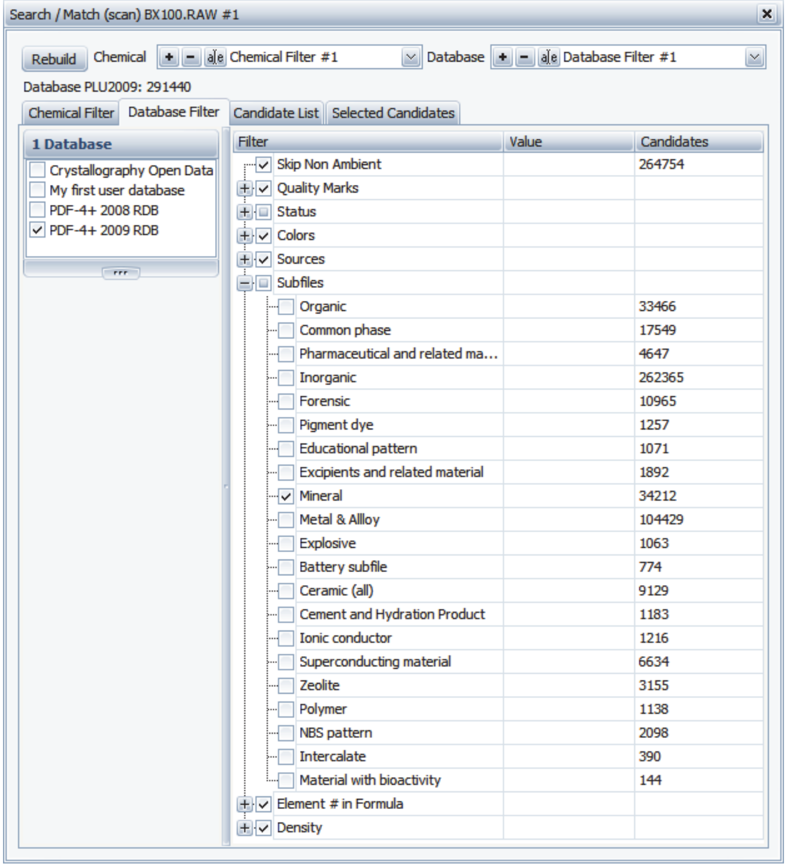


Search / Match (scan) BX100.RAW #1

Chemical: Chemical Filter #1 — Database: Database Filter #1

Database: Rebuild needed

4. In the **Database Filter** tab, select only the **Mineral** subfile.



Search / Match (scan) BX100.RAW #1

Chemical: Chemical Filter #1 — Database: Database Filter #1

Database PLU2009: 291440

1 Database
- ☐ Crystallography Open Data
- ☐ My first user database
- ☐ PDF-4+ 2008 RDB
- ☑ PDF-4+ 2009 RDB

Filter	Value	Candidates
☑ Skip Non Ambient		264754
☑ Quality Marks		
☐ Status		
☑ Colors		
☑ Sources		
☐ Subfiles		
☐ Organic		33466
☐ Common phase		17549
☐ Pharmaceutical and related ma…		4647
☐ Inorganic		262365
☐ Forensic		10965
☐ Pigment dye		1257
☐ Educational pattern		1071
☐ Excipients and related material		1892
☑ Mineral		34212
☐ Metal & Allloy		104429
☐ Explosive		1063
☐ Battery subfile		774
☐ Ceramic (all)		9129
☐ Cement and Hydration Product		1183
☐ Ionic conductor		1216
☐ Superconducting material		6634
☐ Zeolite		3155
☐ Polymer		1138
☐ NBS pattern		2098
☐ Intercalate		390
☐ Material with bioactivity		144
☑ Element # in Formula		
☑ Density		

5. In the **Candidate List** tab, keep the default parameters:
    - ☐ Group duplicates
    - Criterion = **2** (**Neutral**)
    - **Whole Range** selected
    - ☐ Auto

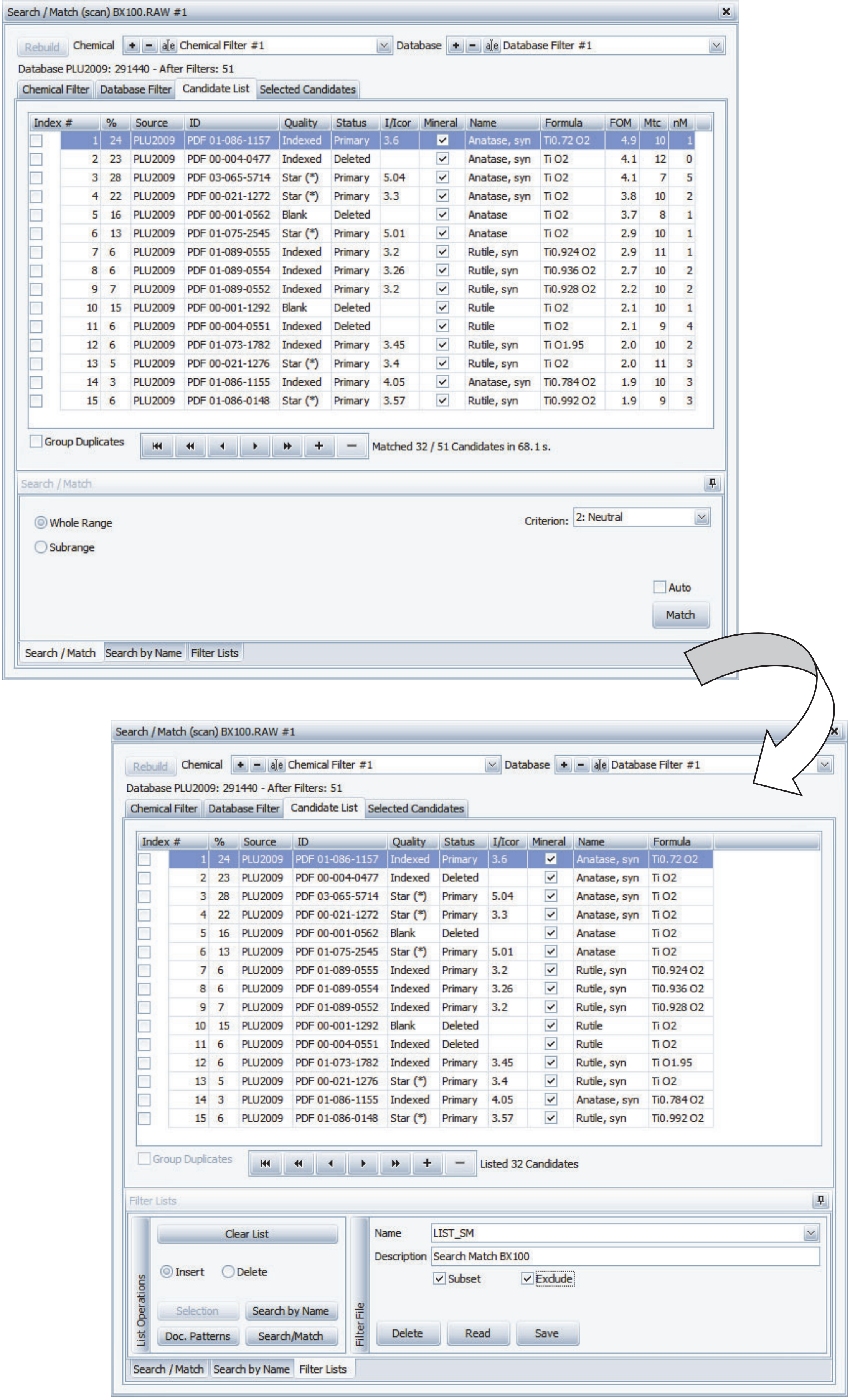
NOTE

The Group duplicates option is not used in this example but this is a practical option which can be used without any risk.

6. Click the **Match** button: 32 candidates are found (with PDF-4+ 2009).
7. Once the search is completed, go to the **Filter Lists** tab. Click the **Search/Match** button: the patterns from the current Search/Match results are added to the Filter list.
8. Enter a name in the **Name** field (limited to 13 characters, spaces are replaced by "_"): *LIST_SM* (for list Search/Match).
9. Enter a description in the **Description** field (optional): *Search Match BX100.*
10. Define the list type. It is recommended to select both types. Select the **Subset** and **Exclude** check boxes.
11. Click the **Save** button to save the filter list.

NOTE

If no description is entered, the name will be used as the list name. If a description is entered, the description will be used as the list name in DIFFRAC.EVA (Database tab of the Settings dialog box, Database filter tab of the Search/match dialog box…).



Database PLU2009: 291440 - After Filters: 51

	Index #	%	Source	ID	Quality	Status	I/Icor	Mineral	Name	Formula	FOM	Mtc	nM
☐	1	24	PLU2009	PDF 01-086-1157	Indexed	Primary	3.6	☑	Anatase, syn	Ti0.72 O2	4.9	10	1
☐	2	23	PLU2009	PDF 00-004-0477	Indexed	Deleted		☑	Anatase, syn	Ti O2	4.1	12	0
☐	3	28	PLU2009	PDF 03-065-5714	Star (*)	Primary	5.04	☑	Anatase, syn	Ti O2	4.1	7	5
☐	4	22	PLU2009	PDF 00-021-1272	Star (*)	Primary	3.3	☑	Anatase, syn	Ti O2	3.8	10	2
☐	5	16	PLU2009	PDF 00-001-0562	Blank	Deleted		☑	Anatase	Ti O2	3.7	8	1
☐	6	13	PLU2009	PDF 01-075-2545	Star (*)	Primary	5.01	☑	Anatase	Ti O2	2.9	10	1
☐	7	6	PLU2009	PDF 01-089-0555	Indexed	Primary	3.2	☑	Rutile, syn	Ti0.924 O2	2.9	11	1
☐	8	6	PLU2009	PDF 01-089-0554	Indexed	Primary	3.26	☑	Rutile, syn	Ti0.936 O2	2.7	10	2
☐	9	7	PLU2009	PDF 01-089-0552	Indexed	Primary	3.2	☑	Rutile, syn	Ti0.928 O2	2.2	10	2
☐	10	15	PLU2009	PDF 00-001-1292	Blank	Deleted		☑	Rutile	Ti O2	2.1	10	1
☐	11	6	PLU2009	PDF 00-004-0551	Indexed	Deleted		☑	Rutile	Ti O2	2.1	9	4
☐	12	6	PLU2009	PDF 01-073-1782	Indexed	Primary	3.45	☑	Rutile, syn	Ti O1.95	2.0	10	2
☐	13	5	PLU2009	PDF 00-021-1276	Star (*)	Primary	3.4	☑	Rutile, syn	Ti O2	2.0	11	3
☐	14	3	PLU2009	PDF 01-086-1155	Indexed	Primary	4.05	☑	Anatase, syn	Ti0.784 O2	1.9	10	3
☐	15	6	PLU2009	PDF 01-086-0148	Star (*)	Primary	3.57	☑	Rutile, syn	Ti0.992 O2	1.9	9	3

☐ Group Duplicates

Matched 32 / 51 Candidates in 68.1 s.

● Whole Range
○ Subrange

Criterion: 2: Neutral

☐ Auto

Database PLU2009: 291440 - After Filters: 51

	Index #	%	Source	ID	Quality	Status	I/Icor	Mineral	Name	Formula
☐	1	24	PLU2009	PDF 01-086-1157	Indexed	Primary	3.6	☑	Anatase, syn	Ti0.72 O2
☐	2	23	PLU2009	PDF 00-004-0477	Indexed	Deleted		☑	Anatase, syn	Ti O2
☐	3	28	PLU2009	PDF 03-065-5714	Star (*)	Primary	5.04	☑	Anatase, syn	Ti O2
☐	4	22	PLU2009	PDF 00-021-1272	Star (*)	Primary	3.3	☑	Anatase, syn	Ti O2
☐	5	16	PLU2009	PDF 00-001-0562	Blank	Deleted		☑	Anatase	Ti O2
☐	6	13	PLU2009	PDF 01-075-2545	Star (*)	Primary	5.01	☑	Anatase	Ti O2
☐	7	6	PLU2009	PDF 01-089-0555	Indexed	Primary	3.2	☑	Rutile, syn	Ti0.924 O2
☐	8	6	PLU2009	PDF 01-089-0554	Indexed	Primary	3.26	☑	Rutile, syn	Ti0.936 O2
☐	9	7	PLU2009	PDF 01-089-0552	Indexed	Primary	3.2	☑	Rutile, syn	Ti0.928 O2
☐	10	15	PLU2009	PDF 00-001-1292	Blank	Deleted		☑	Rutile	Ti O2
☐	11	6	PLU2009	PDF 00-004-0551	Indexed	Deleted		☑	Rutile	Ti O2
☐	12	6	PLU2009	PDF 01-073-1782	Indexed	Primary	3.45	☑	Rutile, syn	Ti O1.95
☐	13	5	PLU2009	PDF 00-021-1276	Star (*)	Primary	3.4	☑	Rutile, syn	Ti O2
☐	14	3	PLU2009	PDF 01-086-1155	Indexed	Primary	4.05	☑	Anatase, syn	Ti0.784 O2
☐	15	6	PLU2009	PDF 01-086-0148	Star (*)	Primary	3.57	☑	Rutile, syn	Ti0.992 O2

☐ Group Duplicates

Listed 32 Candidates

● Insert ○ Delete

Name: LIST_SM

Description: Search Match BX100

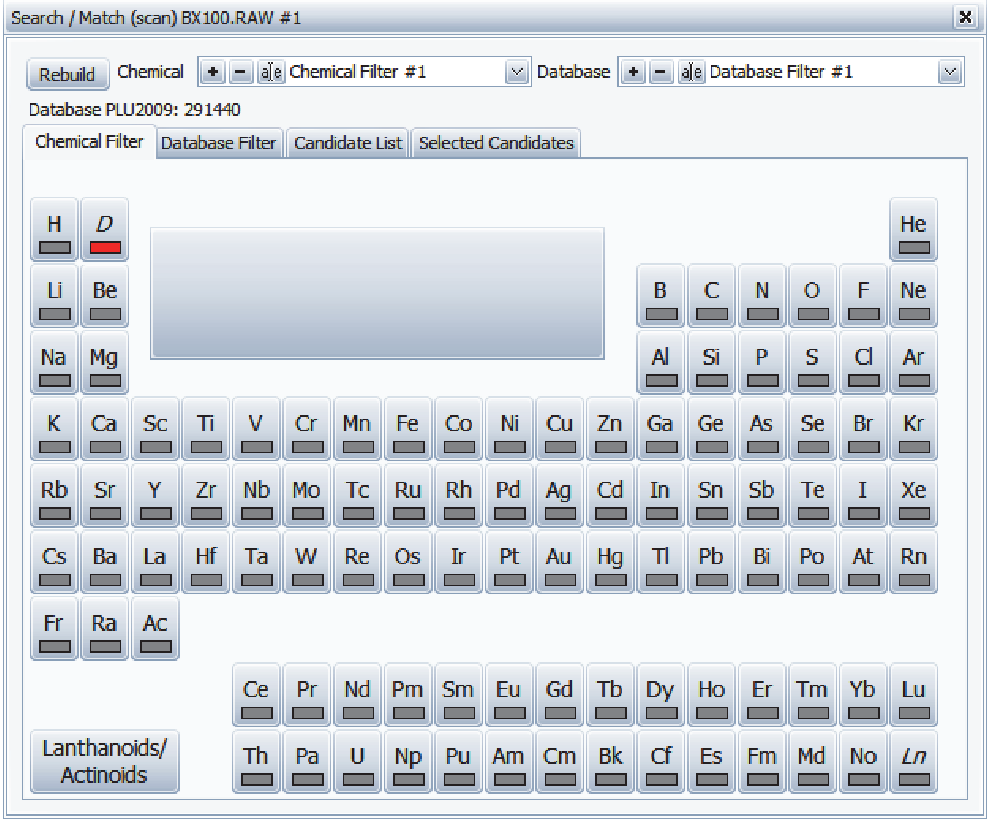
☑ Subset ☑ Exclude

Fig. 30: Adding the Search by Name results to the filter list

Step 3: Using a Filter List

You will be given here an example of Search/Match procedure using a filter list.
Here we are looking for a specific phase which is Anatase.

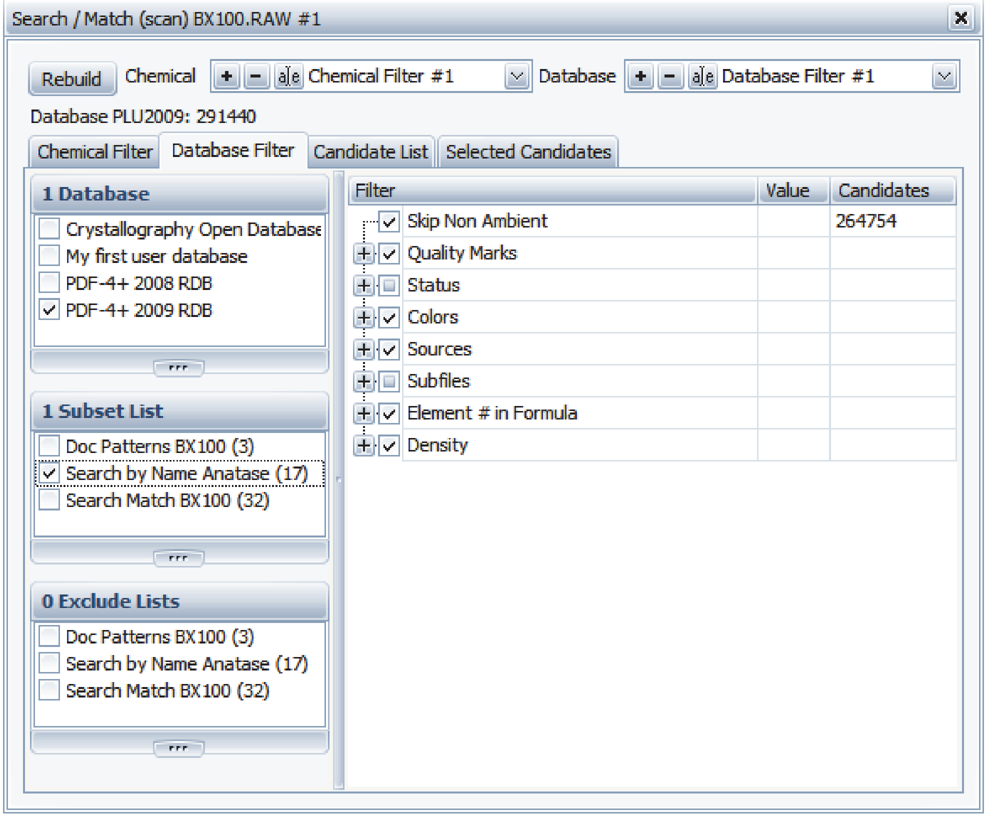
1. Select the BX100.RAW scan in the Data tree.
2. Click **Search / Match (scan)** in the Data Command panel
   — or —
   Right-click the scan, click **Tool** on the context menu and then **Search / Match (scan)** on the related submenu.
   The **Search / Match (scan)** dialog box will be displayed.
3. In the Chemical Filter tab, keep the default parameters:



No chemical filter, except D (deuterium) is Discarded (red).

4. In the Database Filter tab:

- ☑ all Subfiles are selected
- ☑ all Quality Marks are selected
- ☑ all Status are selected except ☐ **A** (alternative) that is cleared
- In addition to the PDF-4+ database, select the ***Search by Name Anatase*** subset list.



Search / Match (scan) BX100.RAW #1

Rebuild Chemical Chemical Filter #1 Database Database Filter #1

Database PLU2009: 291440

Chemical Filter | Database Filter | Candidate List | Selected Candidates

1 Database

- ☐ Crystallography Open Database
- ☐ My first user database
- ☐ PDF-4+ 2008 RDB
- ☑ PDF-4+ 2009 RDB

1 Subset List

- ☐ Doc Patterns BX100 (3)
- ☑ Search by Name Anatase (17)
- ☐ Search Match BX100 (32)

0 Exclude Lists

- ☐ Doc Patterns BX100 (3)
- ☐ Search by Name Anatase (17)
- ☐ Search Match BX100 (32)

Filter	Value	Candidates
☑ Skip Non Ambient		264754
☑ Quality Marks		
☐ Status		
☑ Colors		
☑ Sources		
☐ Subfiles		
☑ Element # in Formula		
☑ Density		

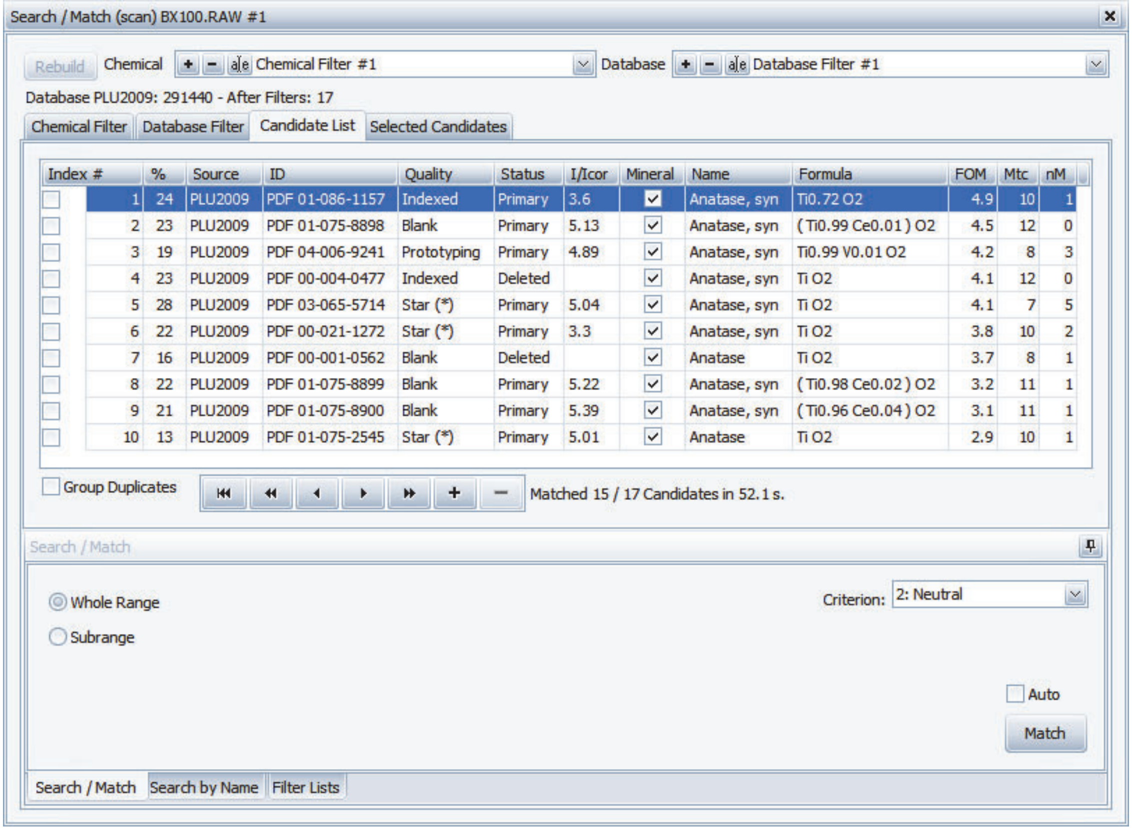
5. In the Candidate List tab, keep the default parameters:

- ☐ Group duplicates
- Criterion = **2** (**Neutral**)
- **Whole Range** selected
- ☐ Auto

NOTE

The Group duplicates option is not used in this example but this is a practical option which can be used without any risk.

6. Click the **Match** button. 15 Anatase candidate patterns are listed (with PDF-4+ 2009).



Search / Match (scan) BX100.RAW #1

Chemical: Chemical Filter #1 Database: Database Filter #1

Database PLU2009: 291440 - After Filters: 17

	Index #	%	Source	ID	Quality	Status	I/Icor	Mineral	Name	Formula	FOM	Mtc	nM
☐	1	24	PLU2009	PDF 01-086-1157	Indexed	Primary	3.6	☑	Anatase, syn	Ti0.72 O2	4.9	10	1
☐	2	23	PLU2009	PDF 01-075-8898	Blank	Primary	5.13	☑	Anatase, syn	(Ti0.99 Ce0.01) O2	4.5	12	0
☐	3	19	PLU2009	PDF 04-006-9241	Prototyping	Primary	4.89	☑	Anatase, syn	Ti0.99 V0.01 O2	4.2	8	3
☐	4	23	PLU2009	PDF 00-004-0477	Indexed	Deleted		☑	Anatase, syn	Ti O2	4.1	12	0
☐	5	28	PLU2009	PDF 03-065-5714	Star (*)	Primary	5.04	☑	Anatase, syn	Ti O2	4.1	7	5
☐	6	22	PLU2009	PDF 00-021-1272	Star (*)	Primary	3.3	☑	Anatase, syn	Ti O2	3.8	10	2
☐	7	16	PLU2009	PDF 00-001-0562	Blank	Deleted		☑	Anatase	Ti O2	3.7	8	1
☐	8	22	PLU2009	PDF 01-075-8899	Blank	Primary	5.22	☑	Anatase, syn	(Ti0.98 Ce0.02) O2	3.2	11	1
☐	9	21	PLU2009	PDF 01-075-8900	Blank	Primary	5.39	☑	Anatase, syn	(Ti0.96 Ce0.04) O2	3.1	11	1
☐	10	13	PLU2009	PDF 01-075-2545	Star (*)	Primary	5.01	☑	Anatase	Ti O2	2.9	10	1

☐ Group Duplicates

Matched 15 / 17 Candidates in 52.1 s.

● Whole Range
○ Subrange

Criterion: 2: Neutral

☐ Auto

Fig. 31: Search/Match results using a Subset list

Creating a User Database

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 Tutorial directory.

Steps:

1. Creating a new EVA document and importing m1.RAW.
2. Automatic matching procedure:

   Identification of the compounds
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. Performing a peak search on LaB6 and creating the corresponding DIF.
8. Adding the LaB6 DIF to the user database.
9. Using the User database during a Search/Match operation.
10. Saving the EVA document.

NOTE

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

This tutorial was prepared using PDF 4+ 2009 as a reference database. The user may have another reference database.

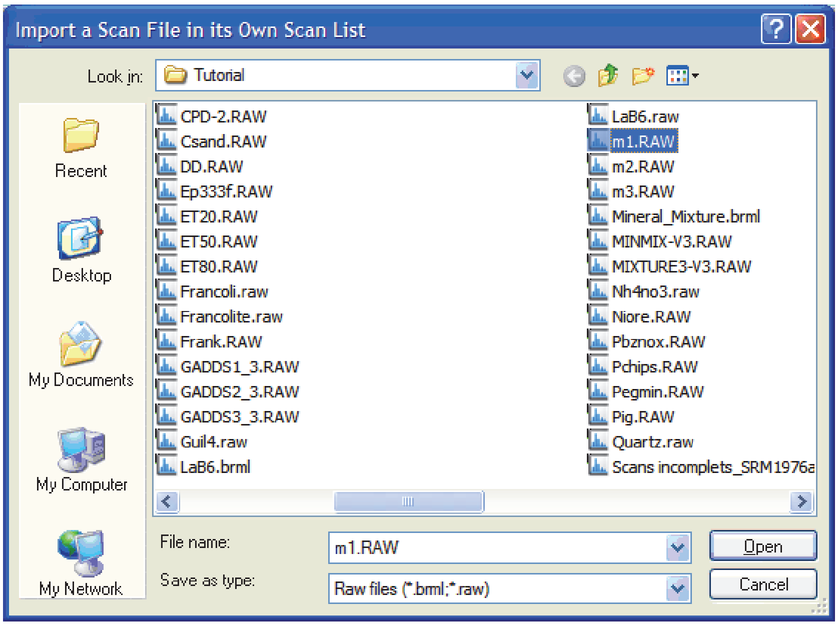
If the user does not have a database, this part of the tutorial using the Search/Match cannot be performed.

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

New button

Import from file button

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



File name: m1.RAW

Save as type: Raw files (*.brml;*.raw)

Fig. 32: Importing the m1.RAW file

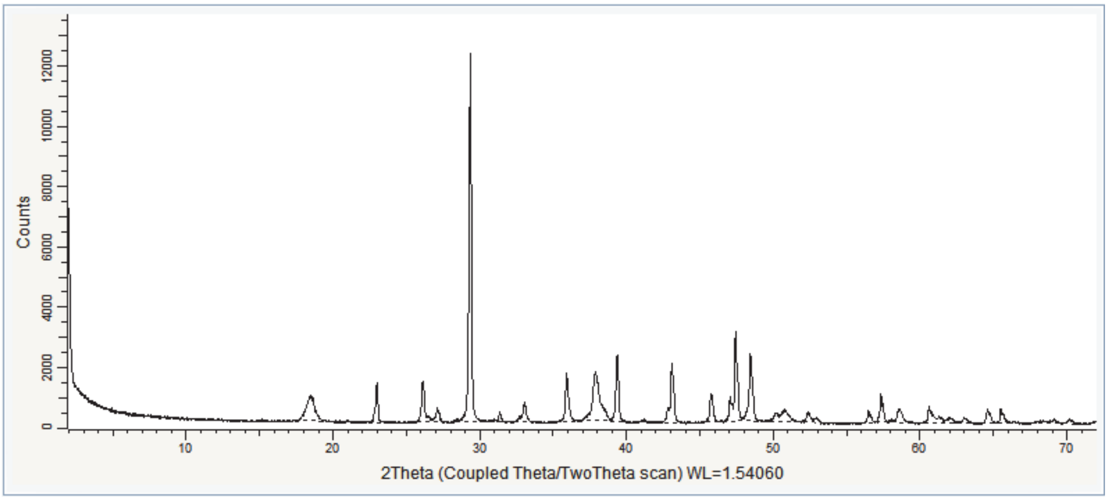


Fig. 33: m1.RAW file imported in the graphical view

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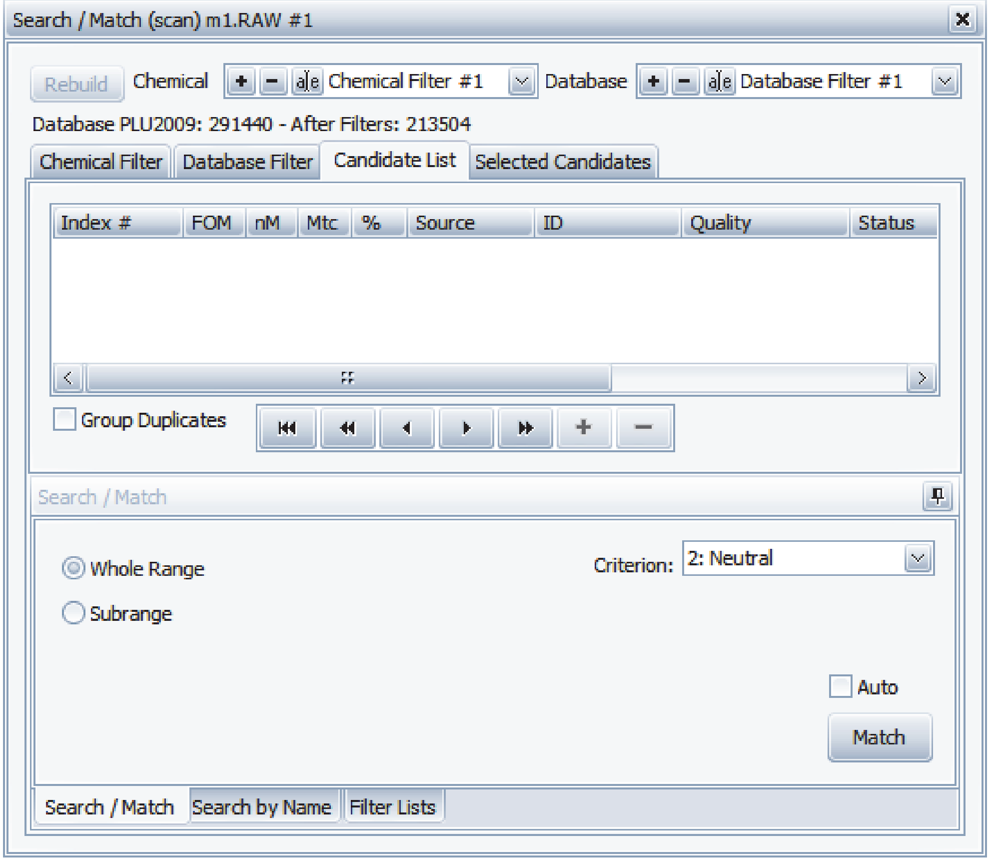
[1] The directory path to the EVA tutorial files is ″C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials″ under Windows XP and ″C:\ProgramData\Bruker AXS\Tutorials″ under Windows 7.

To be able to access the folder via Explorer, select “Display hidden files and folders” in the Folders options.

Step 2: Performing the Automatic Matching Procedure

1. Make sure that the scan has been selected. If the scan has not been chosen select it either in the Data tree or in the graphical view.
2. Click **Search / Match (scan)** in the Data Command panel
   — or —
   right-click the scan, click **Tool** on the context menu and then **Search / Match (scan)** on the related submenu.
   The **Search / Match (scan)** dialog box will be displayed.



Database PLU2009: 291440 - After Filters: 213504

☐ Group Duplicates

● Whole Range
○ Subrange

Criterion: 2: Neutral

☐ Auto

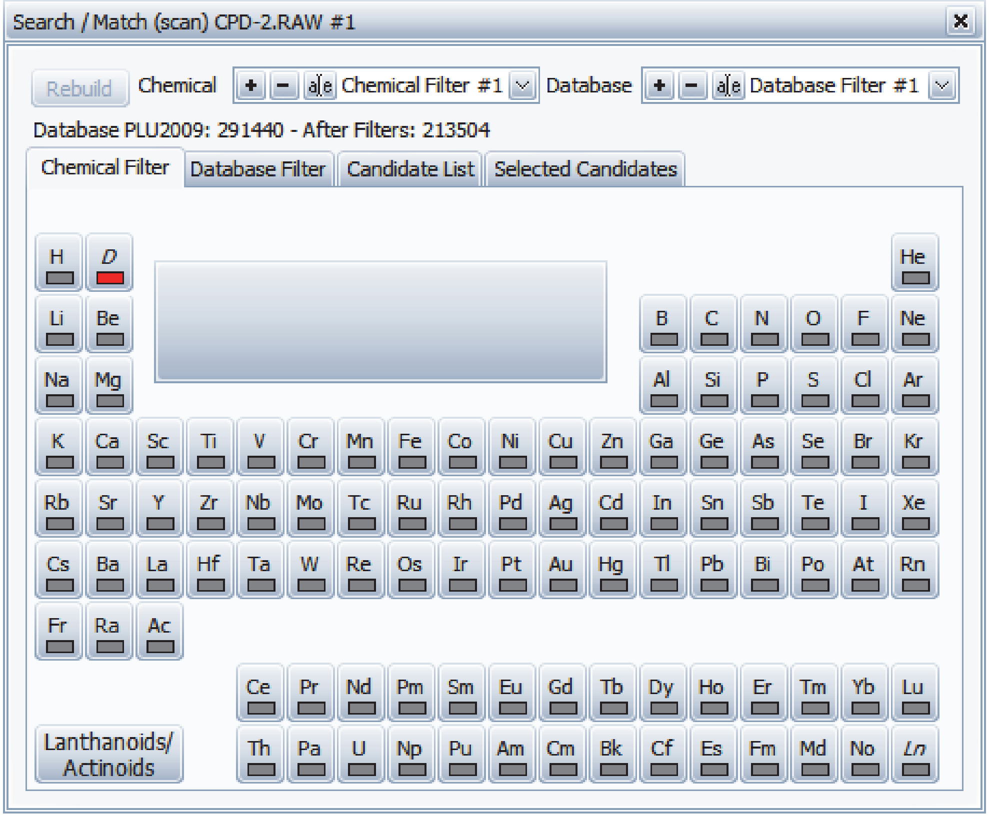
Fig. 34: Search/match dialog box

3. Select the **Auto** check box.
4. Set the parameters for the Search/Match procedure:
   ⇒ In the Candidate List tab:
   - ☐ Group duplicates
   - Criterion = **2** (**Neutral**)
   - **Whole Range** selected

NOTE

The Group duplicates option is not used in this example but this is a practical option which can be used without any risk.

⇒ In the Chemical Filter tab:

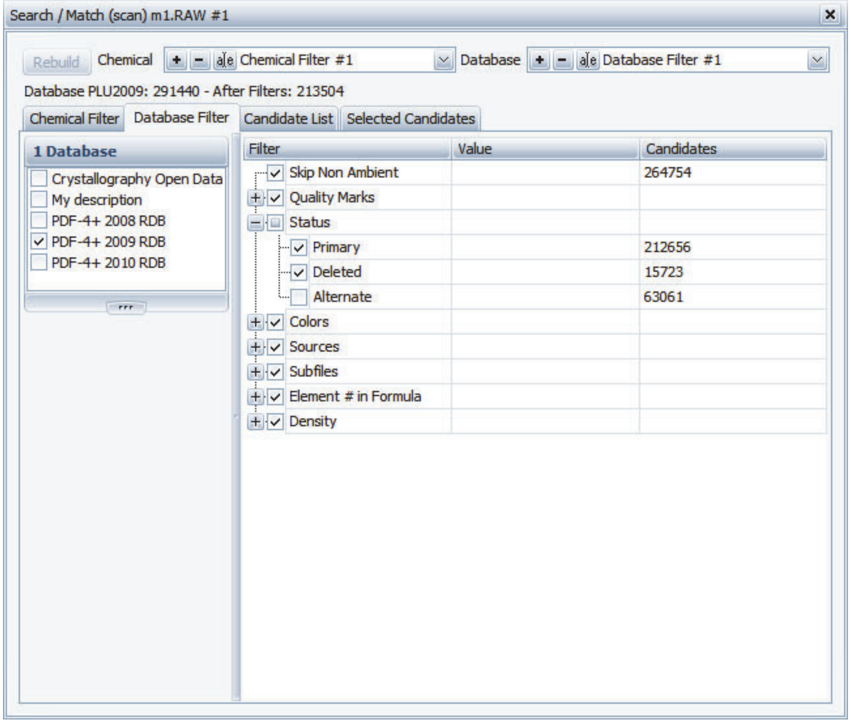


Search / Match (scan) CPD-2.RAW #1

Database PLU2009: 291440 - After Filters: 213504

No chemical filter, except D (deuterium) is Discarded (red)

⇒ In the Database Filter tab:



Search / Match (scan) m1.RAW #1

Rebuild Chemical Chemical Filter #1 Database Database Filter #1

Database PLU2009: 291440 - After Filters: 213504

Chemical Filter | Database Filter | Candidate List | Selected Candidates

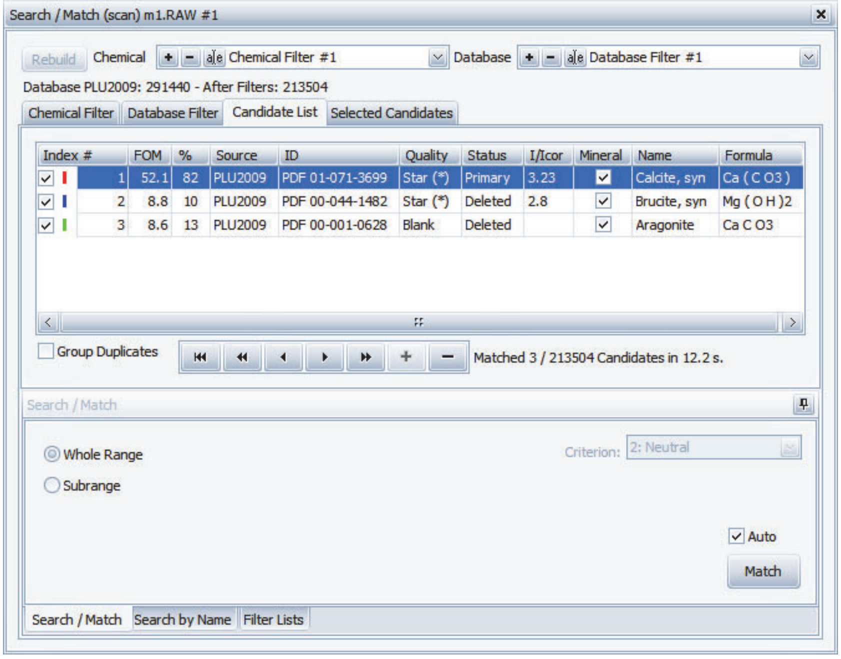
1 Database

- ☐ Crystallography Open Data
- ☐ My description
- ☐ PDF-4+ 2008 RDB
- ☑ PDF-4+ 2009 RDB
- ☐ PDF-4+ 2010 RDB

Filter	Value	Candidates
☑ Skip Non Ambient		264754
☑ Quality Marks		
☐ Status		
☑ Primary		212656
☑ Deleted		15723
☐ Alternate		63061
☑ Colors		
☑ Sources		
☑ Subfiles		
☑ Element # in Formula		
☑ Density		

- ☑ all Subfiles are selected
- ☑ all Quality Marks are selected
- ☑ all Status are selected except ☐ **A** (alternative) which has been cleared

5. Click the **Match** button. The candidates are listed in the Candidate List tab.



Search / Match (scan) m1.RAW #1

Rebuild Chemical Chemical Filter #1 Database Database Filter #1

Database PLU2009: 291440 - After Filters: 213504

Chemical Filter | Database Filter | Candidate List | Selected Candidates

	Index #	FOM	%	Source	ID	Quality	Status	I/Icor	Mineral	Name	Formula
☑	1	52.1	82	PLU2009	PDF 01-071-3699	Star (*)	Primary	3.23	☑	Calcite, syn	Ca (C O3)
☑	2	8.8	10	PLU2009	PDF 00-044-1482	Star (*)	Deleted	2.8	☑	Brucite, syn	Mg (O H)2
☑	3	8.6	13	PLU2009	PDF 00-001-0628	Blank	Deleted		☑	Aragonite	Ca C O3

☐ Group Duplicates

Matched 3 / 213504 Candidates in 12.2 s.

Search / Match

● Whole Range
○ Subrange

Criterion: 2: Neutral

☑ Auto

Match

Search / Match | Search by Name | Filter Lists

Fig. 35: Candidate List with the identified patterns selected

☑ 🟥

Pattern checked

The results of the Automatic Search/Match are displayed in the candidate list. The three patterns identified are automatically checked and added to the data tree and to the graphical view.

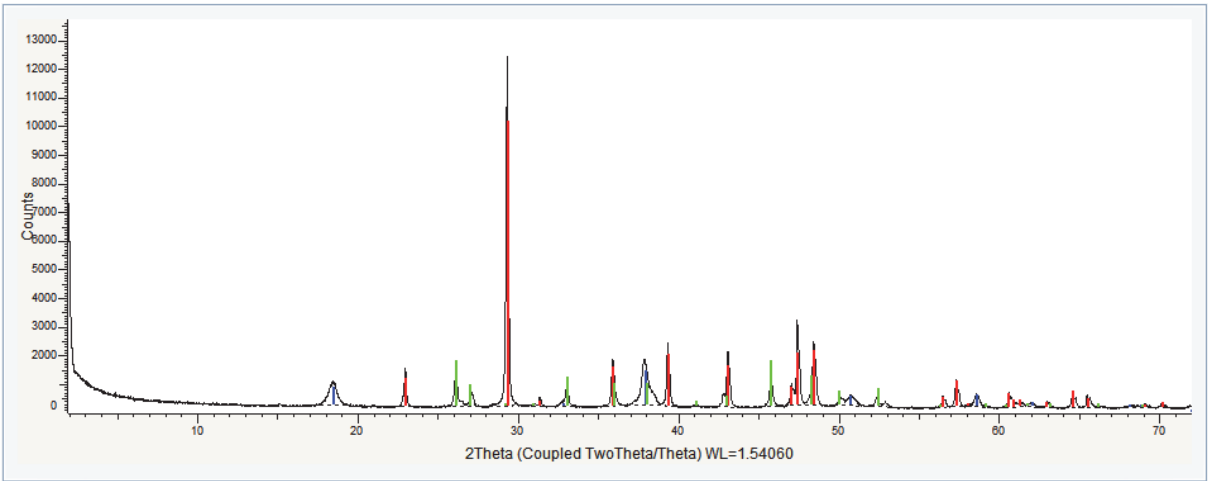
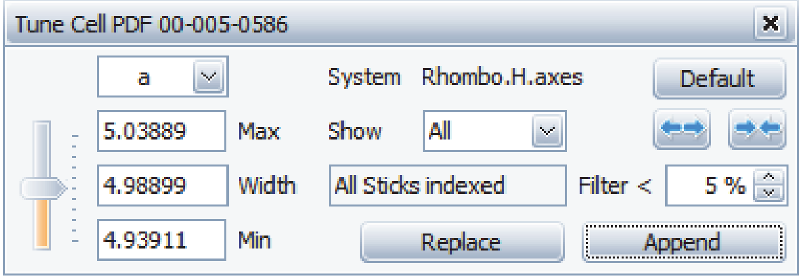


Fig. 36: m1 scan displayed in the graphical view with the three patterns 01-071-3699, 00-044-1482 and 00-001-0628

Step 3: Performing the Tune Cell Operation

1. Select the Calcite pattern in the data tree.
2. Click **Tune Cell** in the Data Command panel
   — or —
   right-click the pattern, then click **Tune Cell** on the context menu.

   The Tune cell dialog box will be displayed.



Tune Cell PDF 00-005-0586

a

System Rhombo.H.axes

5.03889 Max

Show All

4.98899 Width

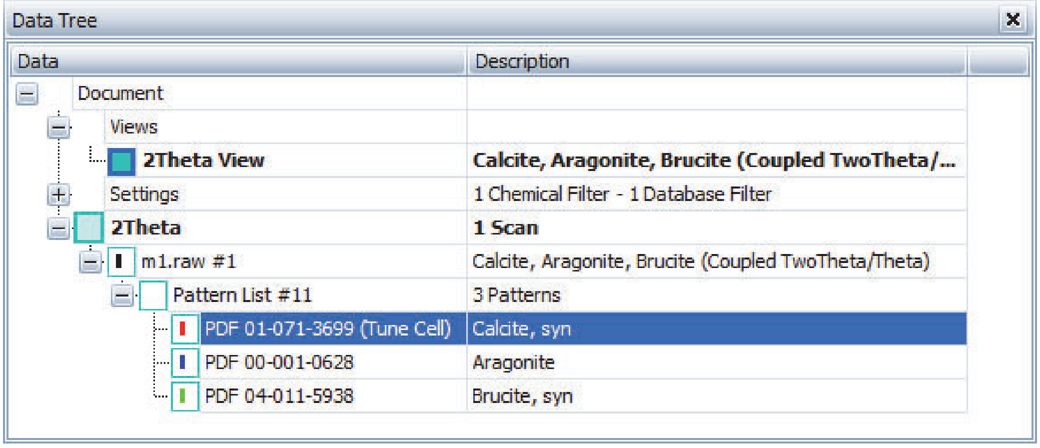
All Sticks indexed

Filter < 5 %

4.93911 Min

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 as well as in the data tree.



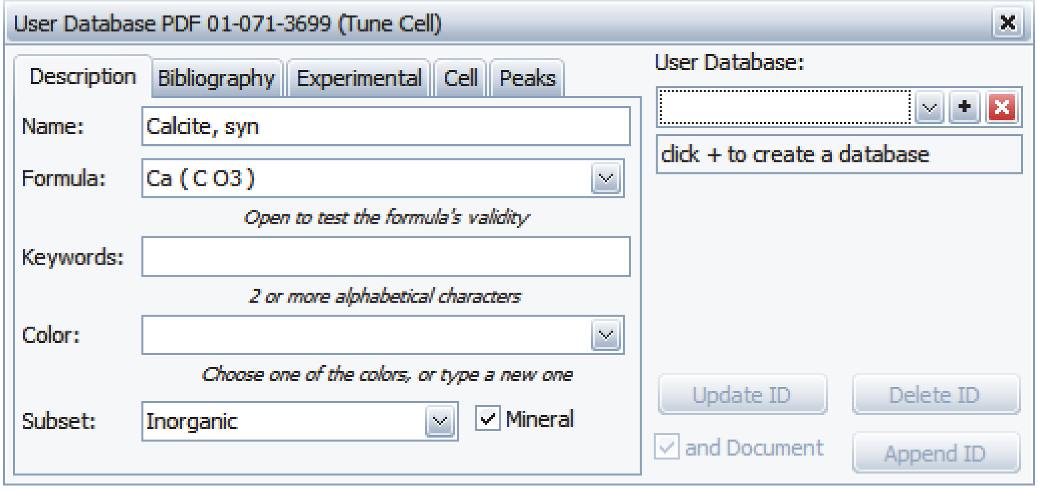
Data Tree

Data	Description
Document	
Views	
2Theta View	Calcite, Aragonite, Brucite (Coupled TwoTheta/...
Settings	1 Chemical Filter - 1 Database Filter
2Theta	1 Scan
m1.raw #1	Calcite, Aragonite, Brucite (Coupled TwoTheta/Theta)
Pattern List #11	3 Patterns
PDF 01-071-3699 (Tune Cell)	Calcite, syn
PDF 00-001-0628	Aragonite
PDF 04-011-5938	Brucite, syn

Step 4: Creating the User Database

1. Click **User Database** in the Data Command panel
— or —
right-click the tuned pattern and click **User Database** on the context menu.

The User Database dialog box will be displayed.



Name: Calcite, syn

Formula: Ca (C O3)

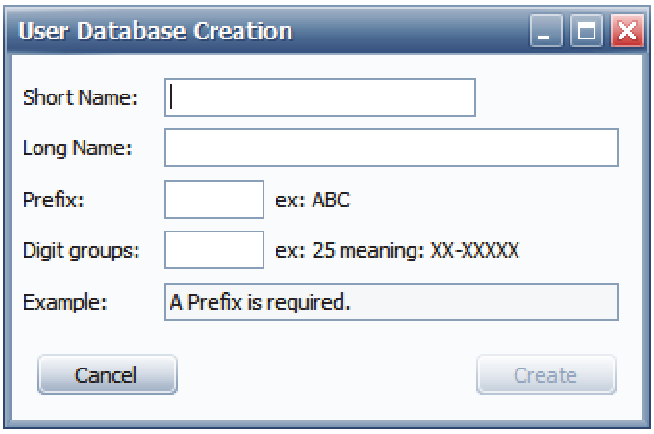
Keywords:

Color:

Subset: Inorganic ☑ Mineral

Fig. 37: User Database dialog box

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



Short Name:

Long Name:

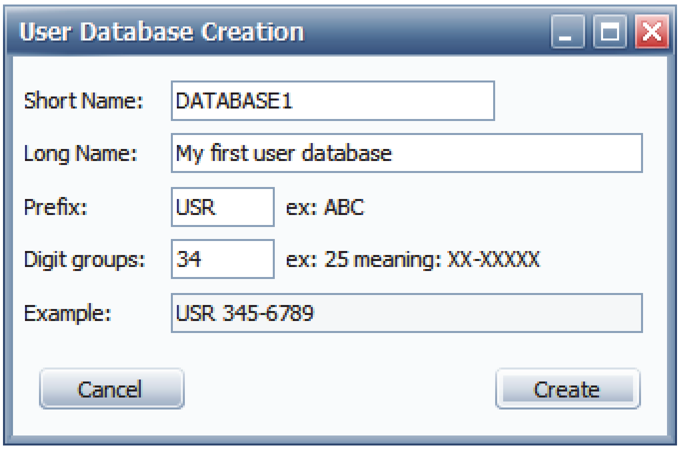
Prefix:

Digit groups:

Example: A Prefix is required.

Fig. 38: 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.
6. The example field will give an example of a pattern name with a prefix and a digits group chosen.



Short Name: DATABASE1

Long Name: My first user database

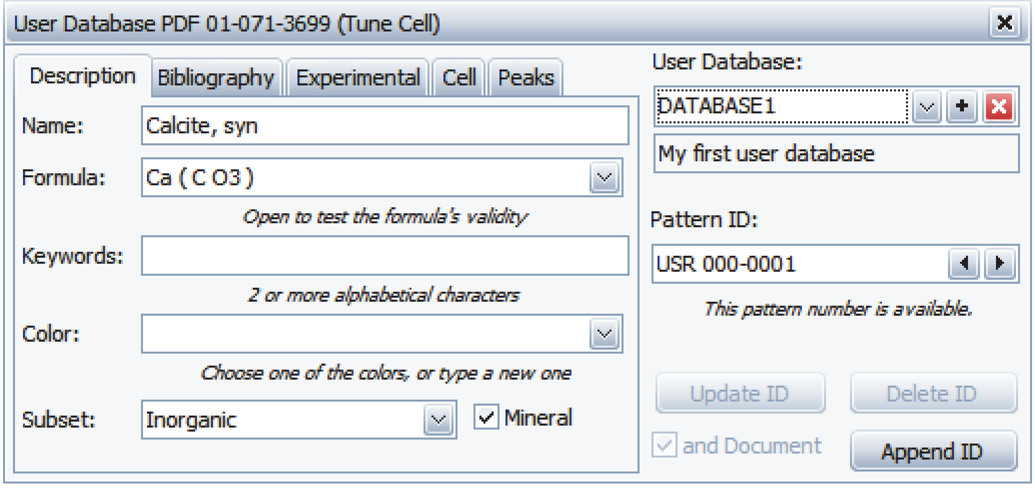
Prefix: USR ex: ABC

Digit groups: 34 ex: 25 meaning: XX-XXXXX

Example: USR 345-6789

7. 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.



Name: Calcite, syn

Formula: Ca (C O3)

Keywords:

Color:

Subset: Inorganic ☑ Mineral

User Database: DATABASE1

My first user database

Pattern ID: USR 000-0001

This pattern number is available.

☑ and Document

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.

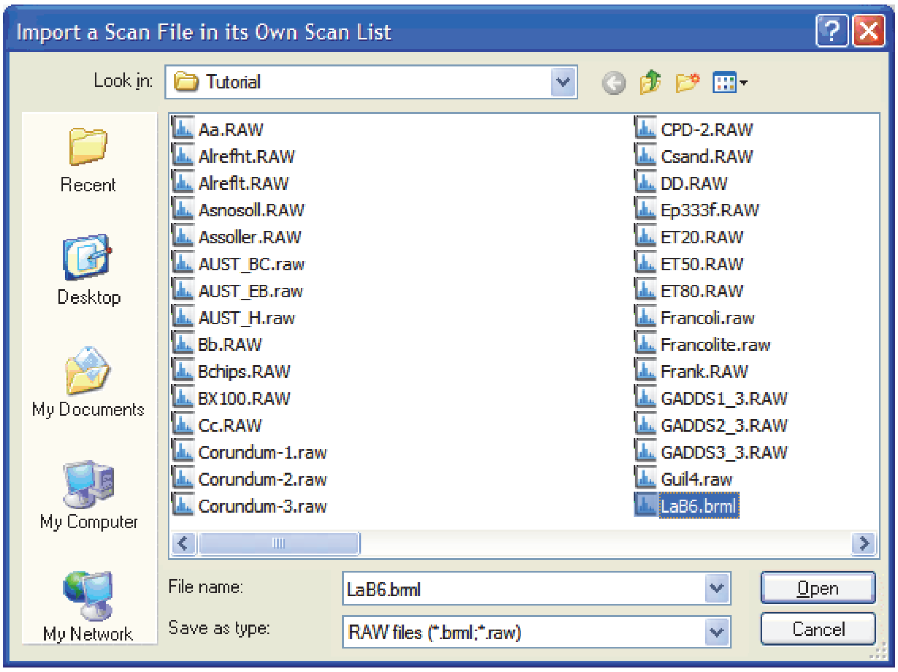
   The User Database dialog box will be closed.
3. Close the document. All the data will be removed from the screen.

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

New button

Import from file button

1. Click **New** on the **File** menu or use the toolbar button. The EVA document will be empty.
2. Click the **Import from file** data command or the **Import from file** button. The Import from files dialog box will be displayed. Search the Tutorials/EVA[1] directory and select the LaB6.BRML file.
3. Click **Open**. The scan LaB6 will be displayed in the graphical view of the EVA document.



File name: LaB6.brml

Save as type: RAW files (*.brml;*.raw)

Fig. 39: Import a Scan File dialog box

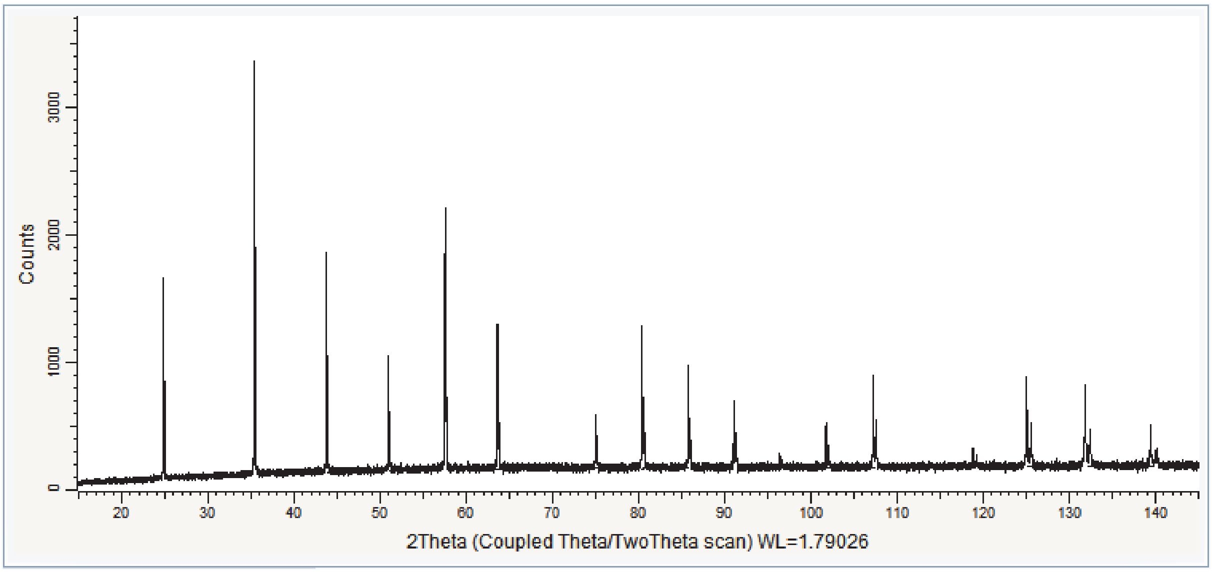


Fig. 40: LaB6 file imported in the graphical view

---

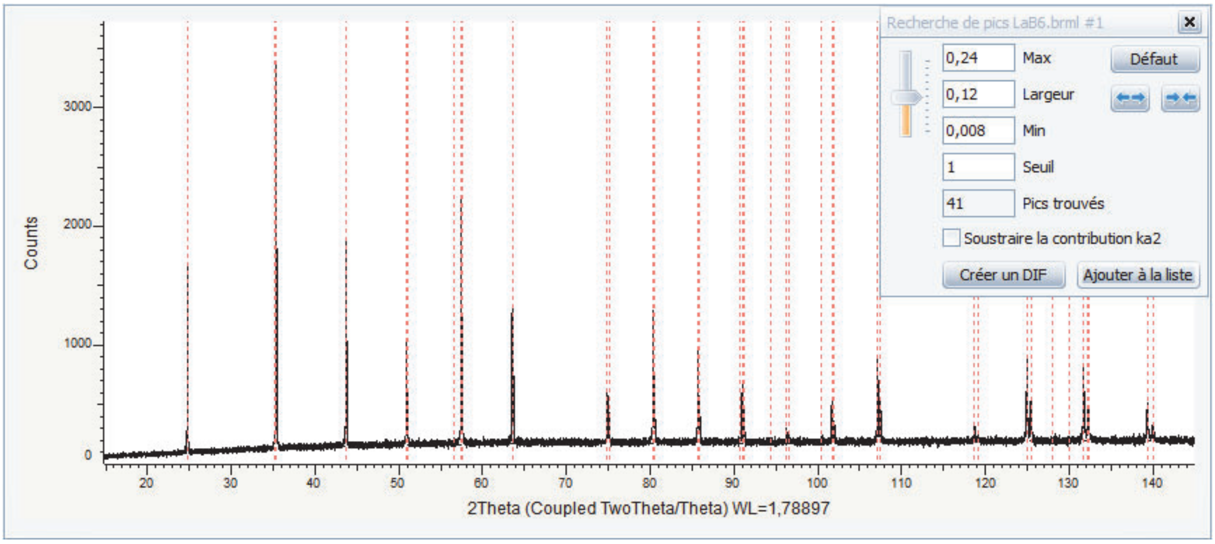
[1] The directory path to the EVA tutorial files is ″C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials″ under Windows XP and ″C:\ProgramData\Bruker AXS\Tutorials″ under Windows 7.

To be able to access the folder via Explorer, select “Display hidden files and folders” in the Folders options.

Step 7: Adding the LaB6 DIF to the User Database

1. Import the LaB6.BRML scan.
2. Make sure the scan has been selected. If no scan has been chosen, select it either in the data tree or in the 1D view.
3. Click **Peak Search** in the Tool list of the Data Command panel
   — 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.



Recherche de pics LaB6.brml #1

0,24 Max

0,12 Largeur

0,008 Min

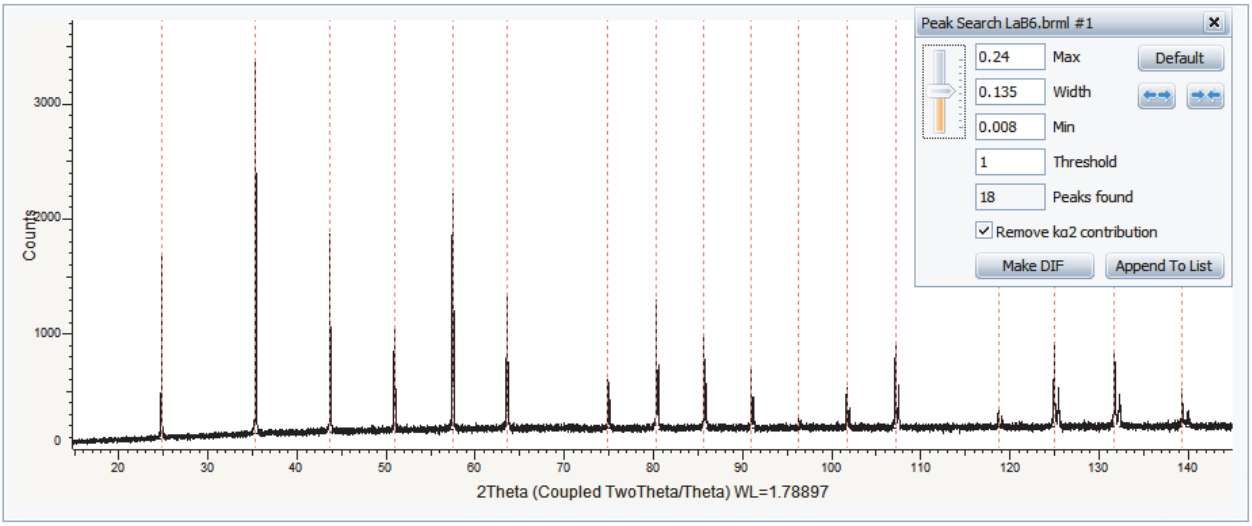
1 Seuil

41 Pics trouvés

☐ Soustraire la contribution ka2

Fig. 41: Peak Search dialog box and graphical view showing the ghost peaks

4. 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.
5. Select the **Remove Ka2 contribution** check box and move the slider to adjust the peaks.



Peak Search LaB6.brml #1

0.24 Max

0.135 Width

0.008 Min

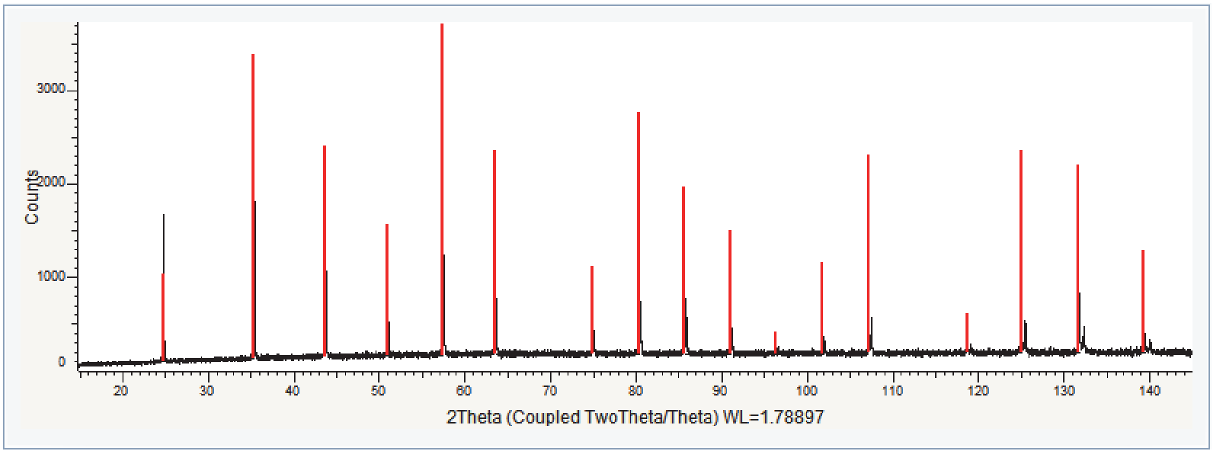
1 Threshold

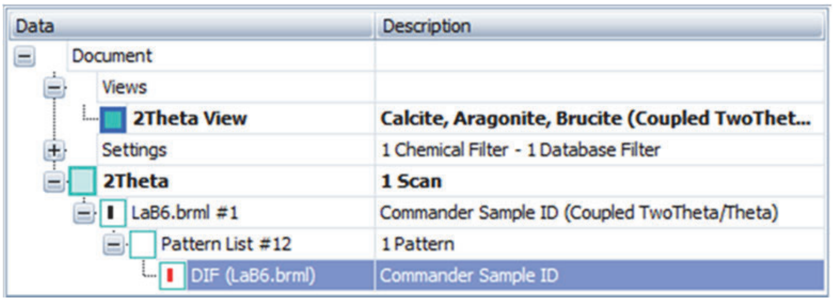
18 Peaks found

☑ Remove kα2 contribution

Fig. 42: Performing a peak search on the LaB6 scan

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

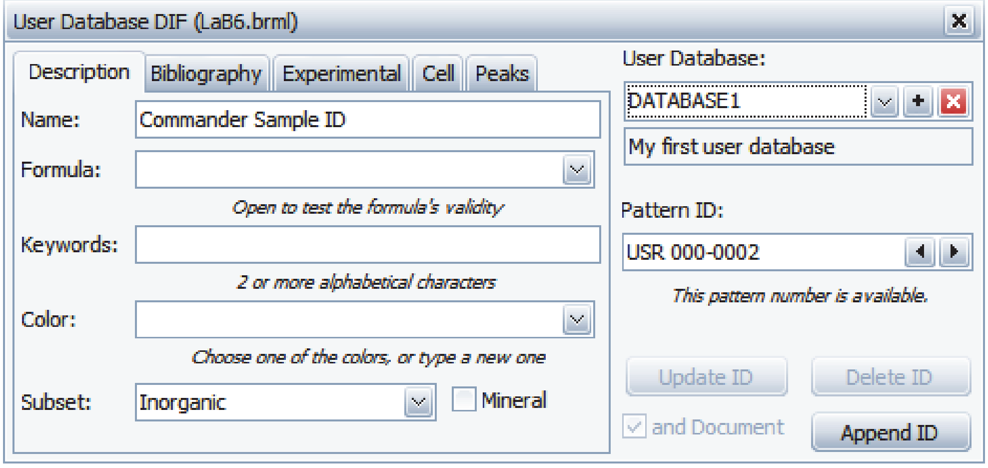




Data	Description
Document	
Views	
2Theta View	**Calcite, Aragonite, Brucite (Coupled TwoThet...**
Settings	1 Chemical Filter - 1 Database Filter
2Theta	**1 Scan**
LaB6.brml #1	Commander Sample ID (Coupled TwoTheta/Theta)
Pattern List #12	1 Pattern
DIF (LaB6.brml)	Commander Sample ID

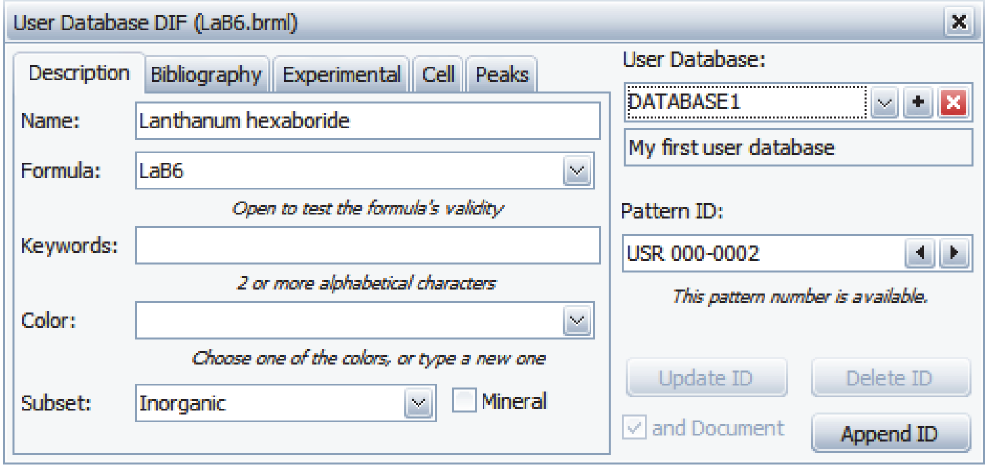
7. Click **User Database** in the Data Command panel
— or —
right-click the DIF and click **User Database** on the context menu.

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).



Name: Commander Sample ID
Formula:
Open to test the formula's validity
Keywords:
2 or more alphabetical characters
Color:
Choose one of the colors, or type a new one
Subset: Inorganic ☐ Mineral
User Database: DATABASE1
My first user database
Pattern ID: USR 000-0002
This pattern number is available.
☑ and Document

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



Name: Lanthanum hexaboride

Formula: LaB6

Keywords:

Color:

Subset: Inorganic ☐ Mineral

User Database: DATABASE1

My first user database

Pattern ID: USR 000-0002

☑ and Document

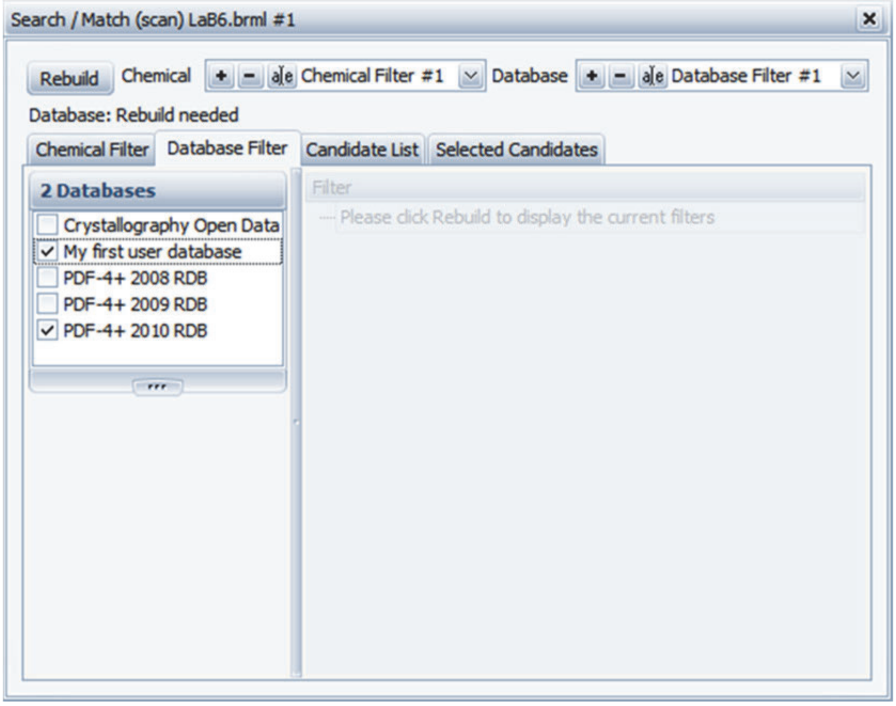
9. Click the **Append ID** button to add the new pattern to the selected user database. The User Database dialog box will be closed.

10. Delete the DIF from the data tree. It will also be removed from the graphical view.

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 (scan)** in the Data Command panel
   — or —
   right-click the current scan, click **Tool** on the menu which appears and then **Search / Match (scan)** on the related submenu.
3. In the Chemical Filter tab, keep the default parameters: no chemical filter, except D (deuterium) is discarded (red).
4. In the Database Filter tab, select *My first user database* in addition to the PDF database (here the PDF-4+ 2009) in the Database list.



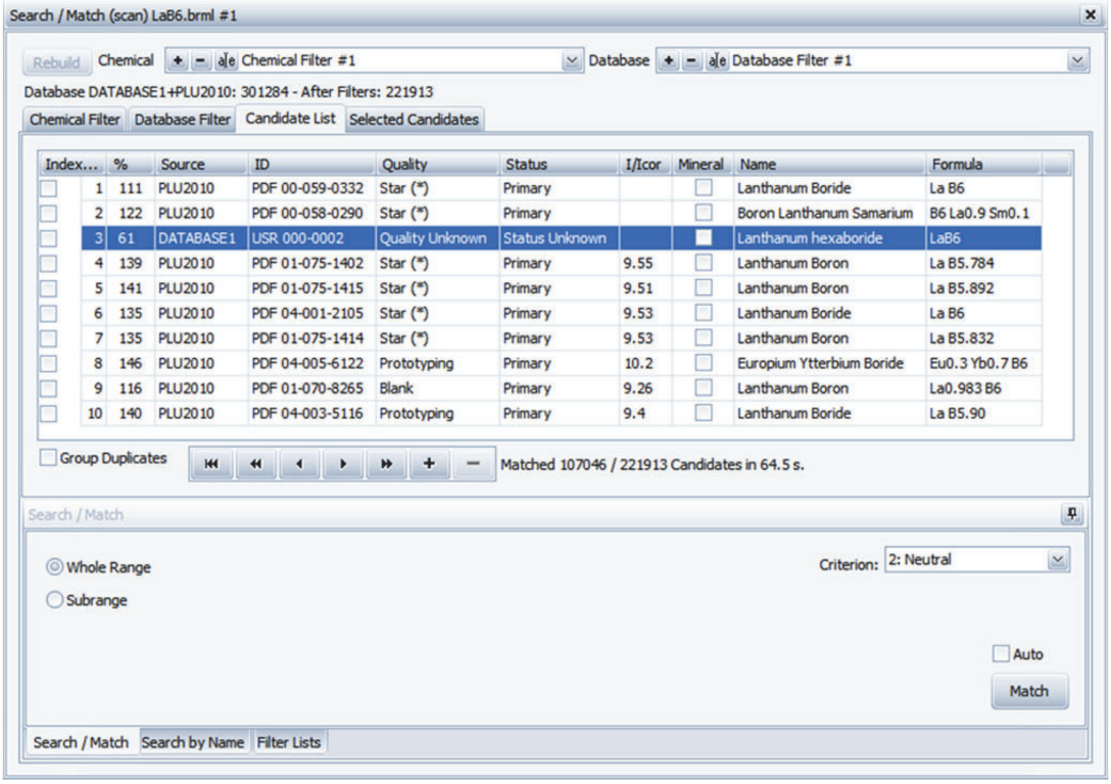
Database: Rebuild needed

2 Databases

- ☐ Crystallography Open Data
- ☑ My first user database
- ☐ PDF-4+ 2008 RDB
- ☐ PDF-4+ 2009 RDB
- ☑ PDF-4+ 2010 RDB

Please click Rebuild to display the current filters

5. In the Candidate List tab, keep the default parameters:
   - ☐ Group duplicates
   - Criterion = **2** (**Neutral**)
   - **Whole Range** selected
   - ☐ Auto
6. Click the **Match** button.



Chemical Filter #1

Database Filter #1

Database DATABASE1+PLU2010: 301284 - After Filters: 221913

	Index...	%	Source	ID	Quality	Status	I/Icor	Mineral	Name	Formula
☐	1	111	PLU2010	PDF 00-059-0332	Star (*)	Primary		☐	Lanthanum Boride	La B6
☐	2	122	PLU2010	PDF 00-058-0290	Star (*)	Primary		☐	Boron Lanthanum Samarium	B6 La0.9 Sm0.1
☐	3	61	DATABASE1	USR 000-0002	Quality Unknown	Status Unknown		☐	Lanthanum hexaboride	LaB6
☐	4	139	PLU2010	PDF 01-075-1402	Star (*)	Primary	9.55	☐	Lanthanum Boron	La B5.784
☐	5	141	PLU2010	PDF 01-075-1415	Star (*)	Primary	9.51	☐	Lanthanum Boron	La B5.892
☐	6	135	PLU2010	PDF 04-001-2105	Star (*)	Primary	9.53	☐	Lanthanum Boride	La B6
☐	7	135	PLU2010	PDF 01-075-1414	Star (*)	Primary	9.53	☐	Lanthanum Boron	La B5.832
☐	8	146	PLU2010	PDF 04-005-6122	Prototyping	Primary	10.2	☐	Europium Ytterbium Boride	Eu0.3 Yb0.7 B6
☐	9	116	PLU2010	PDF 01-070-8265	Blank	Primary	9.26	☐	Lanthanum Boron	La0.983 B6
☐	10	140	PLU2010	PDF 04-003-5116	Prototyping	Primary	9.4	☐	Lanthanum Boride	La B5.90

☐ Group Duplicates

Matched 107046 / 221913 Candidates in 64.5 s.

● Whole Range

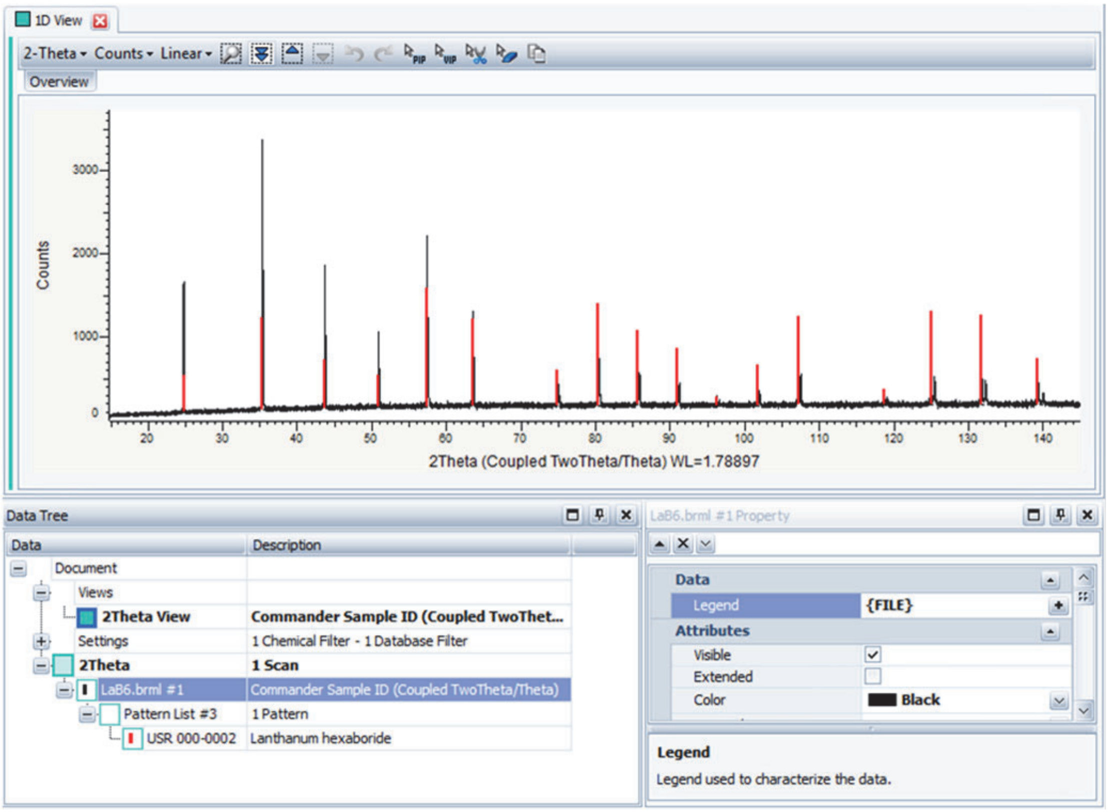
○ Subrange

Criterion: 2: Neutral

☐ Auto

Fig. 43: 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.



Data	Description
Document	
Views	
2Theta View	**Commander Sample ID (Coupled TwoThet...**
Settings	1 Chemical Filter - 1 Database Filter
2Theta	**1 Scan**
LaB6.brml #1	Commander Sample ID (Coupled TwoTheta/Theta)
Pattern List #3	1 Pattern
USR 000-0002	Lanthanum hexaboride

Data

Legend	{FILE}

Attributes

Visible	☑
Extended	☐
Color	■ Black

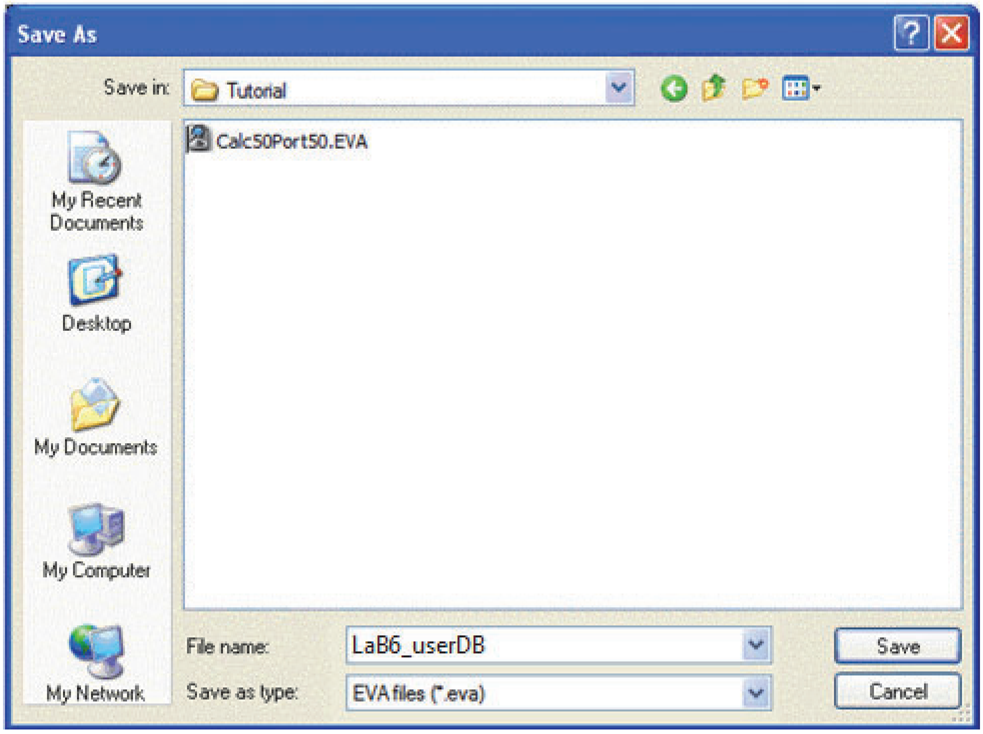
Legend

Legend used to characterize the data.

Fig. 44: User pattern added to the data tree and the graphical view

Step 9: Saving

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



File name: LaB6_userDB

Save as type: EVA files (*.eva)

Fig. 45: Saving LaB6_userDB.EVA document

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:

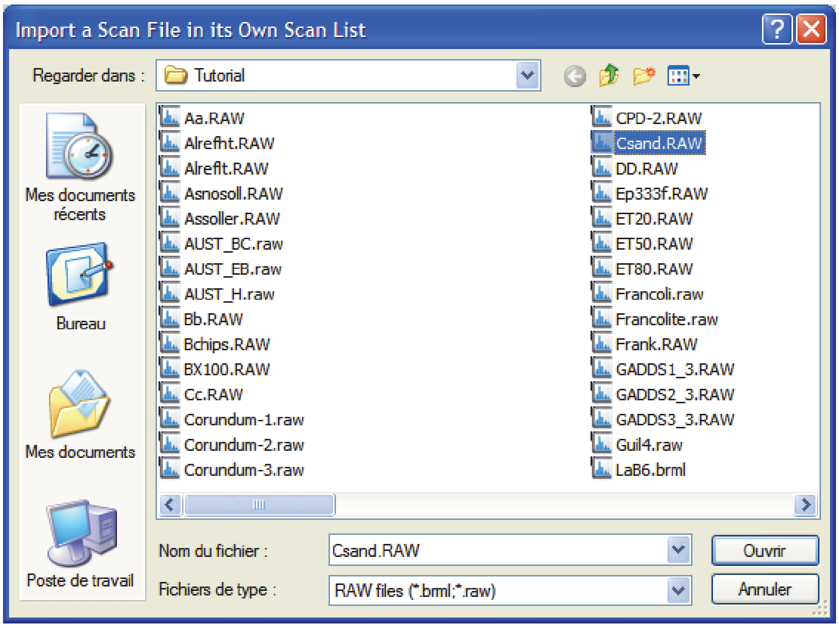
1. Creating a new EVA document and importing Csand.RAW.
2. Setting of the setting the peak search parameters.
3. Appending the peaks.
4. Saving the EVA document containing the scan.

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

New button

Import from file button

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 file** data command or the **Import from file** button. The Import from files dialog box will be displayed.
3. Search the Tutorials/EVA[1] directory and select the Csand.RAW file.
4. Click **Open**. The scan Csand.RAW will be displayed in the graphical view of the EVA document.



Import a Scan File in its Own Scan List

Regarder dans : Tutorial

Nom du fichier : Csand.RAW

Fichiers de type : RAW files (*.brml;*.raw)

Fig. 46: Import a Scan File dialog box

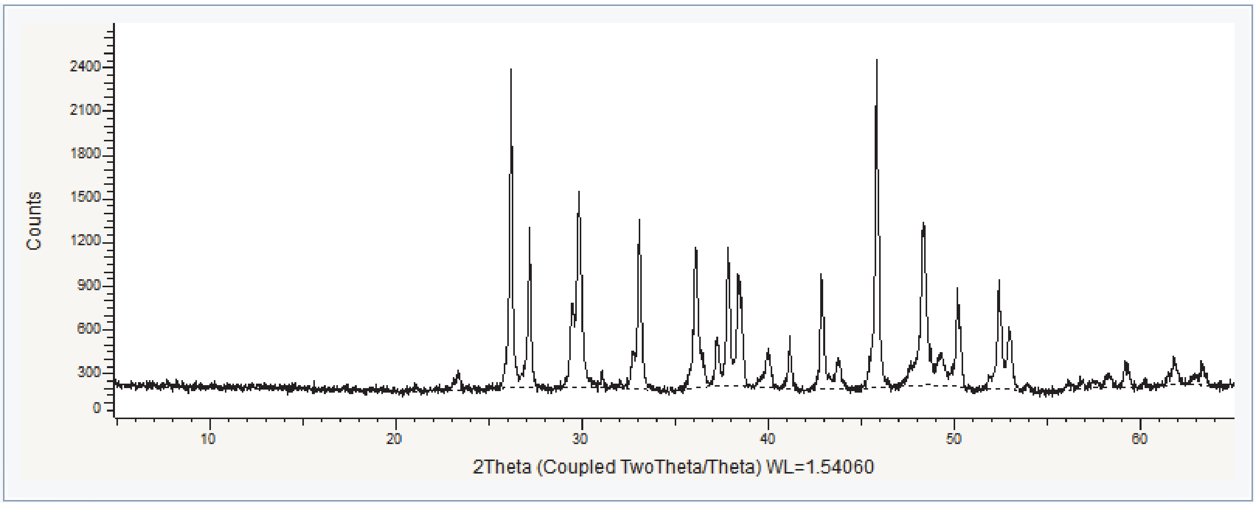


Fig. 47: Csand scan imported in the graphical view

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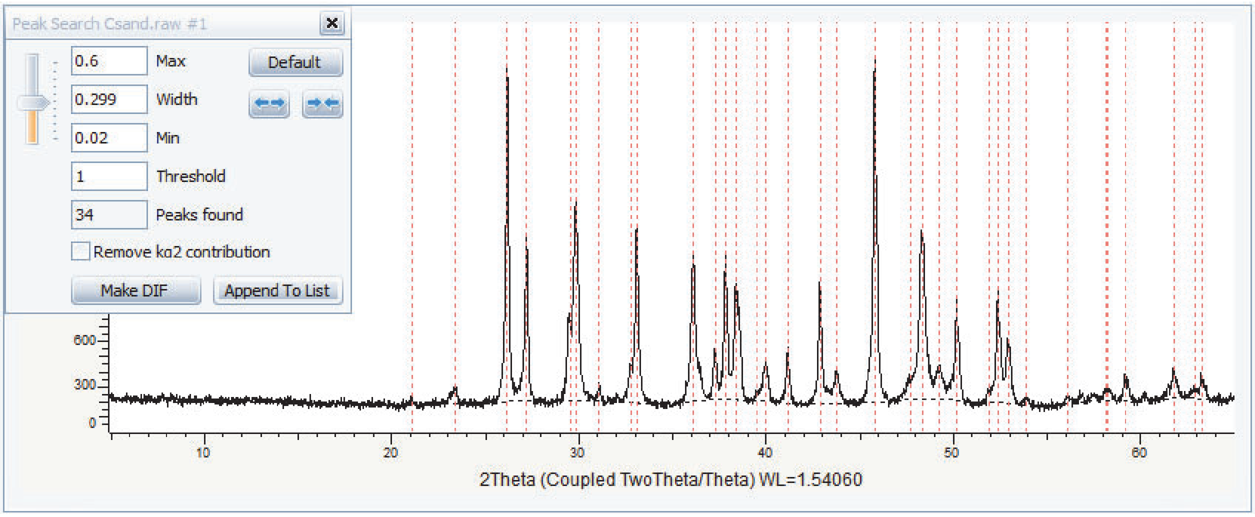
[1] The directory path to the EVA tutorial files is "C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials" under Windows XP and "C:\ProgramData\Bruker AXS\Tutorials" under Windows 7.
To access the folder with the explorer, select "Display hidden files and folders" in the Folders options.

Step 2: Setting the Peak Search Parameters

1. Make certain the scan is 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 —

   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.



Peak Search Csand.raw #1

0.6 Max

0.299 Width

0.02 Min

1 Threshold

34 Peaks found

☐ Remove kα2 contribution

Fig. 48: 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. 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.
4. If the default parameters are satisfactory: click the **Default** button to return to the default parameters.

Step 3: Appending the Peaks

1. To validate the peaks and add them to the graphical view as well as to the data tree, click the **Append to List** button.

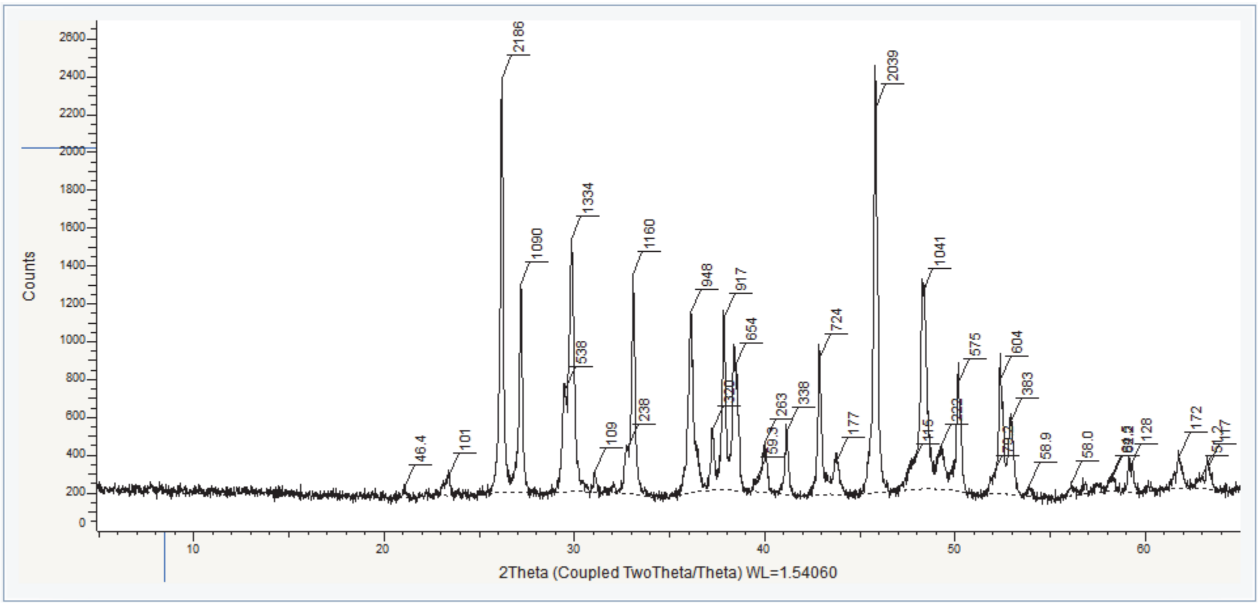
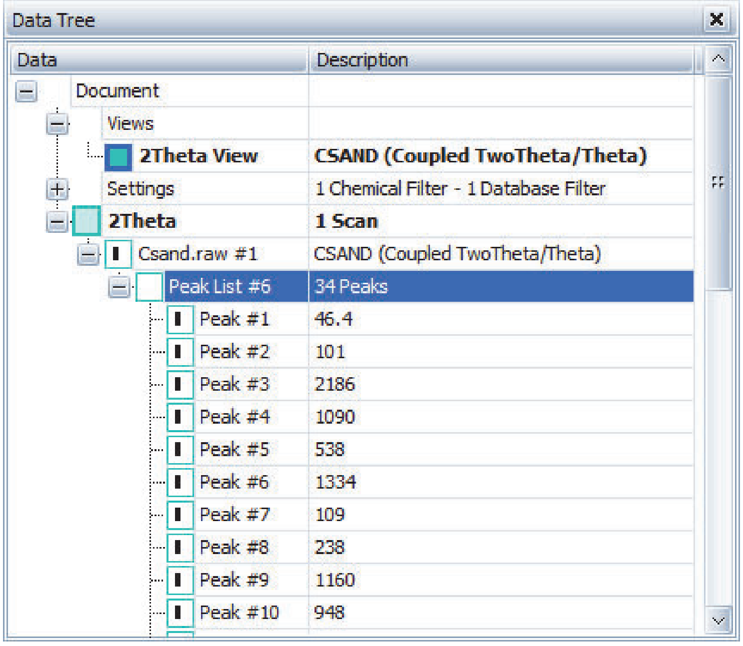


Fig. 49: Peak Search dialog box and graphical view showing the ghost peaks



Data	Description
Document	
Views	
2Theta View	**CSAND (Coupled TwoTheta/Theta)**
Settings	1 Chemical Filter - 1 Database Filter
2Theta	**1 Scan**
Csand.raw #1	CSAND (Coupled TwoTheta/Theta)
Peak List #6	34 Peaks
Peak #1	46.4
Peak #2	101
Peak #3	2186
Peak #4	1090
Peak #5	538
Peak #6	1334
Peak #7	109
Peak #8	238
Peak #9	1160
Peak #10	948

Fig. 50: Peak List added in the Data Tree

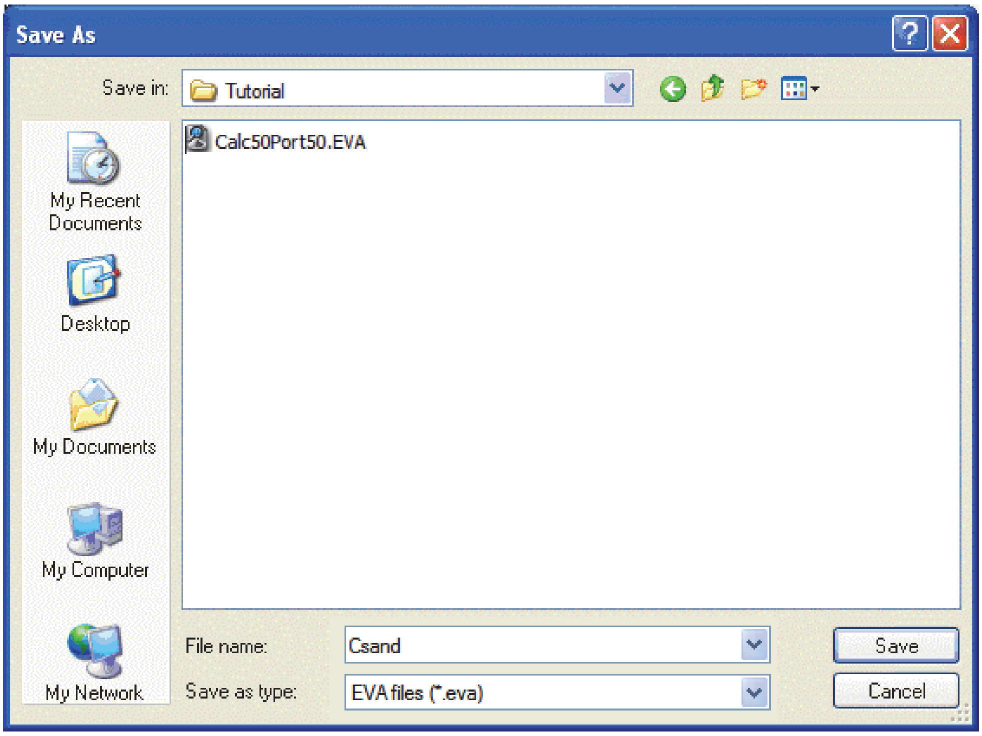
2. You can edit each peak in the Peak Property table. For example you can modify their position or change the layout.

NOTE

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

Step 4: Saving

1. Click **Save As** on the **File** menu. The Save As dialog box will be displayed.
2. Select the appropriate disc drive and directory.
3. Type in the file name.
4. Click **Save**.



Save in: Tutorial

File name: Csand

Save as type: EVA files (*.eva)

Fig. 51: Saving Csand.EVA document

Computing Kα_2 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:

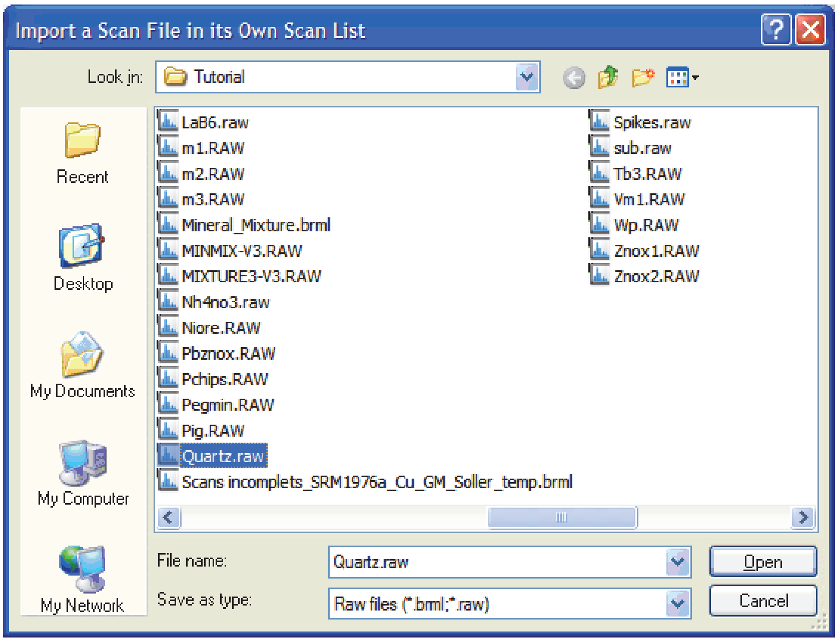
1. Creating a new EVA document and importing Quartz.RAW.
2. Computing the Kα_2 stripping.
3. Saving the EVA document containing the scan.

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

New button

Import from file button

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 file** data command or the **Import from file** button. The Import from files dialog box will be displayed.
3. Search the Tutorials/EVA[1] directory and select the Quartz.RAW file.
4. Click **Open**. The scan Quartz.RAW will be displayed in the graphical view of the EVA document.



File name: Quartz.raw

Save as type: Raw files (*.brml;*.raw)

Fig. 52: Import a Scan File dialog box

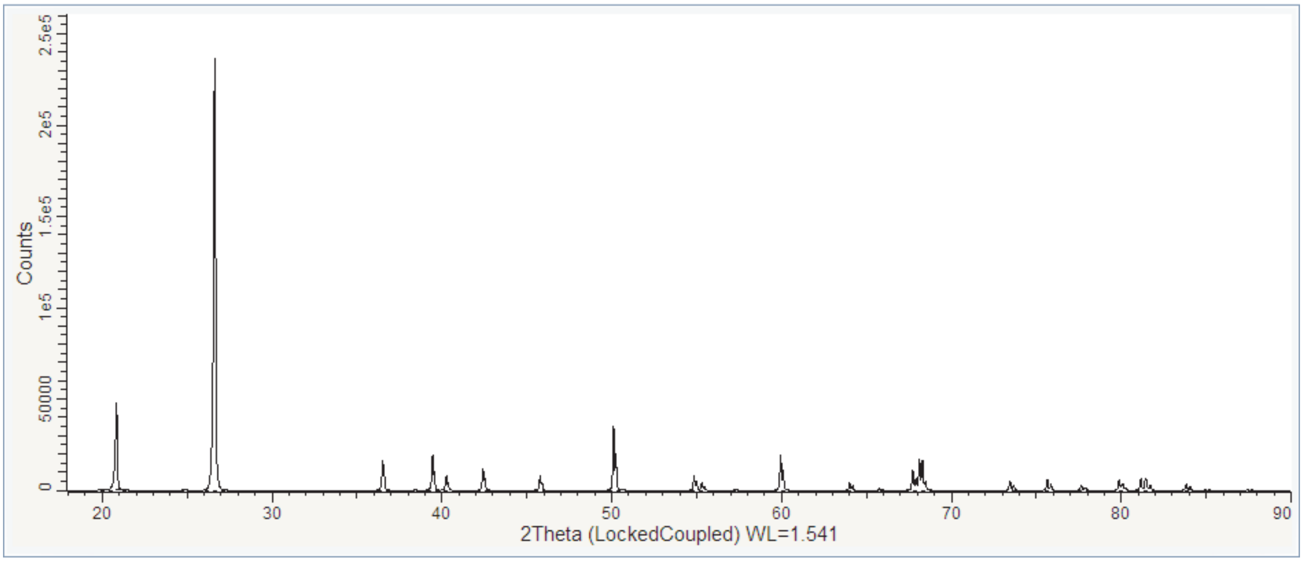


Fig. 53: Quartz scan imported in the graphical view

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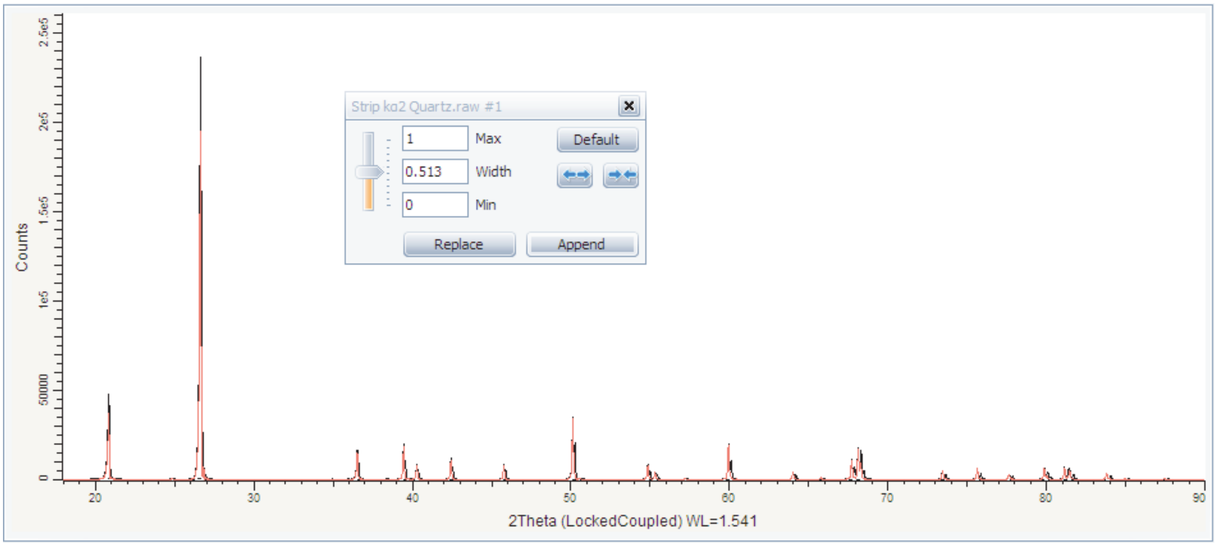
[1] The directory path to the EVA tutorial files is "C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials" under Windows XP and "C:\ProgramData\Bruker AXS\Tutorials" under Windows 7.
To access the folder with the explorer, select "Display hidden files and folders" in the Folders options.

Step 2: Computing the Kα_2 Stripping

1. Make certain the scan is selected; if not, select it either in the data tree or in the 1D view.
2. 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.

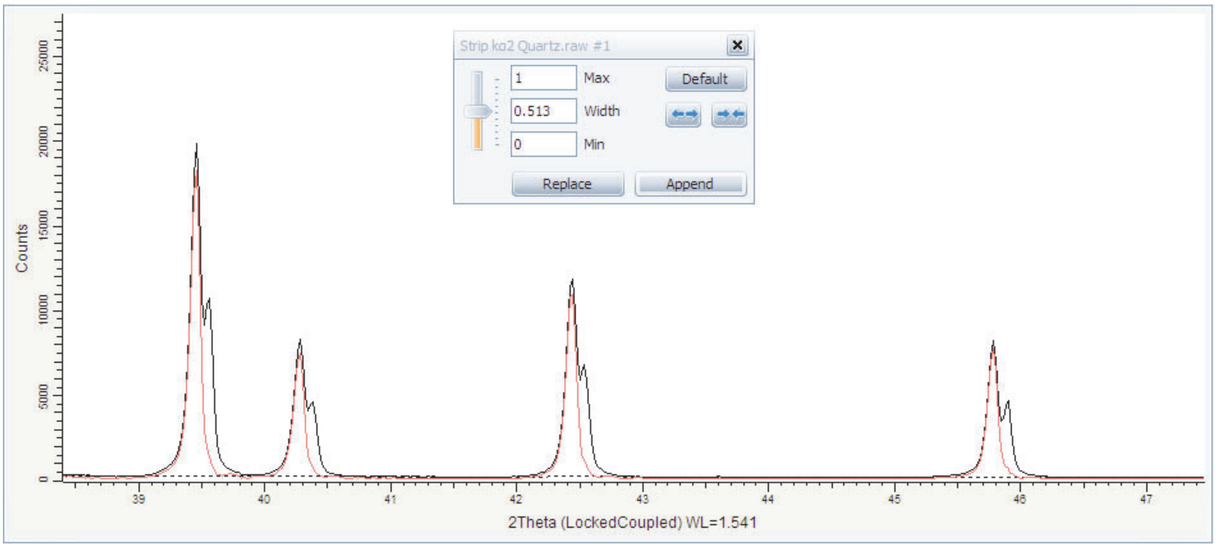


Max: 1
Width: 0.513
Min: 0

Fig. 54: Strip Kα2 dialog box and in the graphical view: ghost Kα2-stripped line

The default parameters are set in the Strip Kα2 dialog box and the ghost line shows the Kα_2-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.



Max: 1
Width: 0.513
Min: 0

Fig. 55: Zoom on the peaks (2θ=38° to 48°)

4. If 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.

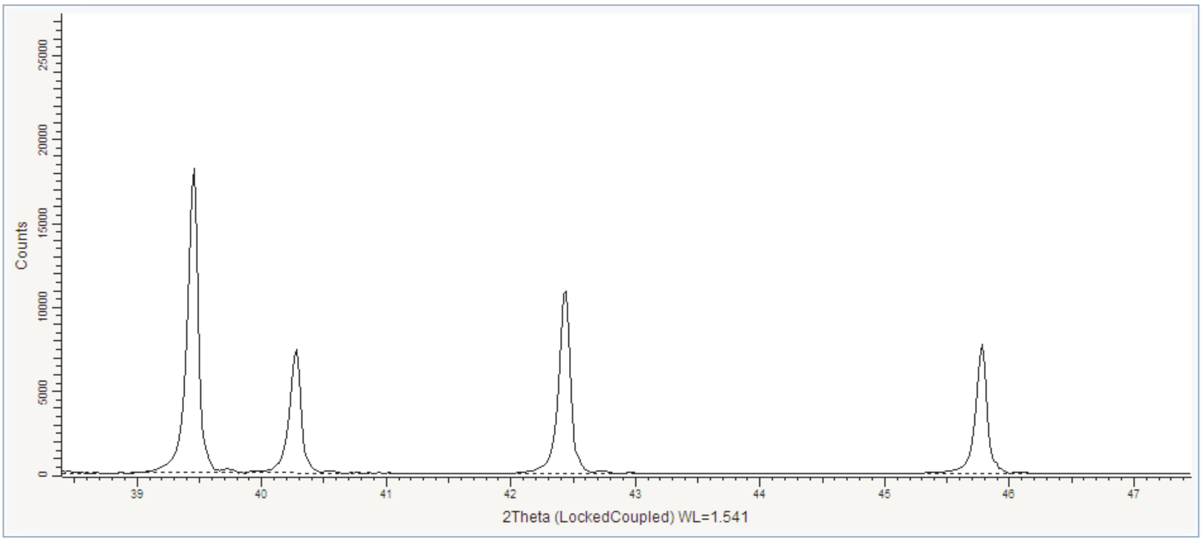
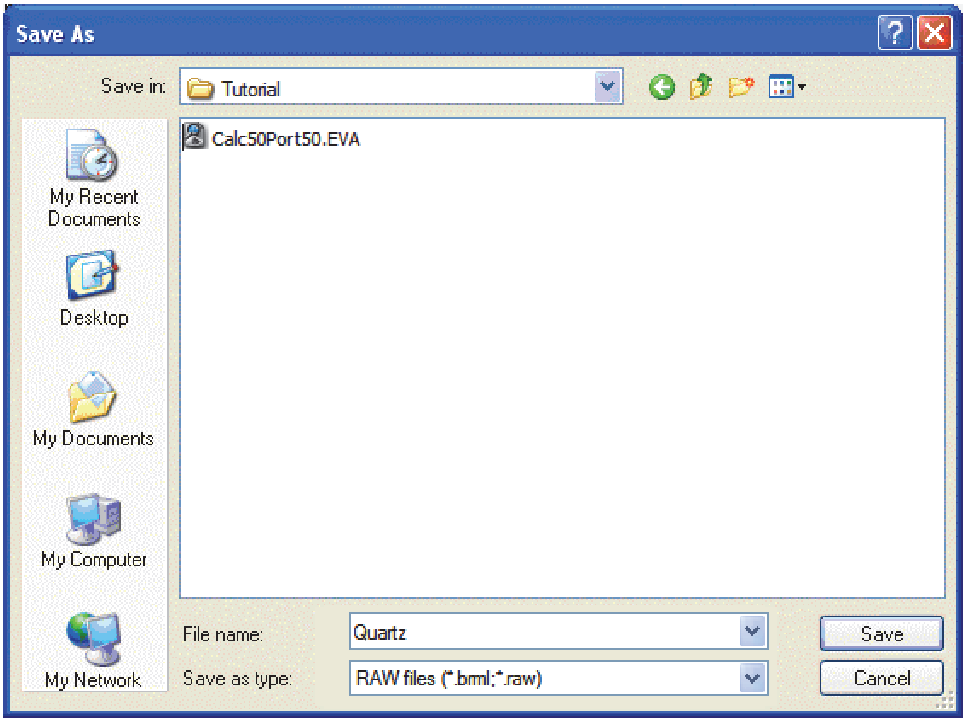


Fig. 56: Original scan replaced with the Kα2 subtracted scan - Zoom on the peaks (2θ=38° to 48°)

Step 3: Saving

1. Click **Save As** on the **File** menu. The Save As dialog box will be displayed.
2. Select the appropriate disc drive and directory.
3. Type in the file name.
4. Click **Save**.



Save in: Tutorial

Calc50Port50.EVA

File name: Quartz

Save as type: RAW files (*.brml;*.raw)

Fig. 57: Saving the Quartz.EVA document

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:

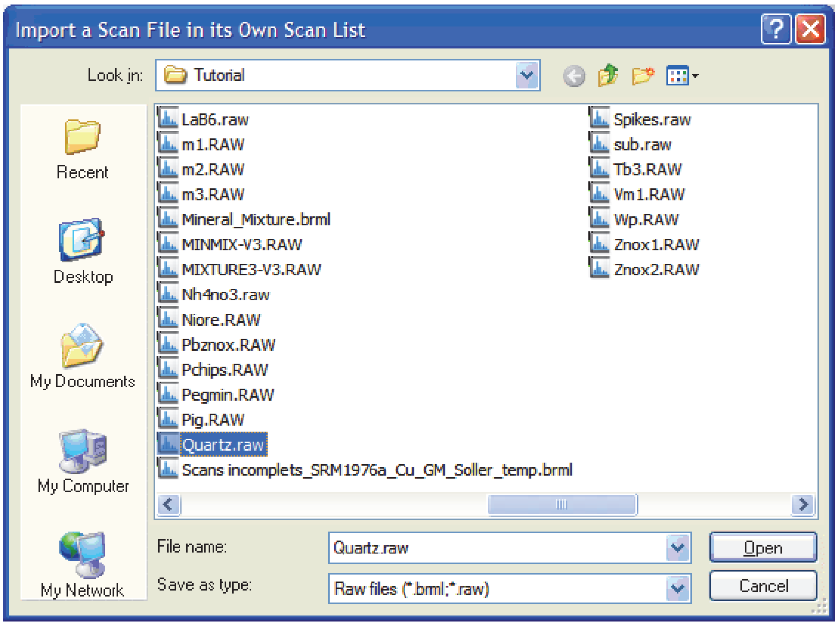
1. Creating a new EVA document and importing Quartz.RAW.
2. Smoothing the scan.
3. Saving the EVA document containing the scan.

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

New button

Import from file button

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 file** data command or the **Import from file** button. The Import from files dialog box will be displayed.
3. Search the Tutorials/EVA[1] directory and select the Quartz.RAW file.
4. Click **Open**. The scan Quartz.RAW will be displayed in the graphical view of the EVA document.



File name: Quartz.raw

Save as type: Raw files (*.brml;*.raw)

Fig. 58: Import a Scan File dialog box

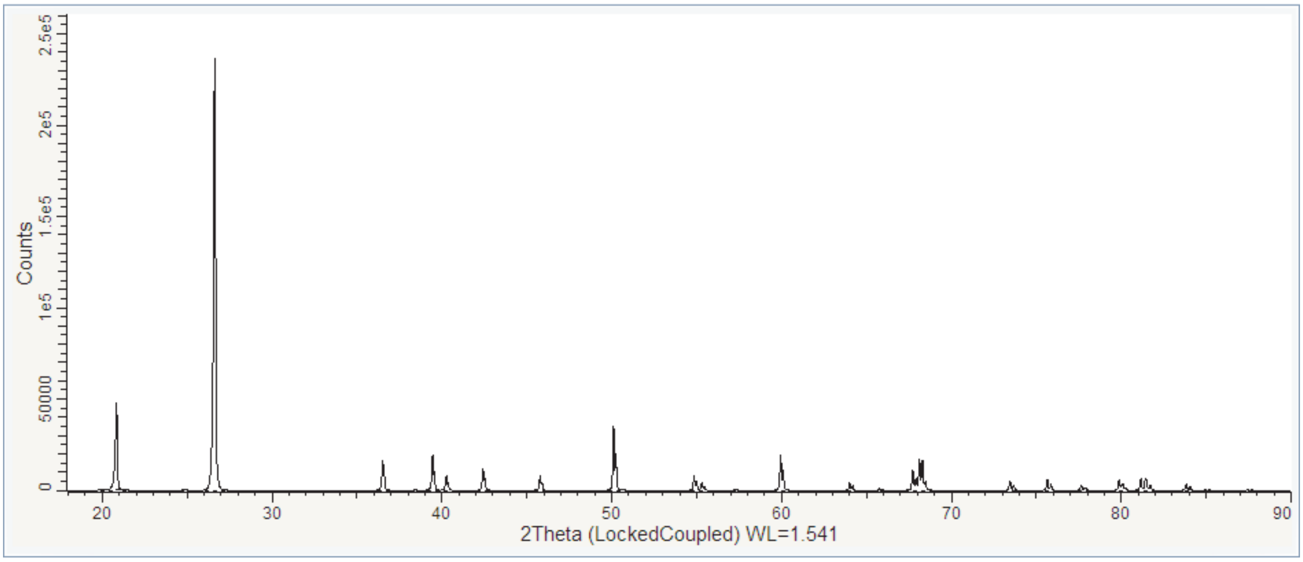


Fig. 59: Quartz scan imported in the graphical view

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[1] 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.

Step 2: Smoothing the Scan

Case #1: Smoothing

1. Make certain the scan is selected; if not, select it either in the data tree or in the 1D view.
2. 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.

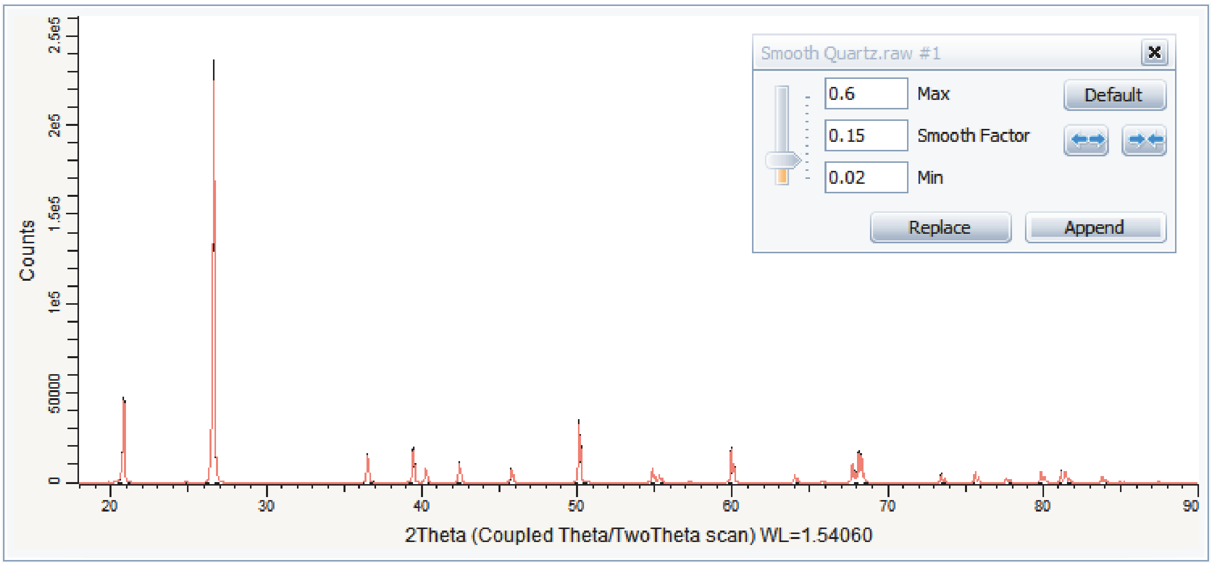

Smooth Quartz.raw #1
0.6 Max
0.15 Smooth Factor
0.02 Min

Fig. 60: Smooth dialog box and in the graphical view: ghost smoothed line

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.

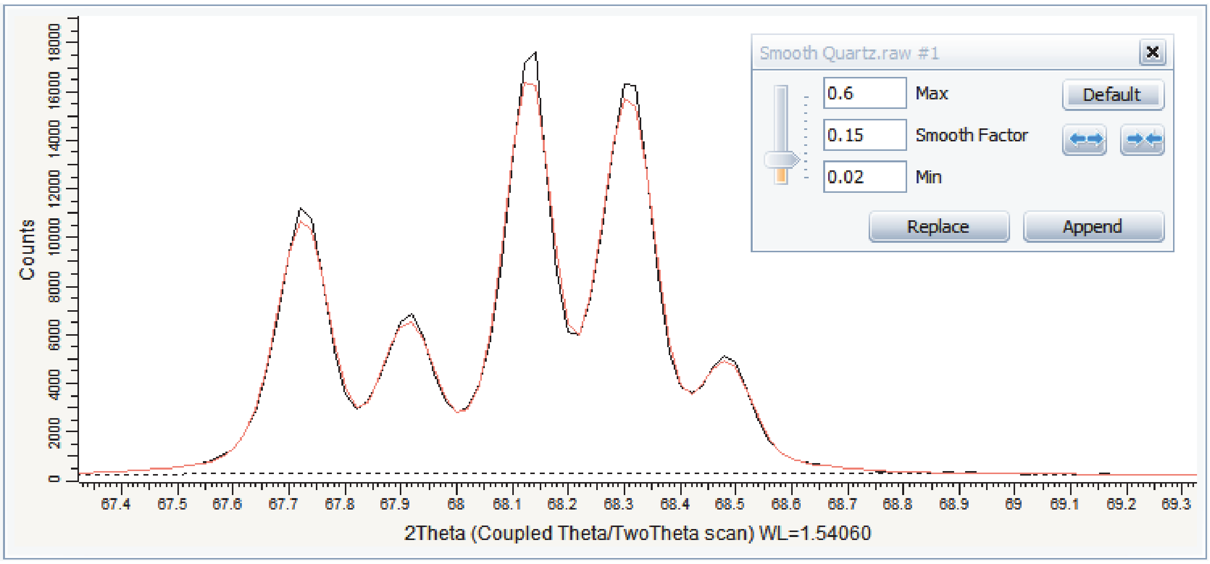

Smooth Quartz.raw #1
0.6 Max
0.15 Smooth Factor
0.02 Min

Fig. 61: Zoom on peaks (2θ=67° to 69°)

4. If the default parameters are satisfactory: click the **Default** button to return to the default parameters.

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.

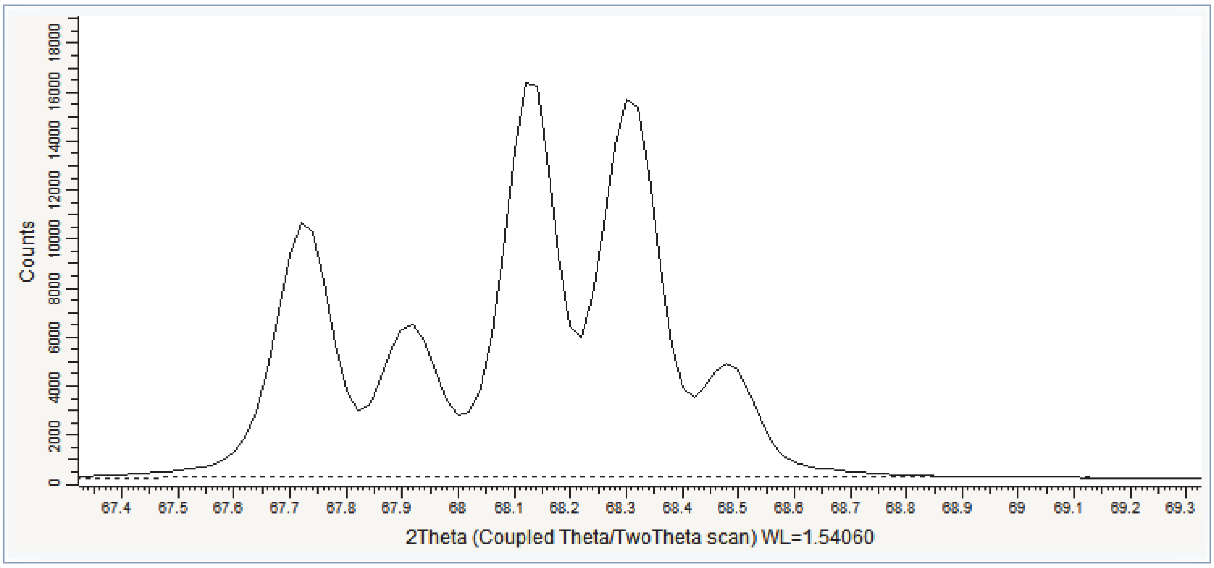
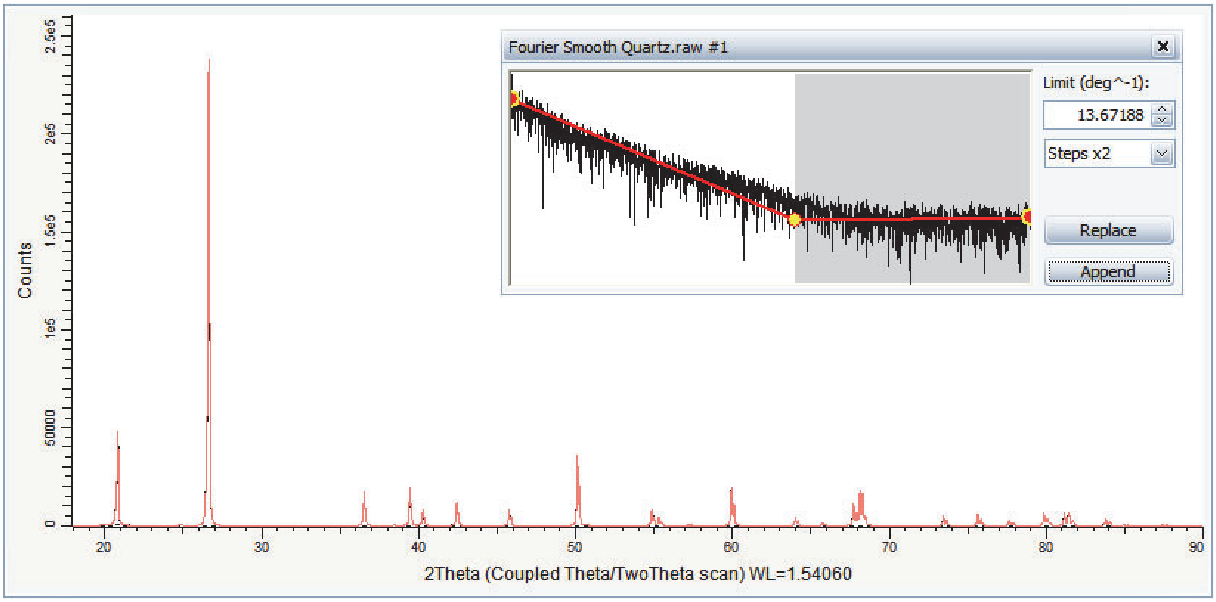


Fig. 62: Original scan replaced with the smoothed scan - Zoom on peaks (2θ=67° to 69°)

<u>Case #2: Fourier Smoothing</u>

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

2. 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.


Fourier Smooth Quartz.raw #1

Limit (deg^-1): 13.67188

Steps x2

Fig. 63: Smooth dialog box and in the graphical view: ghost smoothed line

3. Automatic adjustments are done. The ghost line shows the smoothed line in the graphical view.

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.

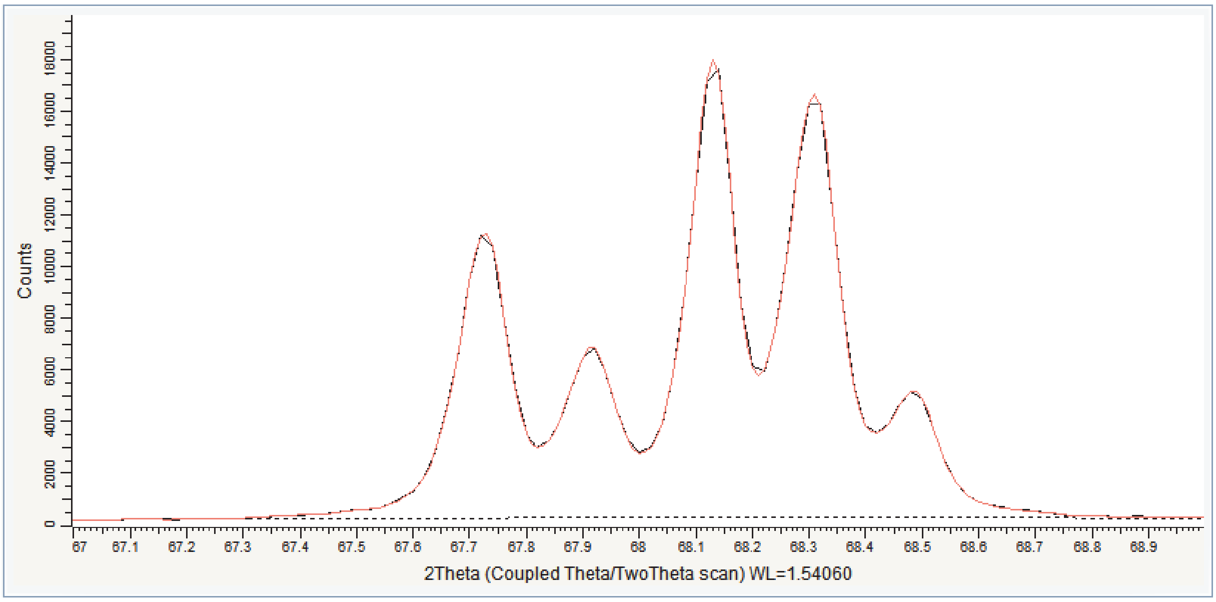


Fig. 64: Zoom on peaks (2θ=67° to 69°)

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.

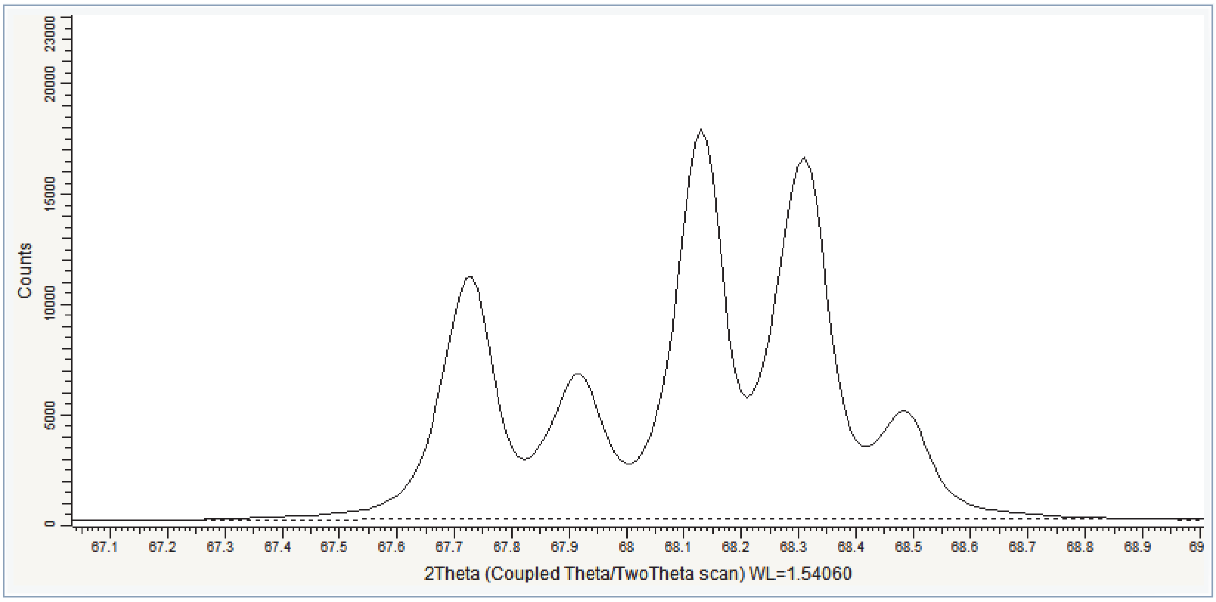
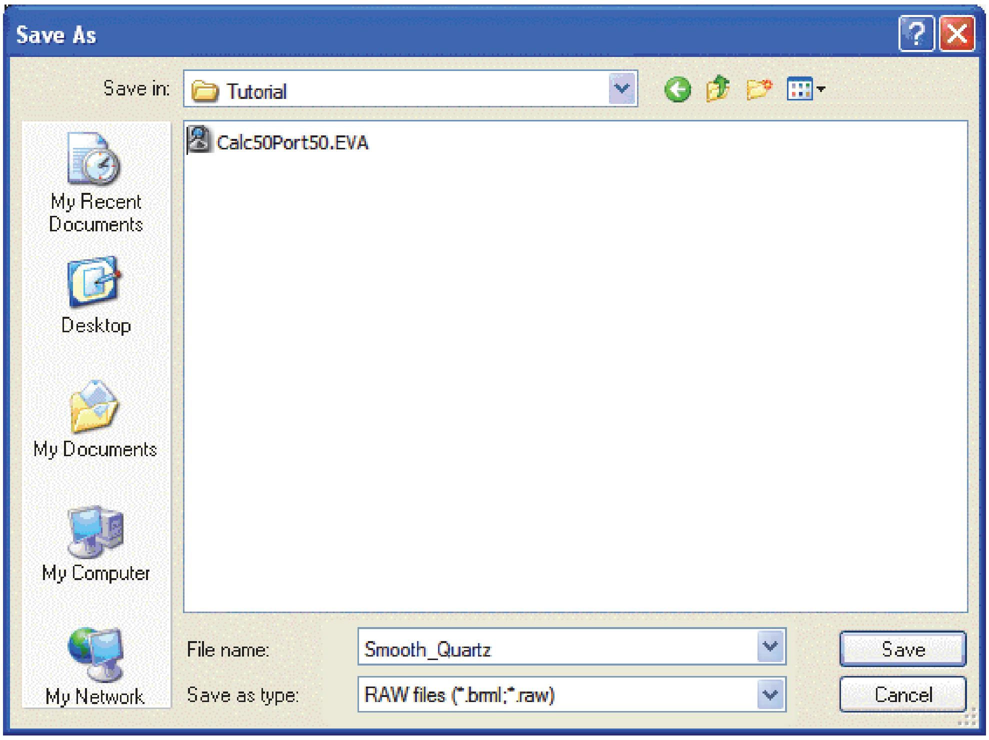


Fig. 65: Original scan replaced with the smoothed scan - Zoom on peaks (2θ=67° to 69°)

Step 3: Saving

1. Click **Save As** on the **File** menu. The Save As dialog box will be displayed.
2. Select the appropriate disc drive and directory.
3. Type in the file name.
4. Click **Save**.



File name: Smooth_Quartz

Save as type: RAW files (*.brml;*.raw)

Fig. 66: Saving the Smooth_Quartz.EVA document

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:

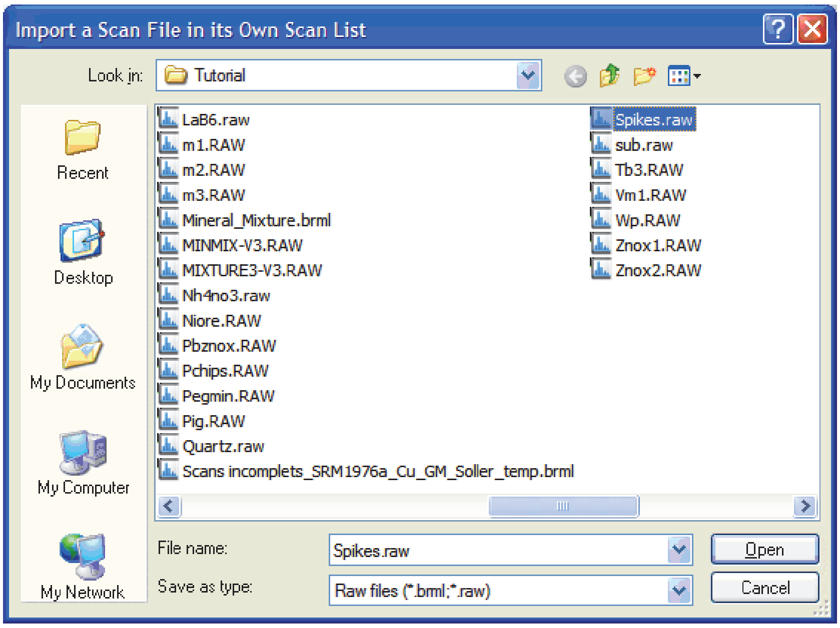
1. Creating a new EVA document and importing Spikes.RAW.
2. Removing the aberrant points.
3. Saving the EVA document containing the scan.

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

New button

Import from file button

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 file** data command or the **Import from file** button. The Import from files dialog box will be displayed.
3. Search the Tutorials/EVA[1] directory and select the Spikes.RAW file.
4. Click **Open**. The scan Spikes.RAW will be displayed in the graphical view of the EVA document.


Import a Scan File in its Own Scan List

Look in: Tutorial

File name: Spikes.raw

Save as type: Raw files (*.brml;*.raw)

Fig. 67: Import a Scan File dialog box

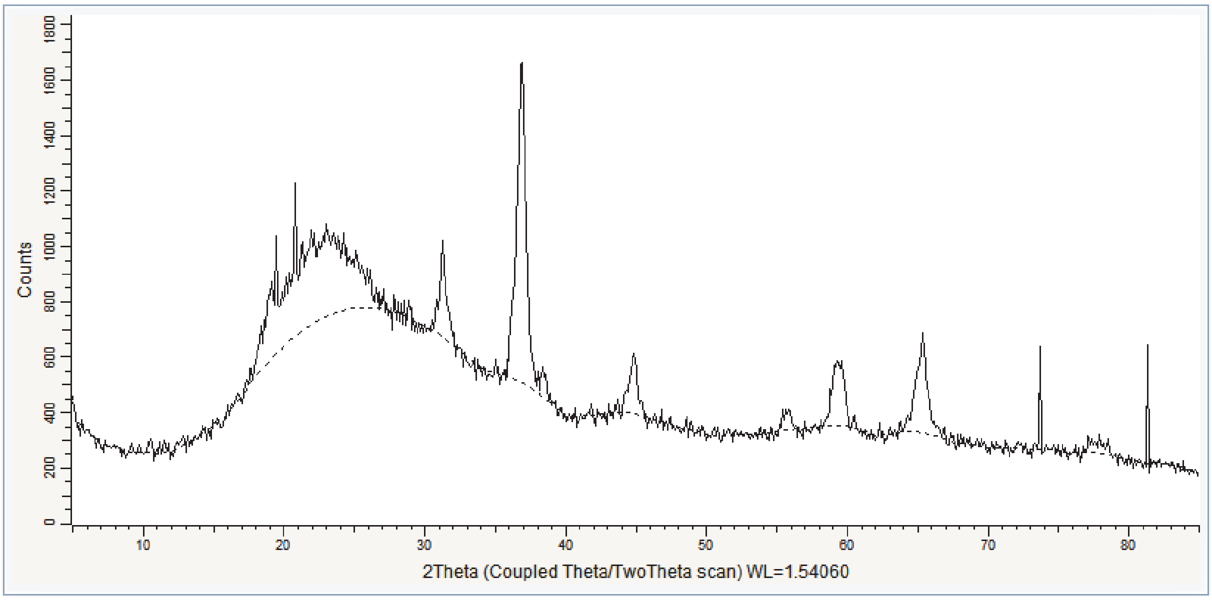


Fig. 68: Spikes scan imported in the graphical view

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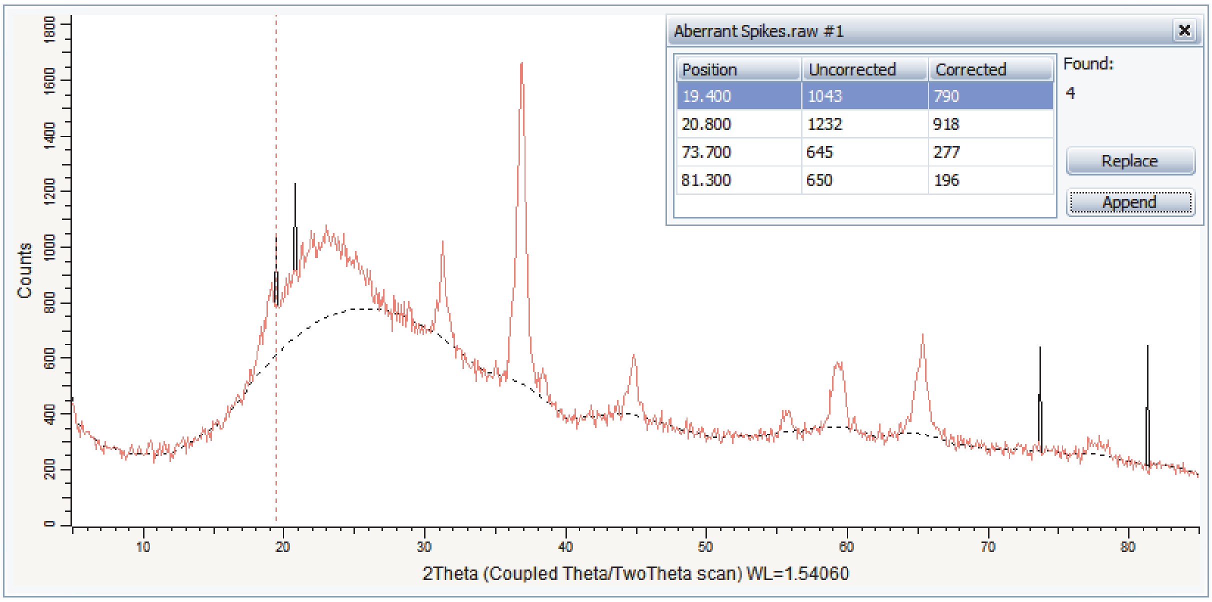
[1] The directory path to the EVA tutorial files is "C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials" under Windows XP and "C:\ProgramData\Bruker AXS\Tutorials" under Windows 7.
To access the folder with the explorer, select "Display hidden files and folders" in the Folders options.

Step 2: Removing Aberrant Points

1. Make certain the scan is selected; if not, select it either in the data tree or in the 1D view.
2. 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.



Aberrant Spikes.raw #1

Position	Uncorrected	Corrected
19.400	1043	790
20.800	1232	918
73.700	645	277
81.300	650	196

Found:
4

Fig. 69: Aberrant dialog box and graphical view displaying a ghost line with the aberrant points removed

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.

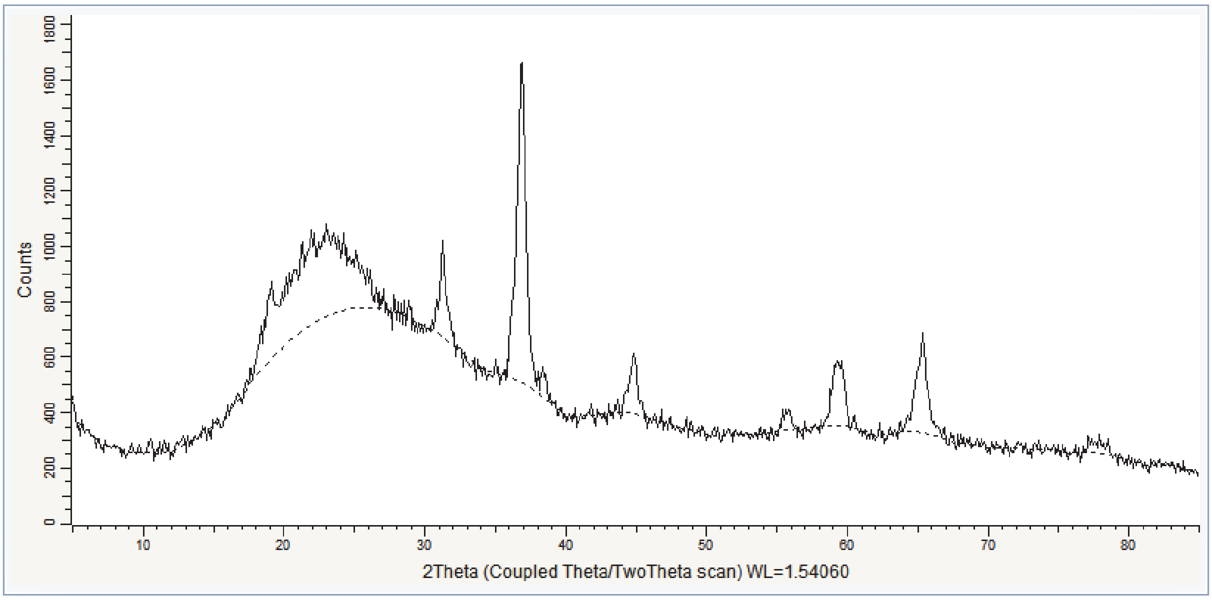
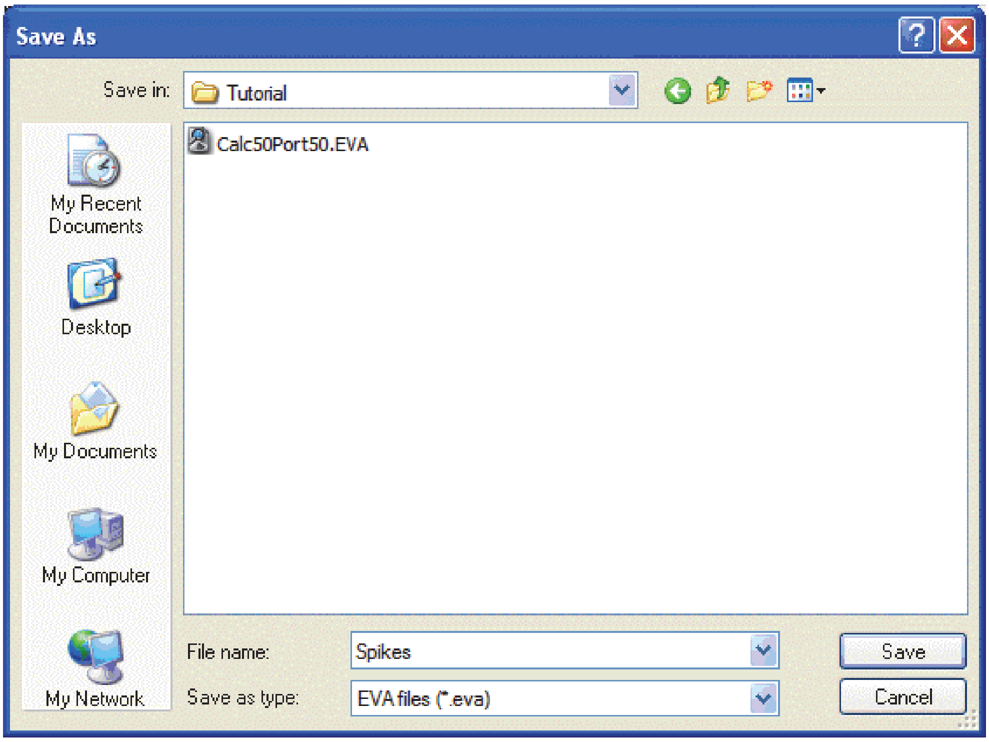


Fig. 70: Original scan replaced with the corrected scan

Step 3: Saving

1. Click **Save As** on the **File** menu. The Save As dialog box will be displayed.
2. Select the appropriate disc drive and directory.
3. Type in the file name.
4. Click **Save**.



File name: Spikes

Save as type: EVA files (*.eva)

Fig. 71: Saving the Spikes.EVA document

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:

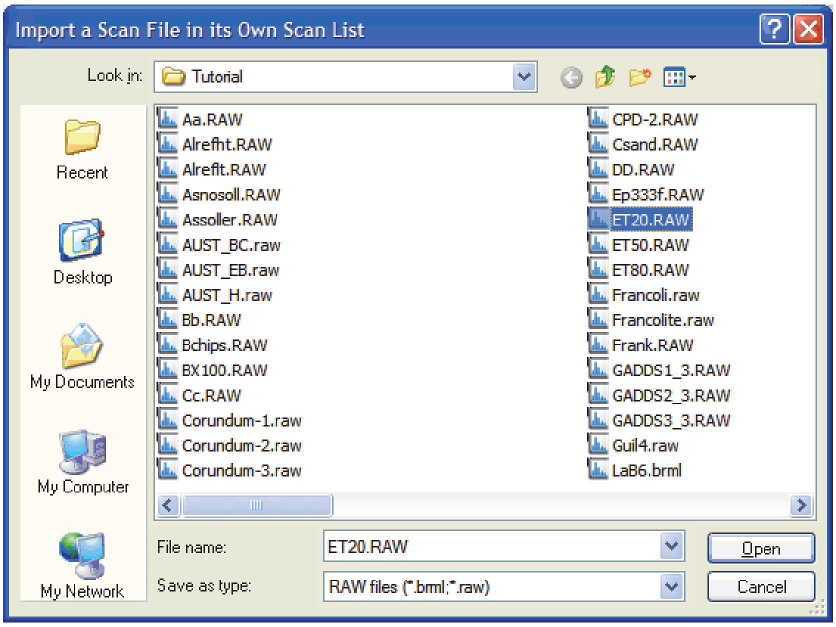
1. Creating a new EVA document and importing ET20.RAW.
2. Selecting and computing an area.
3. Saving the EVA document containing the scan.

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

New button

Import from file button

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 file** data command or the **Import from file** button. The Import from files dialog box will be displayed.
3. Search the Tutorials/EVA[1] directory and select the ET20.RAW file.
4. Click **Open**. The scan ET20 will be displayed in the graphical view of the EVA document.



Import a Scan File in its Own Scan List

Look in: Tutorial

File name: ET20.RAW

Save as type: RAW files (*.brml;*.raw)

Fig. 72: Import a Scan File dialog box

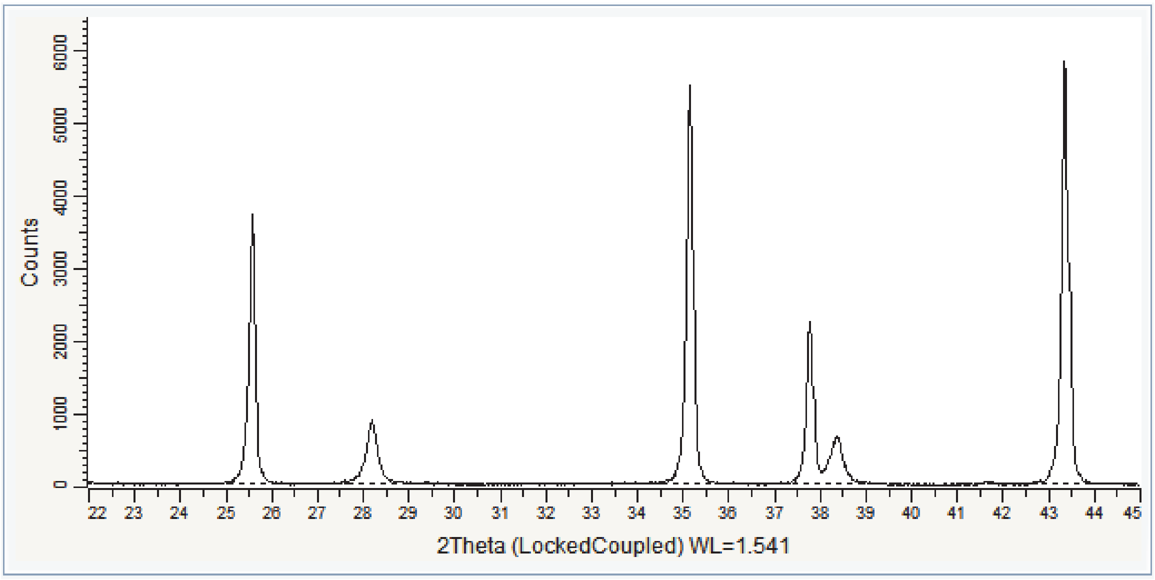


Fig. 73: ET20.RAW file imported in the graphical view

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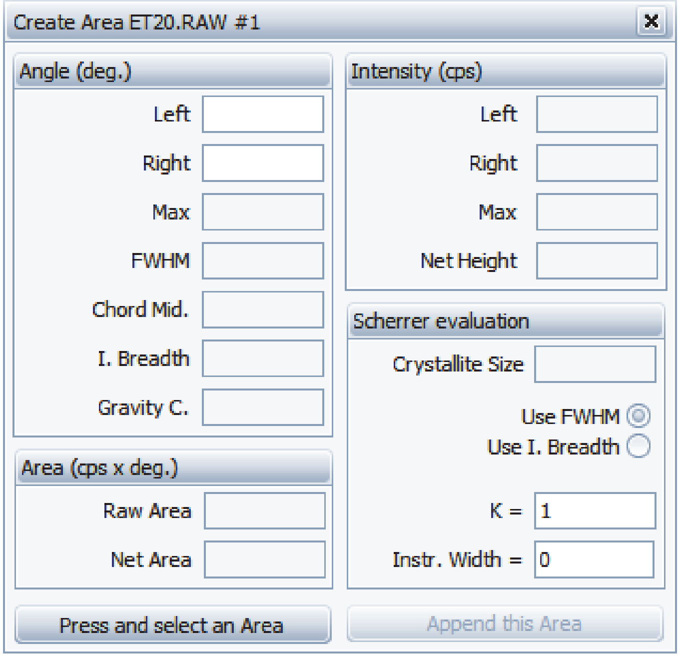
[1] The directory path to the EVA tutorial files is "C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials" under Windows XP and "C:\ProgramData\Bruker AXS\Tutorials" under Windows 7.
To access the folder with the explorer, select "Display hidden files and folders" in the Folders options.

Step 2: Selecting and Computing an Area

1. Make certain the scan is selected; if not, select it either in the data tree or in the 1D view.
2. Click **Create Area** in the Tool list of the Data Command panel,
   — 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.



Use FWHM ●
Use I. Breadth ○
K = 1
Instr. Width = 0

Fig. 74: Create Area dialog box

3. 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.

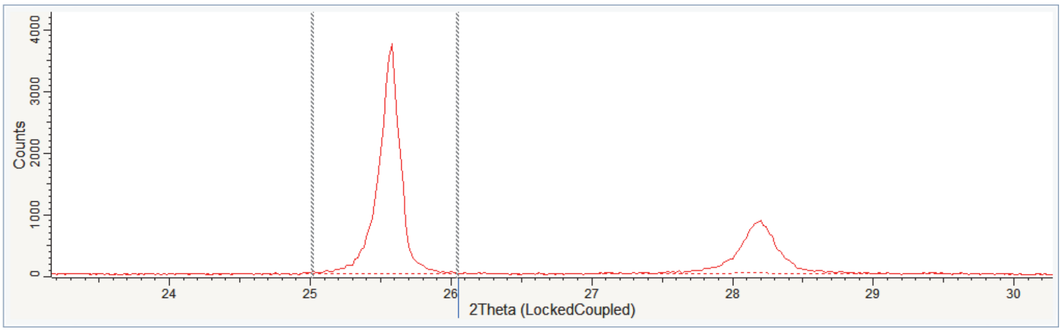


Fig. 75: Selecting an area

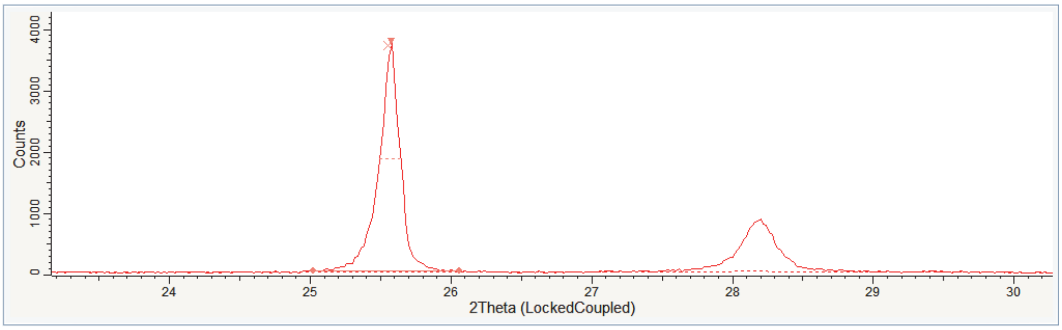
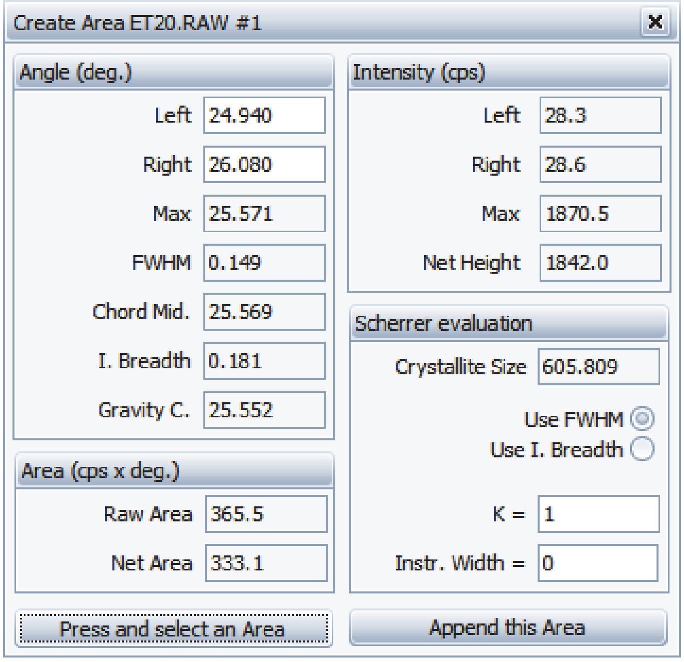


Fig. 76: Area selected

You can modify the area by dragging any filled circle of the area bottom line.

The results are displayed in the dialog box.



Angle (deg.)

Left 24.940
Right 26.080
Max 25.571
FWHM 0.149
Chord Mid. 25.569
I. Breadth 0.181
Gravity C. 25.552

Area (cps x deg.)

Raw Area 365.5
Net Area 333.1

Intensity (cps)

Left 28.3
Right 28.6
Max 1870.5
Net Height 1842.0

Scherrer evaluation

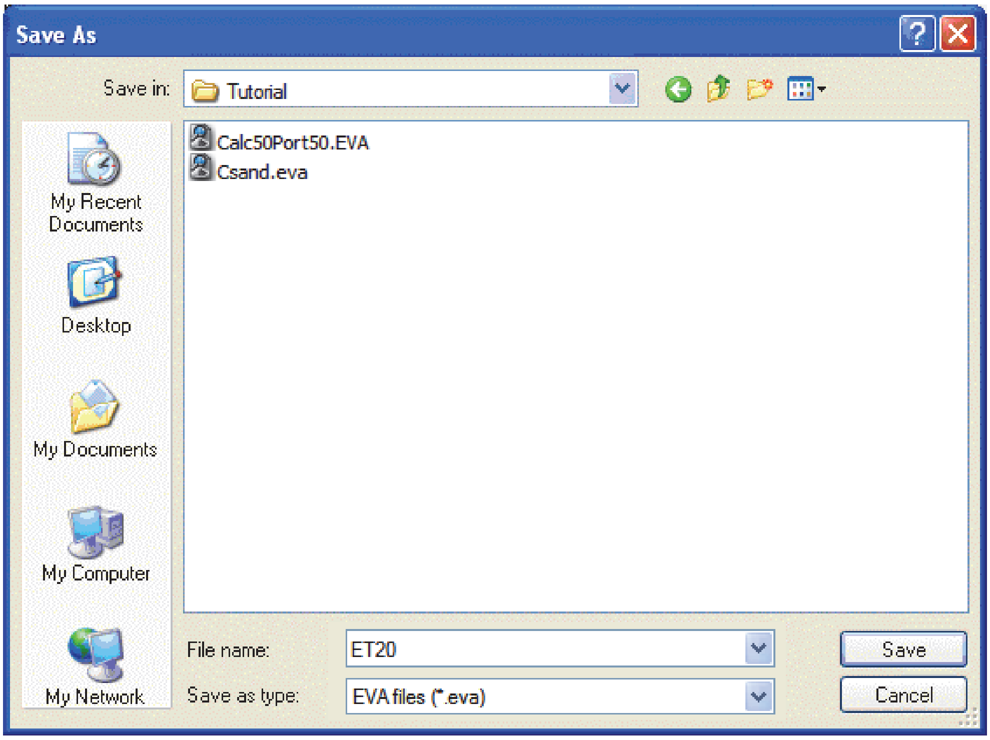
Crystallite Size 605.809
Use FWHM ●
Use I. Breadth ○
K = 1
Instr. Width = 0

Fig. 77: 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.

Step 3: Saving

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



Save in: Tutorial

Calc50Port50.EVA
Csand.eva

File name: ET20

Save as type: EVA files (*.eva)

Fig. 78: Saving ET20.EVA document

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:

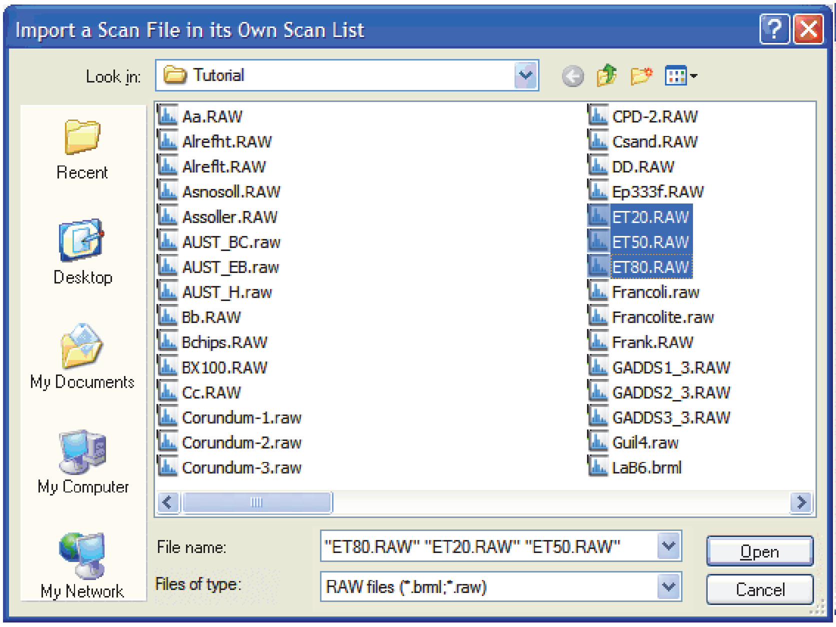
1. Creating a new EVA document and importing ET20.RAW, ET50.RAW and ET80.RAW.
2. Adding the scans.
3. Saving the EVA document containing the scans.

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

New button

Import from file button

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 file** data command or the **Import from file** button. The Import from files dialog box will be displayed. Search the Tutorials/EVA[1] directory and multi-select the ET20.RAW, ET50.RAW and ET80.RAW files.
3. Click **Open**. The scan ET20, ET50 and ET80 will be displayed in the graphical view of the EVA document.



Look in: Tutorial

File name: "ET80.RAW" "ET20.RAW" "ET50.RAW"

Files of type: RAW files (*.brml;*.raw)

Fig. 79: Import a Scan File dialog box

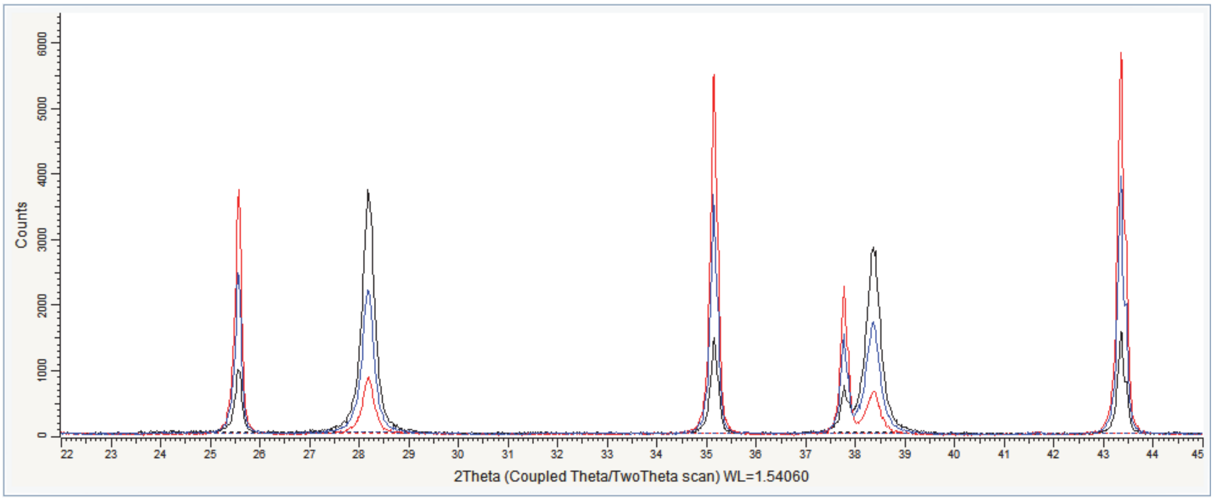


Fig. 80: ET20.RAW, ET50.RAW and ET80.RAW files imported in the graphical view

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[1] 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.

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 —
   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.

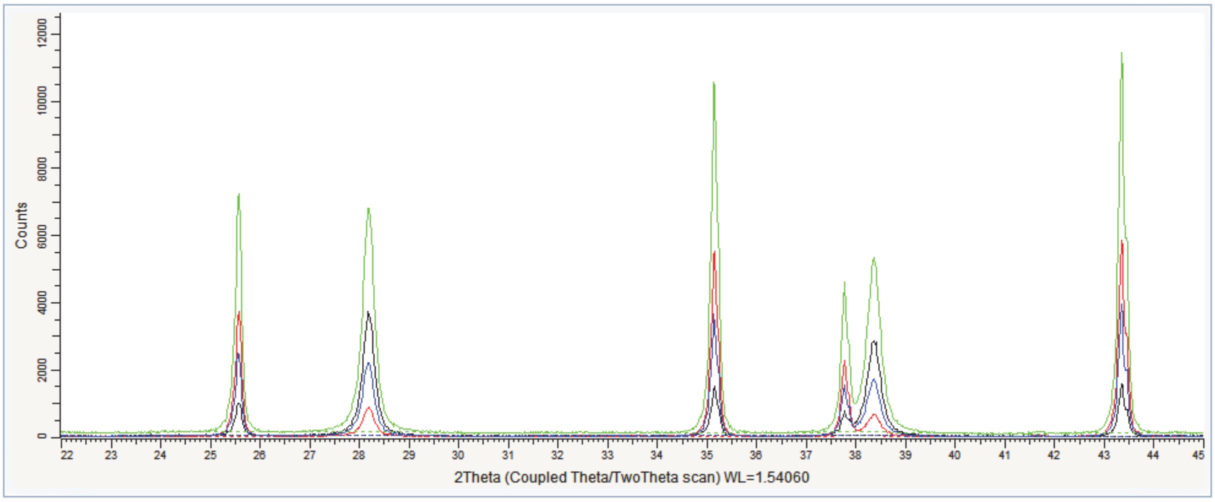
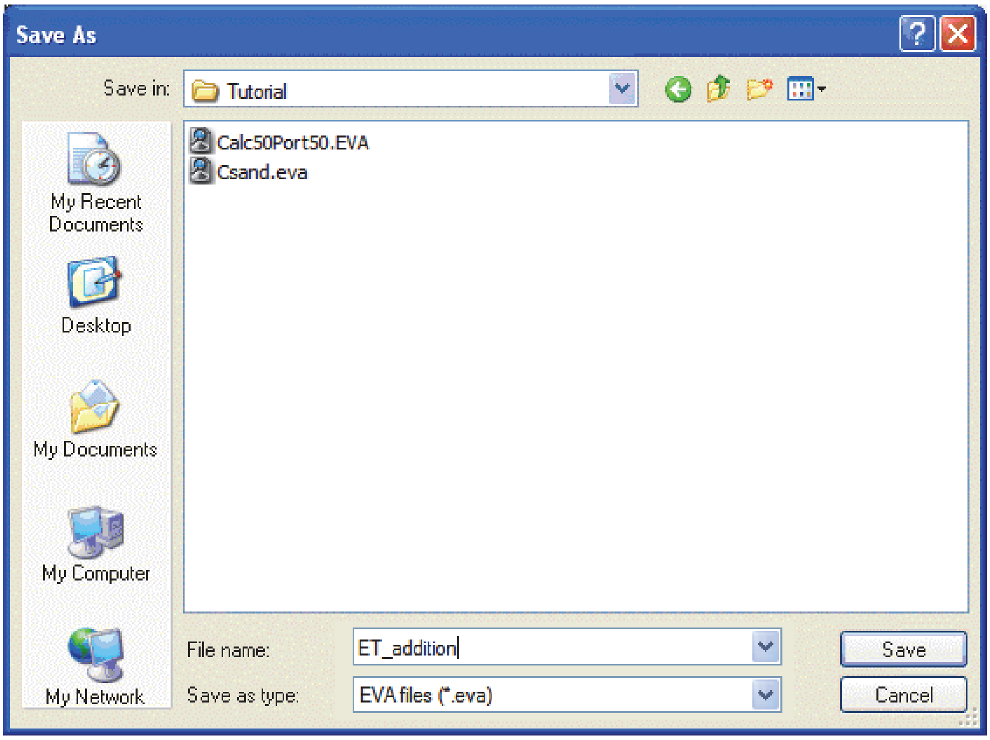


Fig. 81: Original scans and the scan resulting from the addition

Step 3: Saving

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



File name: ET_addition

Save as type: EVA files (*.eva)

Fig. 82: Saving ET_addition.EVA document

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:

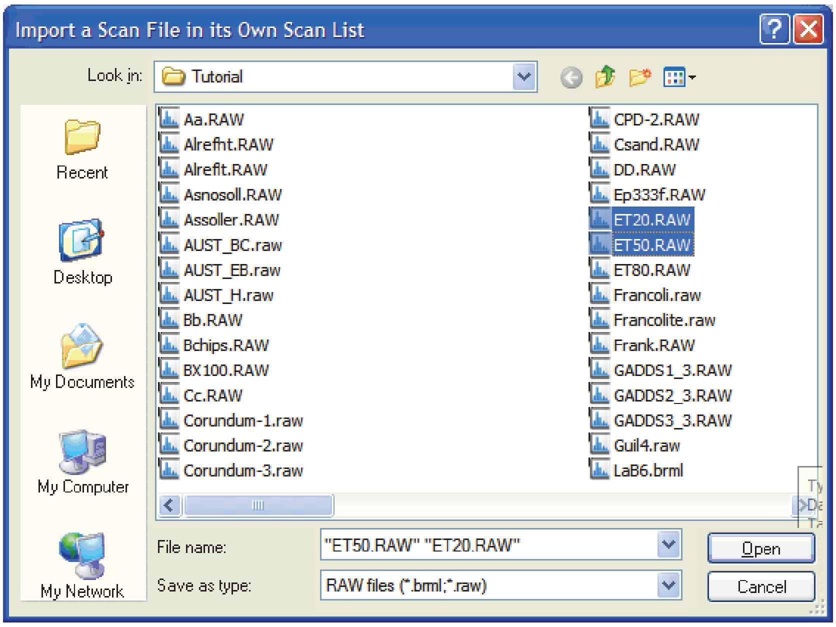
1. Creating a new EVA document and importing ET20.RAW and ET50.RAW.
2. Subtracting the scans.
3. Saving the EVA document containing the scans.

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

New button

Import from file button

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 file** data command or the **Import from file** button. The Import from files dialog box will be displayed. Search the Tutorials/EVA[1] directory and multi-select the files ET20.RAW and ET50.RAW.
3. Click **Open**. The scans ET20 and ET50 will be displayed in the graphical view of the EVA document. Select the **Display Legend** check box to display the legend in the graphical view.



Import a Scan File in its Own Scan List

Look in: Tutorial

Aa.RAW	CPD-2.RAW
Alrefht.RAW	Csand.RAW
Alrefit.RAW	DD.RAW
Asnosoll.RAW	Ep333f.RAW
Assoller.RAW	ET20.RAW
AUST_BC.raw	ET50.RAW
AUST_EB.raw	ET80.RAW
AUST_H.raw	Francoli.raw
Bb.RAW	Francolite.raw
Bchips.RAW	Frank.RAW
BX100.RAW	GADDS1_3.RAW
Cc.RAW	GADDS2_3.RAW
Corundum-1.raw	GADDS3_3.RAW
Corundum-2.raw	Guil4.raw
Corundum-3.raw	LaB6.brml

File name: "ET50.RAW" "ET20.RAW"

Save as type: RAW files (*.brml;*.raw)

Fig. 83: Import a Scan File dialog box

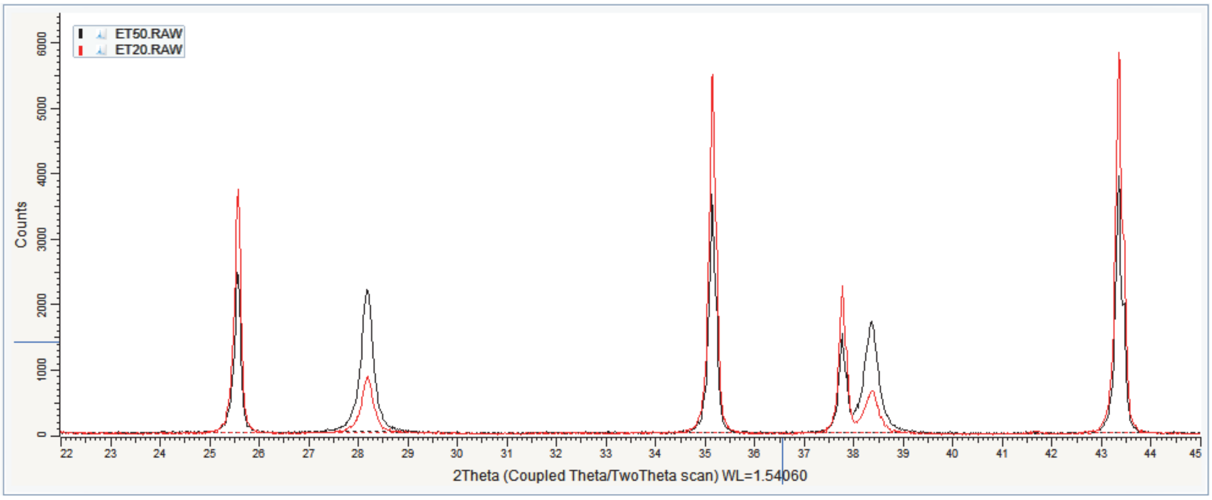


Fig. 84: ET20.RAW and ET50.RAW files imported in the graphical view

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[1] 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.

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 —

   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.

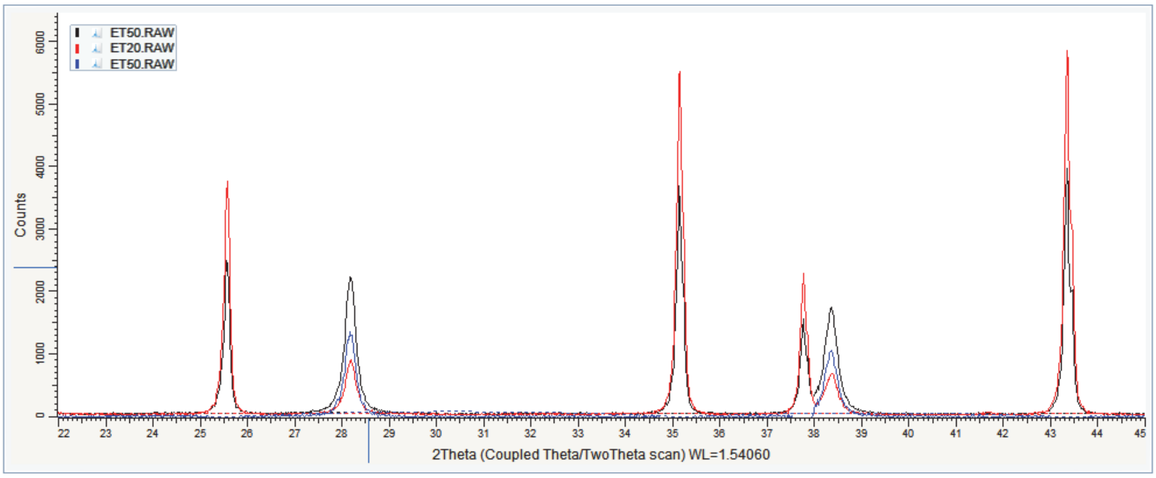


Fig. 85: Original scans and the scan resulting from the subtraction

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 —

   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.

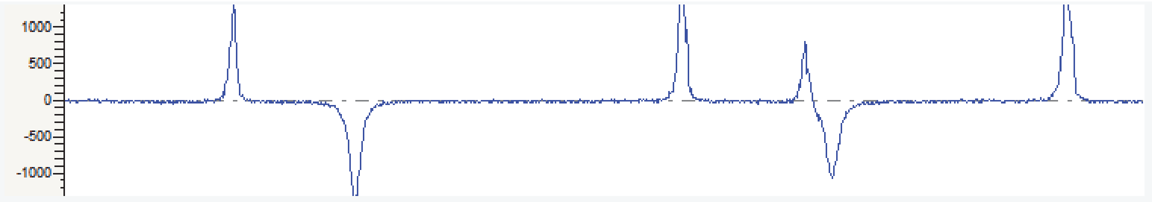
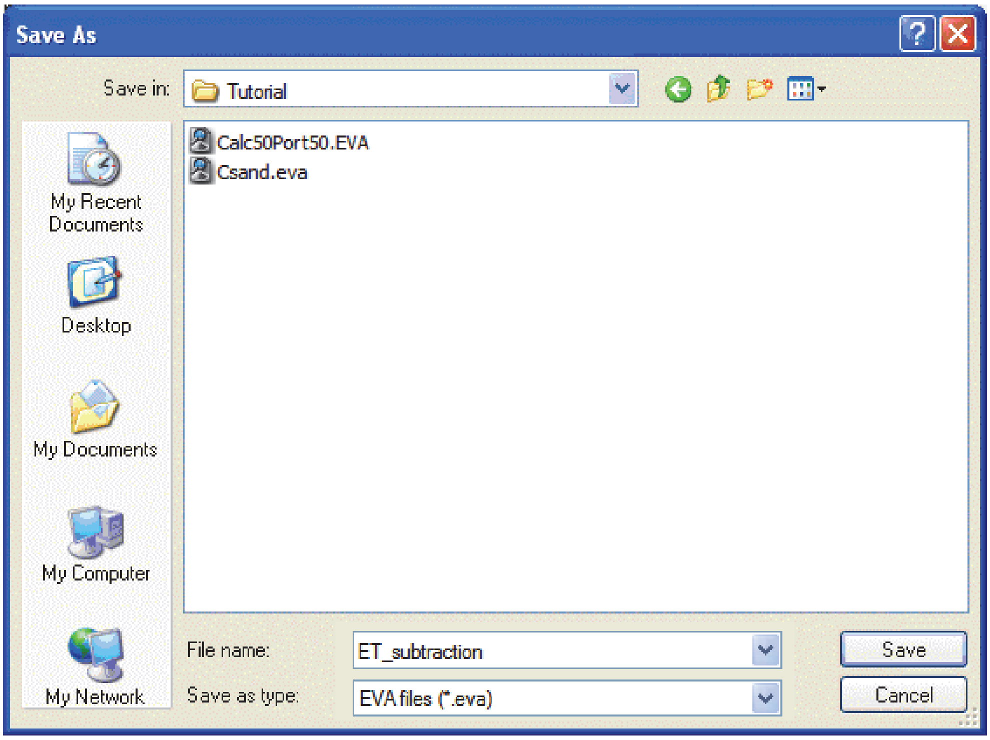


Fig. 86: Difference curve displayed in the extended view

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

Step 3: Saving

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



File name: ET_subtraction

Save as type: EVA files (*.eva)

Fig. 87: Saving ET_subtraction.EVA document

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:

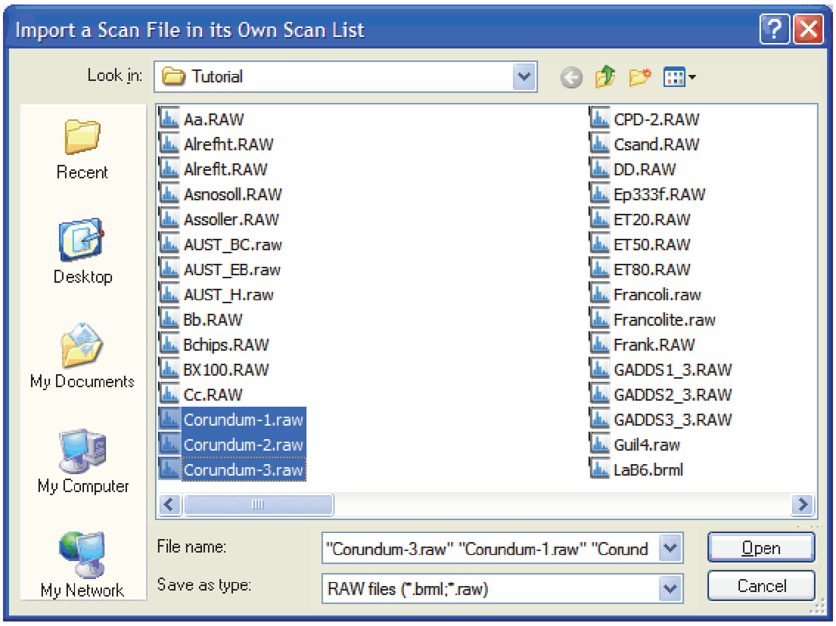
1. Creating a new EVA document and importing Corundum-1.RAW, Corundum-2.RAW and Corundum-3.RAW.
2. Merging the scans.
3. Saving the EVA document containing the scans.

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

New button

Import from file button

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 file** data command or the **Import from file** button. The Import from files dialog box will be displayed. Search the Tutorials/EVA[1] directory and multi-select the files Corundum-1.RAW, Corundum-2.RAW and Corundum-3.RAW.
3. Click **Open**. The scans Corundum-1, Corundum-2 and Corundum-3 will be displayed in the graphical view of the EVA document.



Look in: Tutorial

Aa.RAW
Alrefht.RAW
Alrefit.RAW
Asnosoll.RAW
Assoller.RAW
AUST_BC.raw
AUST_EB.raw
AUST_H.raw
Bb.RAW
Bchips.RAW
BX100.RAW
Cc.RAW
Corundum-1.raw
Corundum-2.raw
Corundum-3.raw
CPD-2.RAW
Csand.RAW
DD.RAW
Ep333f.RAW
ET20.RAW
ET50.RAW
ET80.RAW
Francoli.raw
Francolite.raw
Frank.RAW
GADDS1_3.RAW
GADDS2_3.RAW
GADDS3_3.RAW
Guil4.raw
LaB6.brml

File name: "Corundum-3.raw" "Corundum-1.raw" "Corund

Save as type: RAW files (*.brml;*.raw)

Fig. 88: Import a Scan File dialog box

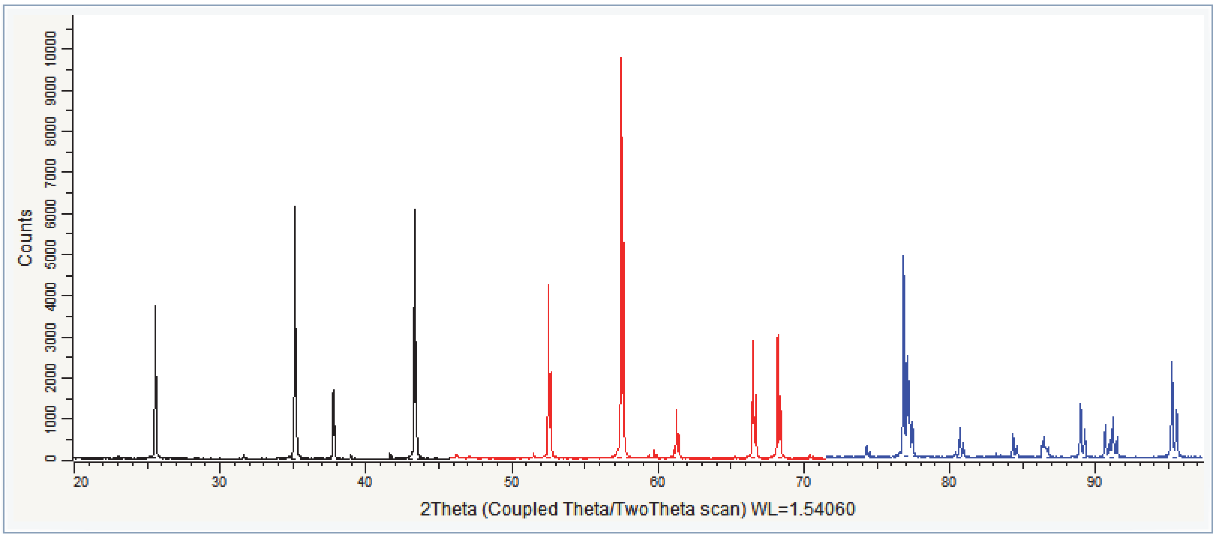


Fig. 89: Corundum-1.RAW, Corundum-2.RAW and Corundum-3 files imported in the graphical view

---

[1] 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.

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 —
   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.

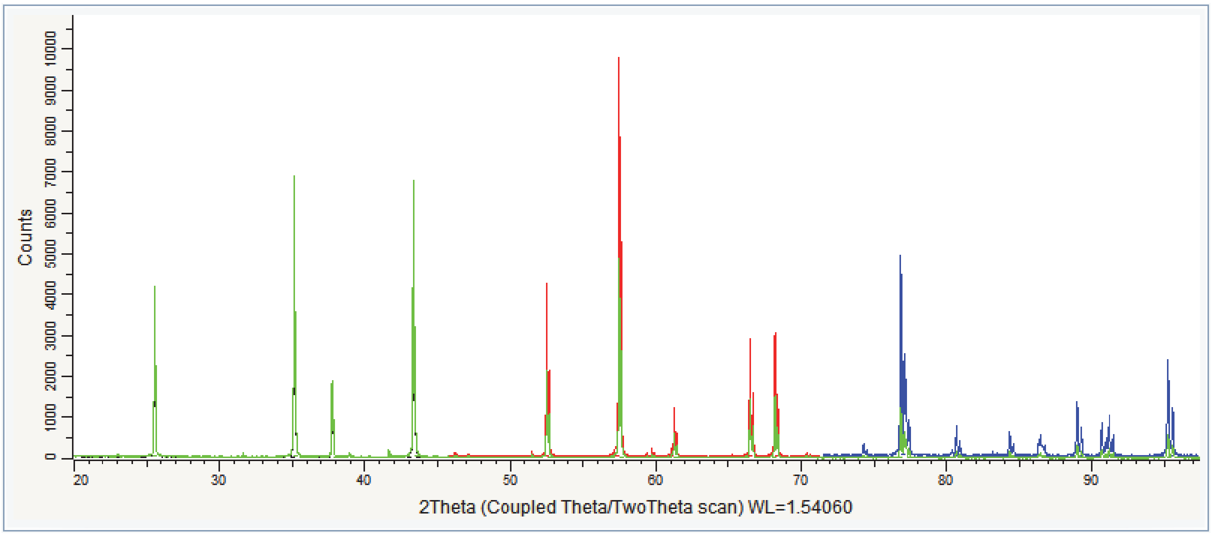
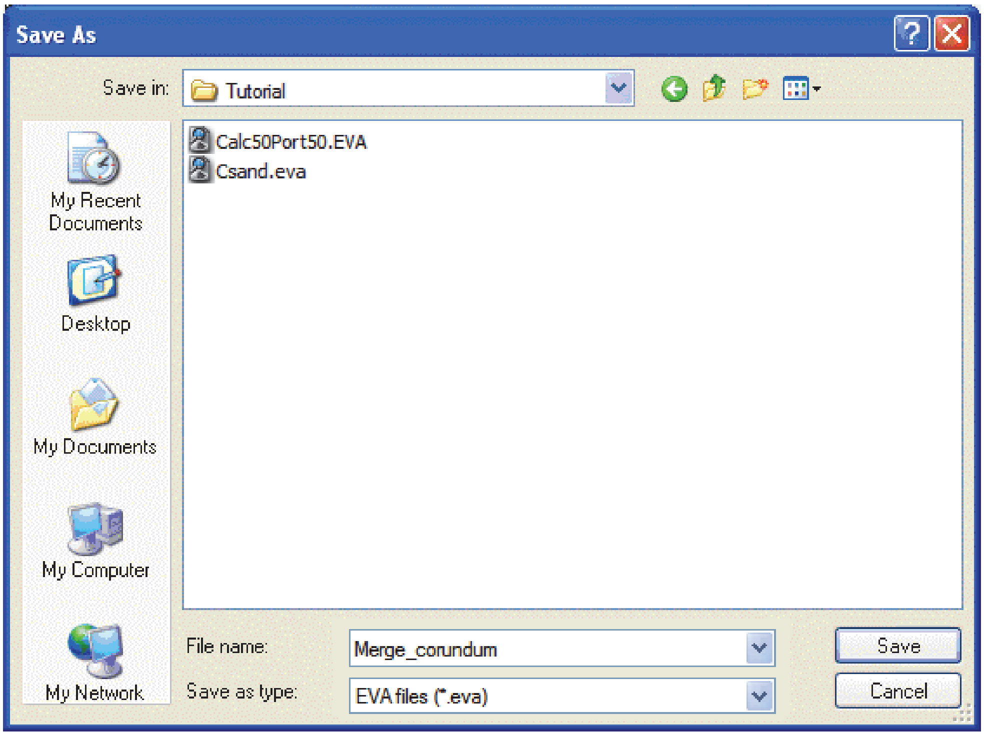


Fig. 90: Original scans and the scan resulting from the merging

Step 3: Saving

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



File name: Merge_corundum

Save as type: EVA files (*.eva)

Fig. 91: Saving Merge_corundum.EVA document

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:

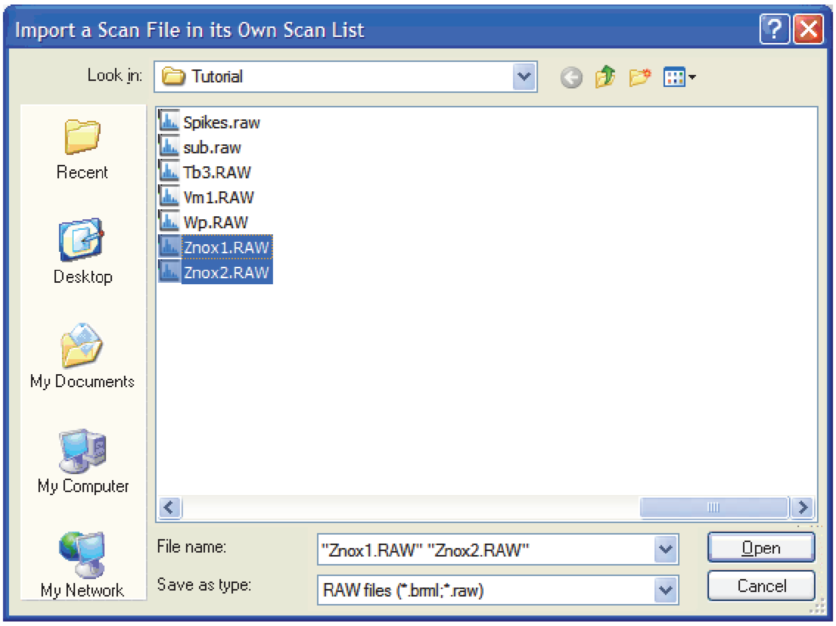
1. Creating a new EVA document and importing Znox1.RAW and Znox2.RAW.
2. Normalizing the scans.
3. Saving the EVA document containing the scans.

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

New button

Import from file button

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 file** data command or the **Import from file** button. The Import from files dialog box will be displayed. Search the Tutorials/EVA[1] directory and multi-select the Znox1.RAW and Znox2.RAW.
3. Click **Open**. The scans Znox1.RAW and Znox2.RAW will be displayed in the graphical view of the EVA document.



Look in: Tutorial

File name: "Znox1.RAW" "Znox2.RAW"

Save as type: RAW files (*.brml;*.raw)

Fig. 92: Import a Scan File dialog box

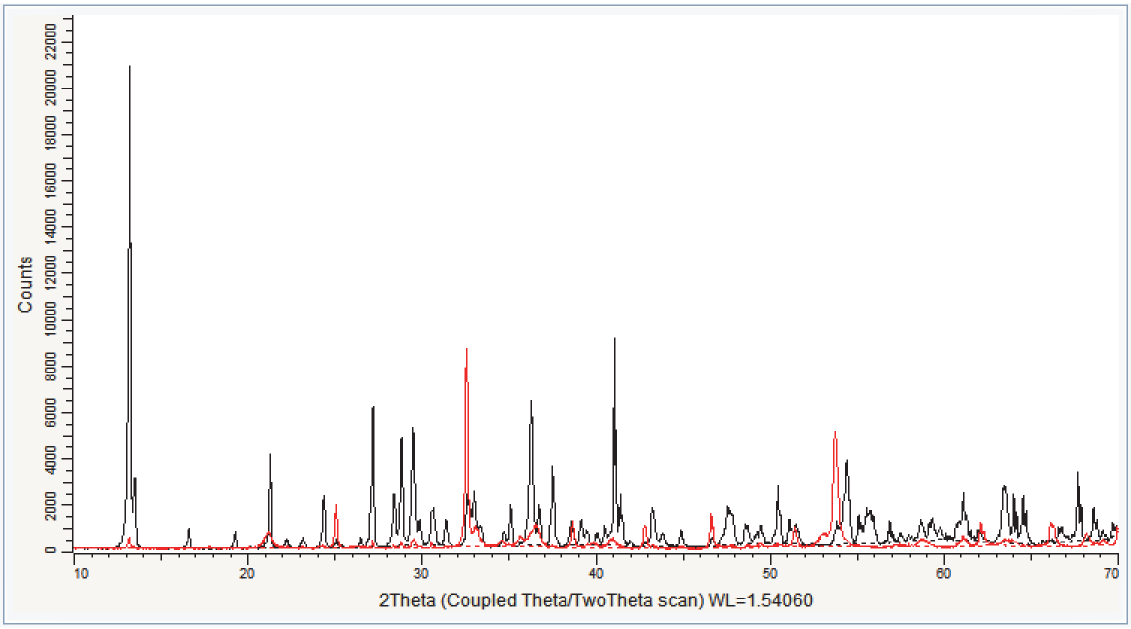


Fig. 93: Znox1.RAW (in red) and Znox2.RAW (in black) files imported in the graphical view

---

[1] 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.

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: the related context menu is displayed.
3. Point to **Normalize all visible scans** and on the sub-menu, click the **Normalize on scan Znox2.RAW** command.
4. The scans are normalized on the maximum of the Znox2 scan:

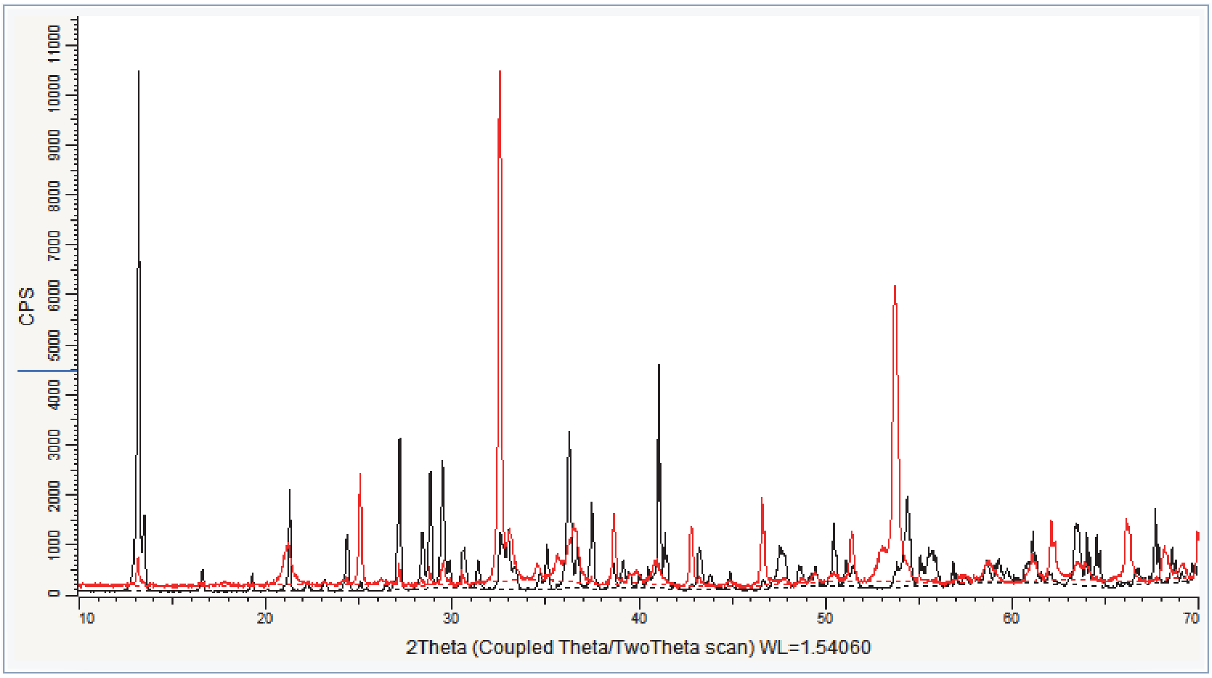
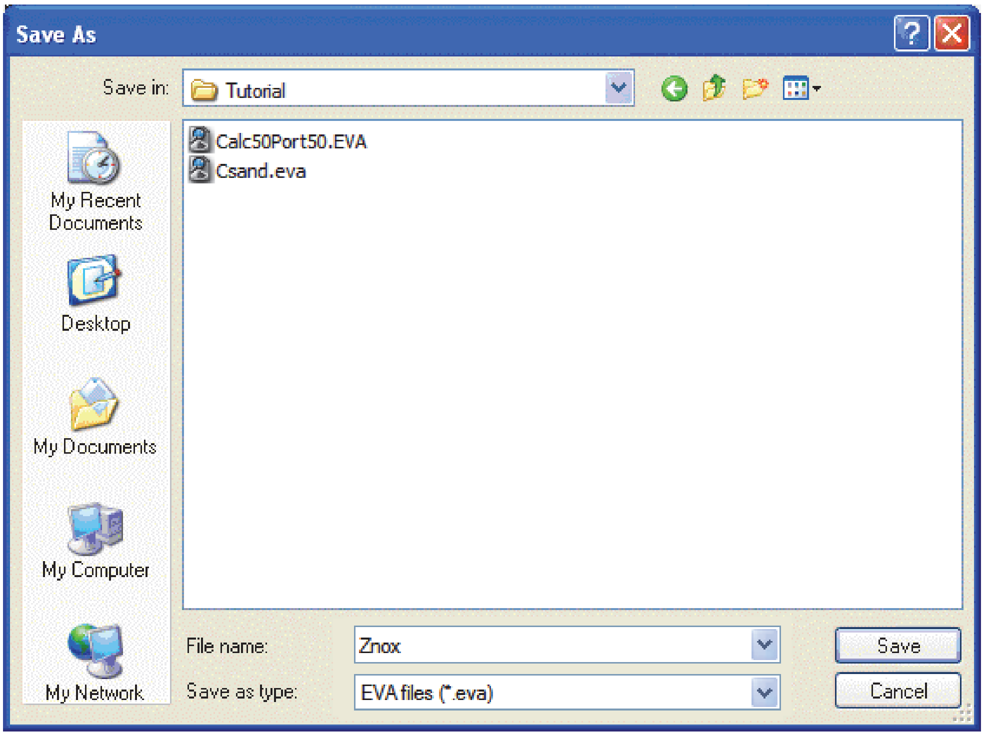


Fig. 94: Original scans and the scan resulting from normalizing

Step 3: Saving

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



Save in: Tutorial

Calc50Port50.EVA

Csand.eva

File name: Znox

Save as type: EVA files (*.eva)

Fig. 95: Saving Znox.EVA document

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:

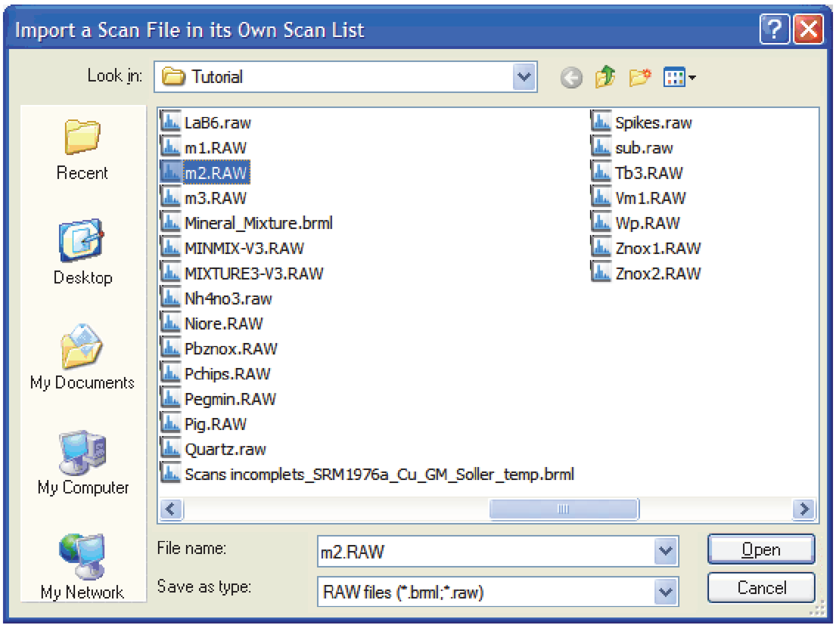
1. Creating a new EVA document and importing m2.RAW.
2. Computing the crystallinity.
3. Checking the calculation.
4. Saving the EVA document containing the scans.

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

New button

Import from file button

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 file** data command or the **Import from file** button. The Import from files dialog box will be displayed. Search the Tutorials/EVA[1] directory and select the m2.RAW file.
3. Click **Open**. The scan m2 will be displayed in the graphical view of the EVA document.



Import a Scan File in its Own Scan List

Look in: Tutorial

LaB6.raw
m1.RAW
m2.RAW
m3.RAW
Mineral_Mixture.brml
MINMIX-V3.RAW
MIXTURE3-V3.RAW
Nh4no3.raw
Niore.RAW
Pbznox.RAW
Pchips.RAW
Pegmin.RAW
Pig.RAW
Quartz.raw
Scans incomplets_SRM1976a_Cu_GM_Soller_temp.brml
Spikes.raw
sub.raw
Tb3.RAW
Vm1.RAW
Wp.RAW
Znox1.RAW
Znox2.RAW

File name: m2.RAW

Save as type: RAW files (*.brml;*.raw)

Fig. 96: Import a Scan File dialog box

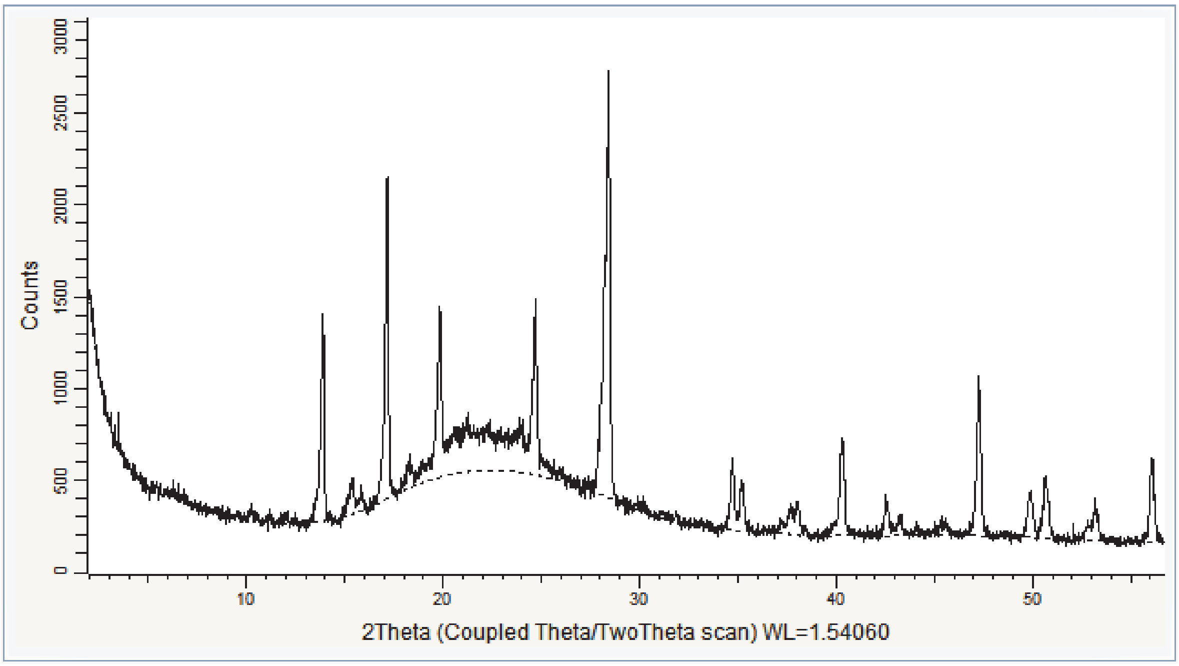


Fig. 97: m2 file imported in the graphical view

---

[1] 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.

Step 2: Computing the Crystallinity

1. Make certain the m2 scan is selected in the data tree.
2. Adjust the background. To do so:
   - Click **Background** in the Tool list of the Data Command panel
     — 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.
   - Adjust the background curvature as shown below.

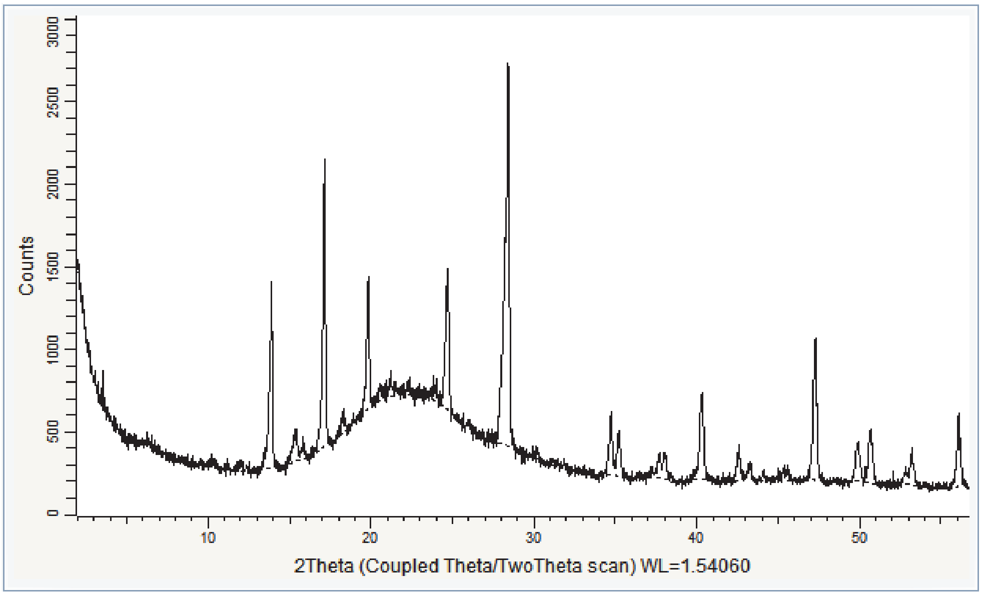
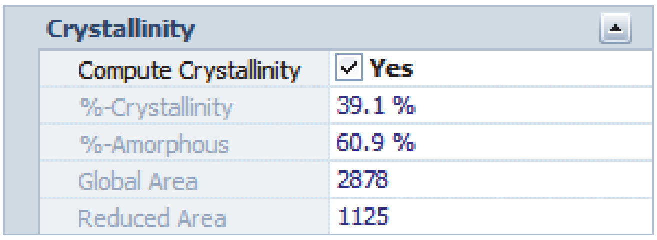


Fig. 98: Background adjusted

3. Select the **Compute Crystallinity** check box in the Scan Property table
   The crystallinity percentage is automatically computed and given below in the table.



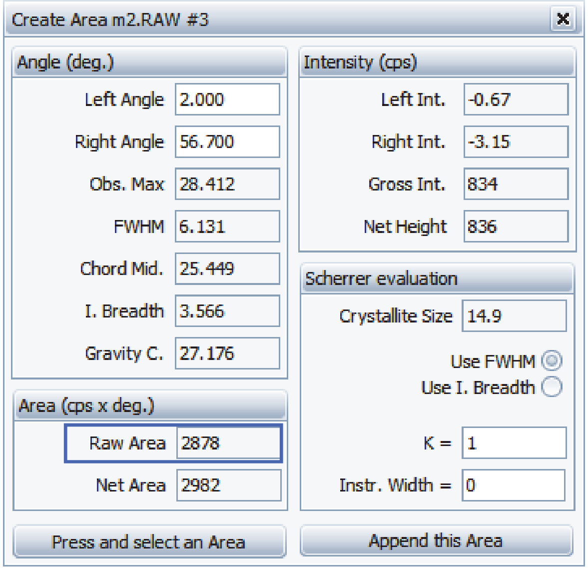
Crystallinity

Compute Crystallinity	☑ **Yes**
%-Crystallinity	39.1 %
%-Amorphous	60.9 %
Global Area	2878
Reduced Area	1125

Step 3: Checking the Results

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

1. Make certain the m2 scan is selected in the data tree.
2. Click **Background** in the Tool list of the Data Command panel
   — or —
   Right-click the scan in the data tree and then click **Tool** on the context menu. Click **Background** on the Tool submenu.
3. Set the curvature to the minimum of 0.01.
4. Click the **Append Background** button to create a scan from the background line: this scan will be named m2.RAW #2 by default.
5. Subtract this scan (m2.RAW #2) from the initial m2.RAW scan (m2.RAW #1). See the tutorial chapter “Subtracting Scans” on page 86 to know how to proceed. It gives you a new scan which is listed in the data tree as m2.RAW #3.
6. Select the scan resulting from the subtraction if it is not already selected. Compute the area on the whole range. To do so:
   - Click **Create Area** in the Tool list of the Data Command panel
     — 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.
   - 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.



Create Area m2.RAW #3

Angle (deg.)
Left Angle 2.000
Right Angle 56.700
Obs. Max 28.412
FWHM 6.131
Chord Mid. 25.449
I. Breadth 3.566
Gravity C. 27.176

Area (cps x deg.)
Raw Area 2878
Net Area 2982

Intensity (cps)
Left Int. -0.67
Right Int. -3.15
Gross Int. 834
Net Height 836

Scherrer evaluation
Crystallite Size 14.9
Use FWHM ●
Use I. Breadth ○
K = 1
Instr. Width = 0

You can check if this value is equal to the global area value given automatically by the program which is 2878 cps x deg.

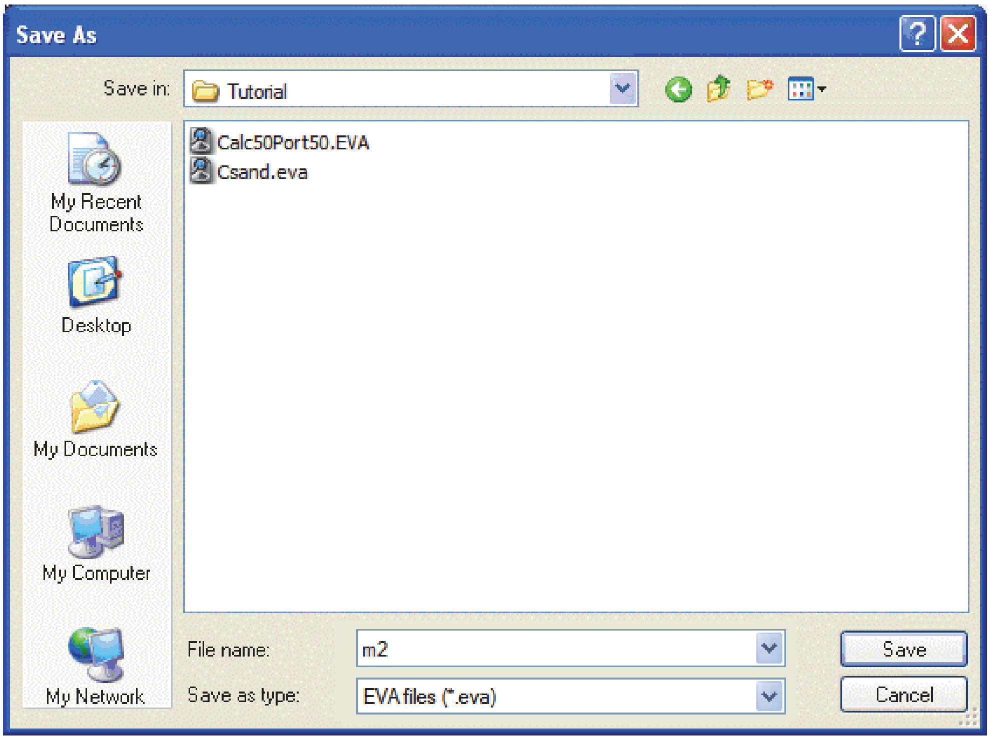
7. You can compute the Reduced area the same way but using the adjusted background. The raw area value found is equal to the reduced area value which is 1125 cps x deg. From this you can finally compute the crystallinity using the following formulas:

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

%Crystallinity=100 - %Amorphous

Step 4: Saving

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



File name: m2

Save as type: EVA files (*.eva)

Fig. 99: Saving m2.EVA document

Simulating a Slit Mode

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:

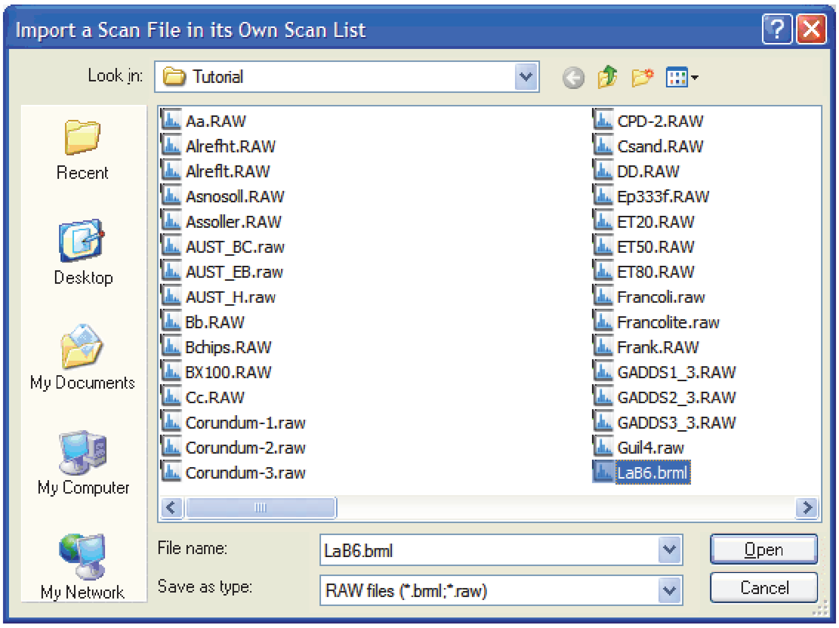
1. Creating a new EVA document and importing LaB6.BRML.
2. Performing the Search/Match operation.
3. Simulating a slit mode.
4. Saving the EVA document containing the scans.

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

New button

Import from file button

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 file** data command or the **Import from file** button. The Import from files dialog box will be displayed. Search the Tutorials/EVA[1] directory and select the LaB6.BRML file.
3. Click **Open**. The scan LaB6 will be displayed in the graphical view of the EVA document.


Import a Scan File in its Own Scan List

Look in: Tutorial

File name: LaB6.brml

Save as type: RAW files (*.brml;*.raw)

Fig. 100: Import a Scan File dialog box

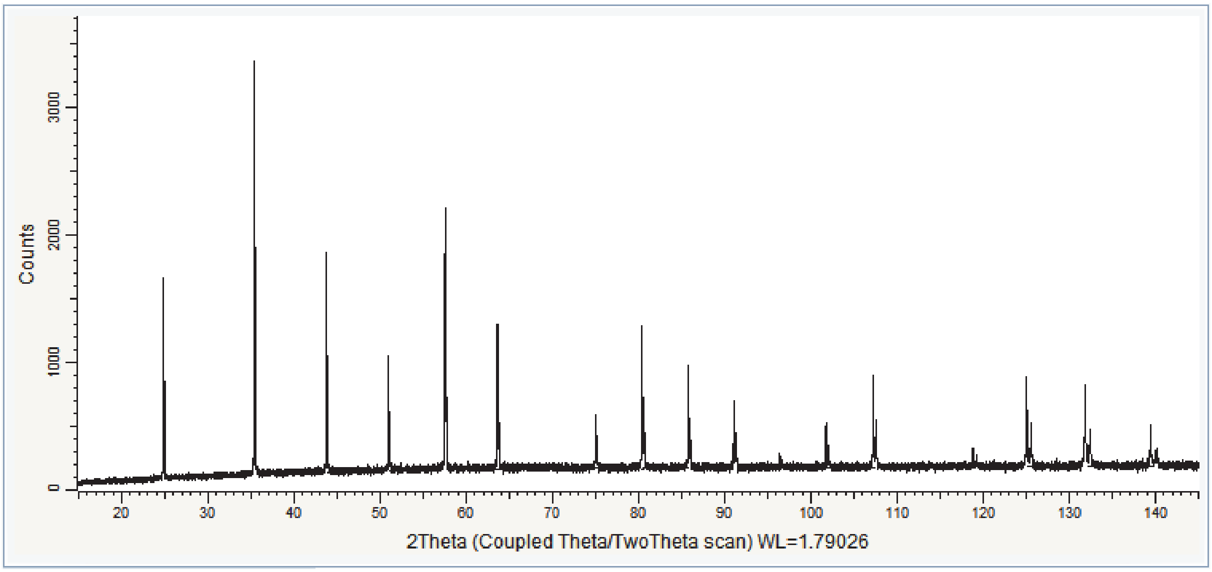


Fig. 101: LaB6 file imported in the graphical view

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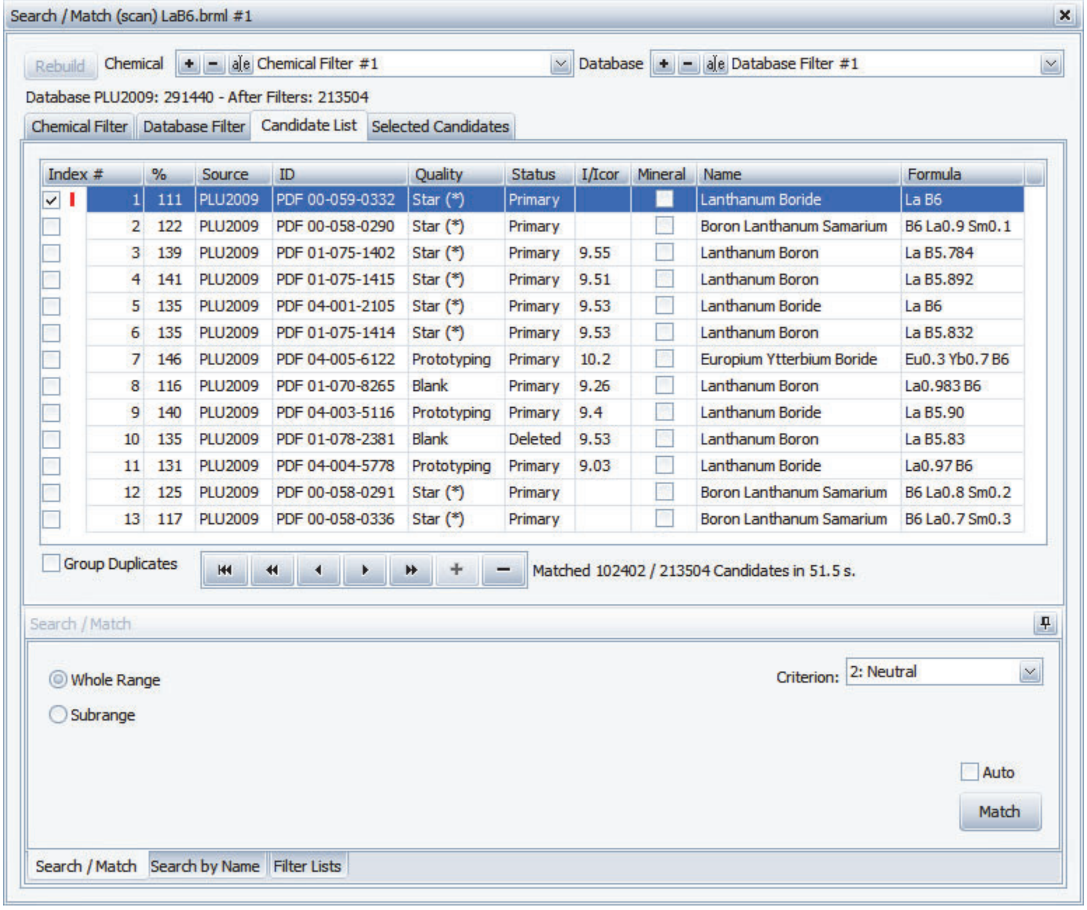
[1] The directory path to the EVA tutorial files is "C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials" under Windows XP and "C:\ProgramData\Bruker AXS\Tutorials" under Windows 7.
To access the folder with the explorer, select "Display hidden files and folders" in the Folders options.

Step 2: Performing the Search/Match Operation

1. Make certain the LaB6 scan is selected in the data tree.
2. Keep the default search parameters and run a search. Here are the results obtained:



Chemical Filter #1

Database Filter #1

Database PLU2009: 291440 - After Filters: 213504

	Index #	%	Source	ID	Quality	Status	I/Icor	Mineral	Name	Formula
☑	1	111	PLU2009	PDF 00-059-0332	Star (*)	Primary		☐	Lanthanum Boride	La B6
☐	2	122	PLU2009	PDF 00-058-0290	Star (*)	Primary		☐	Boron Lanthanum Samarium	B6 La0.9 Sm0.1
☐	3	139	PLU2009	PDF 01-075-1402	Star (*)	Primary	9.55	☐	Lanthanum Boron	La B5.784
☐	4	141	PLU2009	PDF 01-075-1415	Star (*)	Primary	9.51	☐	Lanthanum Boron	La B5.892
☐	5	135	PLU2009	PDF 04-001-2105	Star (*)	Primary	9.53	☐	Lanthanum Boride	La B6
☐	6	135	PLU2009	PDF 01-075-1414	Star (*)	Primary	9.53	☐	Lanthanum Boron	La B5.832
☐	7	146	PLU2009	PDF 04-005-6122	Prototyping	Primary	10.2	☐	Europium Ytterbium Boride	Eu0.3 Yb0.7 B6
☐	8	116	PLU2009	PDF 01-070-8265	Blank	Primary	9.26	☐	Lanthanum Boron	La0.983 B6
☐	9	140	PLU2009	PDF 04-003-5116	Prototyping	Primary	9.4	☐	Lanthanum Boride	La B5.90
☐	10	135	PLU2009	PDF 01-078-2381	Blank	Deleted	9.53	☐	Lanthanum Boron	La B5.83
☐	11	131	PLU2009	PDF 04-004-5778	Prototyping	Primary	9.03	☐	Lanthanum Boride	La0.97 B6
☐	12	125	PLU2009	PDF 00-058-0291	Star (*)	Primary		☐	Boron Lanthanum Samarium	B6 La0.8 Sm0.2
☐	13	117	PLU2009	PDF 00-058-0336	Star (*)	Primary		☐	Boron Lanthanum Samarium	B6 La0.7 Sm0.3

☐ Group Duplicates

Matched 102402 / 213504 Candidates in 51.5 s.

● Whole Range
○ Subrange

Criterion: 2: Neutral

☐ Auto

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 of the pattern.

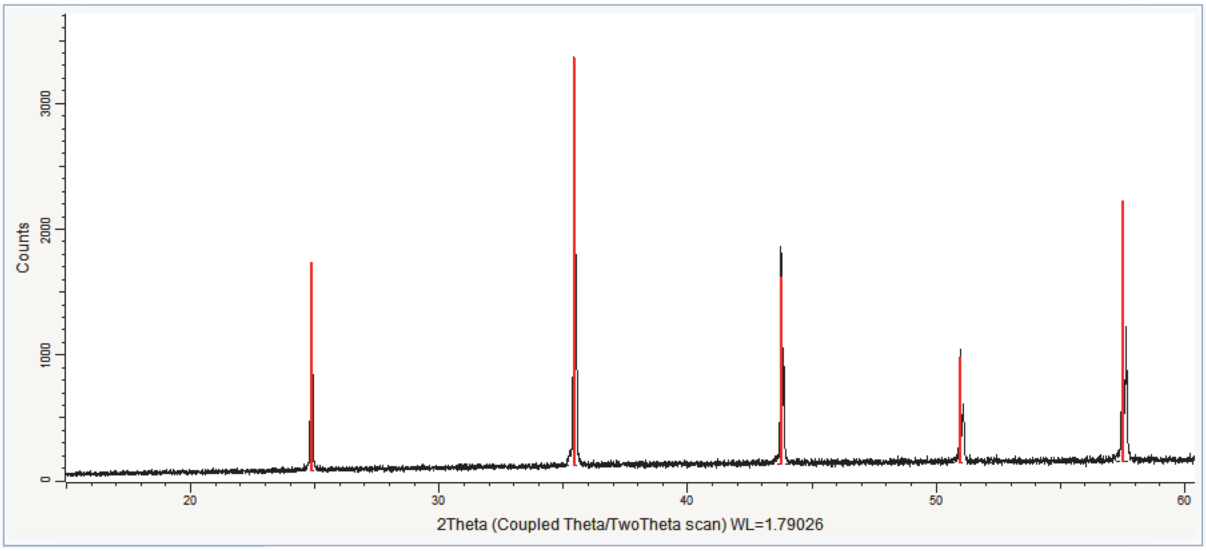


Fig. 102: Zoom on the scan and the pattern (2θ=20° to 60°)

Step 3: Simulating a Slit Mode

1. Make certain the LaB6 scan is selected in the data tree.
2. In the Scan Property Table, change the **Simul. Slit Mode** property from **Variable** to **Fixed**.
3. The intensities of the scan will be recalculated. The other scan related data, a pattern in this example, will be projected as well.

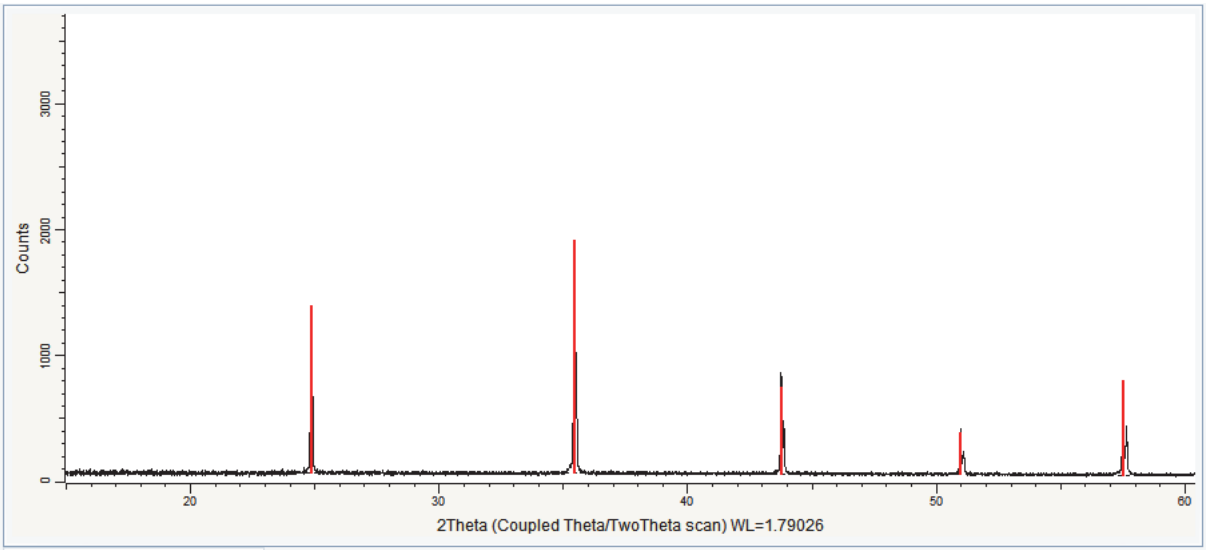
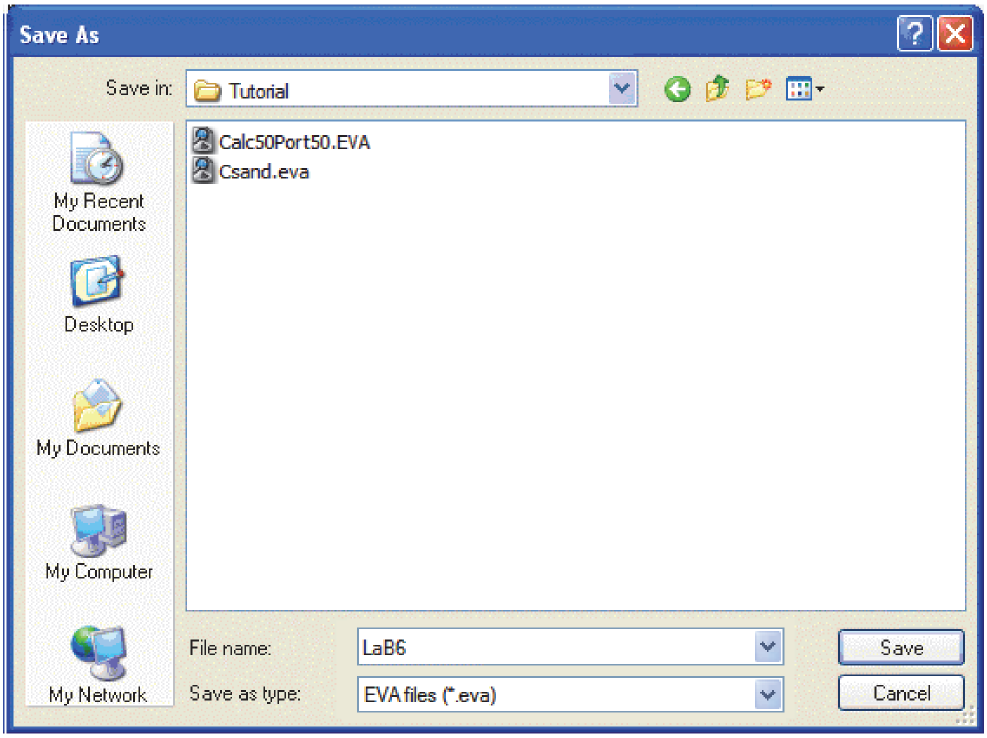


Fig. 103: Zoom on the scan and the pattern (2θ=20° to 60°)

Step 4: Saving

5. Click **Save As** on the **File** menu. The Save As dialog box will be displayed.
6. Select the appropriate disc drive and directory.
7. Type in the file name. (To overwrite an .EVA file, use the same name).
8. Click **Save**.



Save in: Tutorial

Calc50Port50.EVA
Csand.eva

File name: LaB6

Save as type: EVA files (*.eva)

Fig. 104: Saving LaB6.EVA document

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

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.

NOTE

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

This tutorial was prepared using PDF 4+ 2009 as a reference database. You may have another reference database.

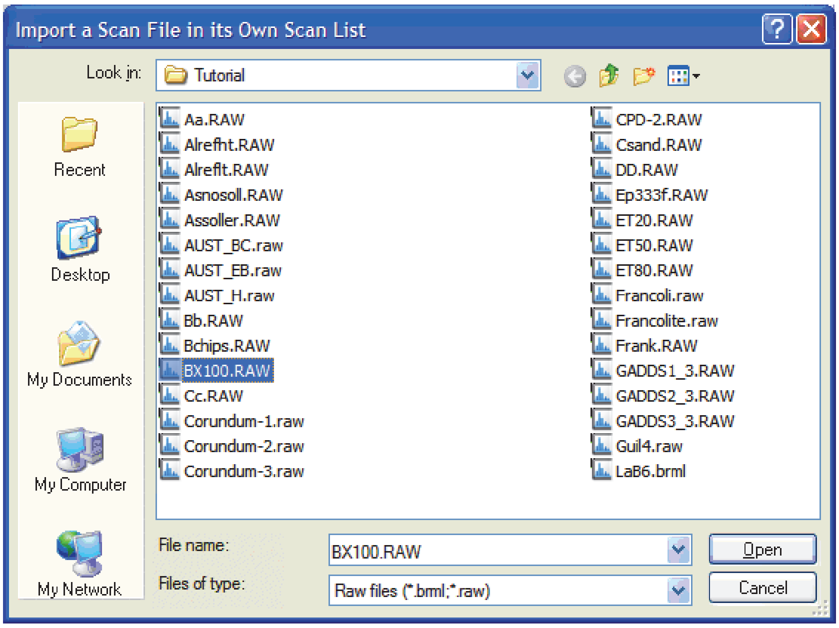
If you have no database, you cannot perform this part of the tutorial using the Search/Match.

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

New button

Import from file button

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 file** data command or the **Import from file** button. The Import from files dialog box will be displayed. Search the Tutorials/EVA[1] directory and select the BX100.RAW file.
3. Click **Open**. The scan BX100 will be displayed in the graphical view of the EVA document.



Look in: Tutorial

Aa.RAW
Alrefht.RAW
Alrefit.RAW
Asnosoll.RAW
Assoller.RAW
AUST_BC.raw
AUST_EB.raw
AUST_H.raw
Bb.RAW
Bchips.RAW
BX100.RAW
Cc.RAW
Corundum-1.raw
Corundum-2.raw
Corundum-3.raw
CPD-2.RAW
Csand.RAW
DD.RAW
Ep333f.RAW
ET20.RAW
ET50.RAW
ET80.RAW
Francoli.raw
Francolite.raw
Frank.RAW
GADDS1_3.RAW
GADDS2_3.RAW
GADDS3_3.RAW
Guil4.raw
LaB6.brml

File name: BX100.RAW

Files of type: Raw files (*.brml;*.raw)

Fig. 105: Import a Scan File dialog box

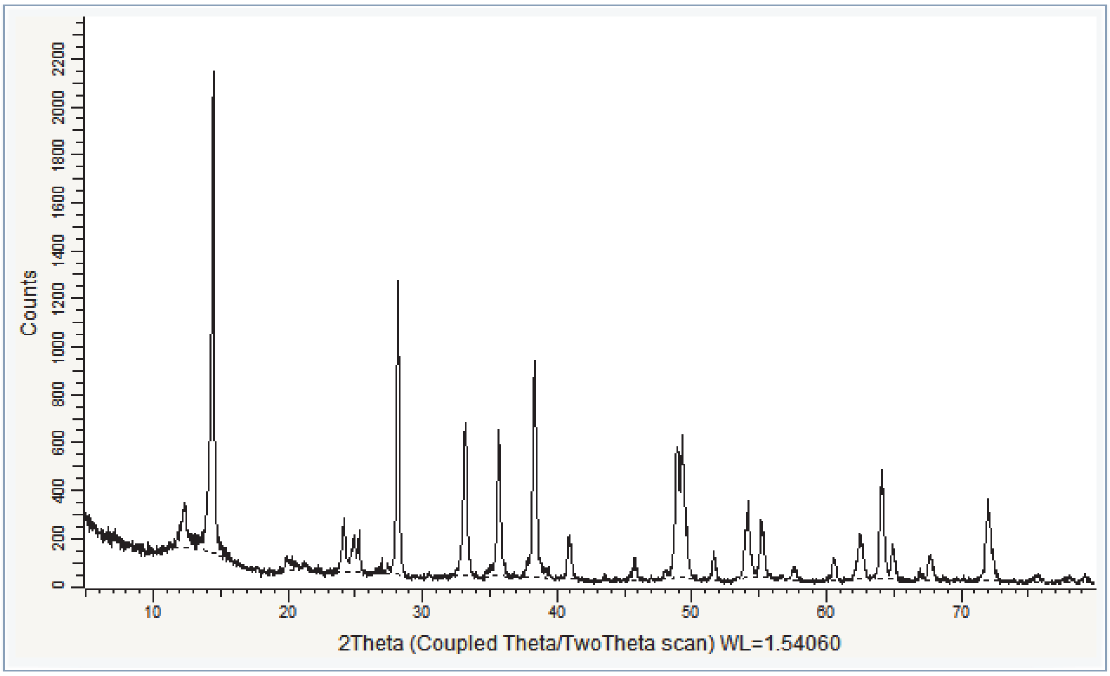


Fig. 106: BX100.RAW imported in the graphical view

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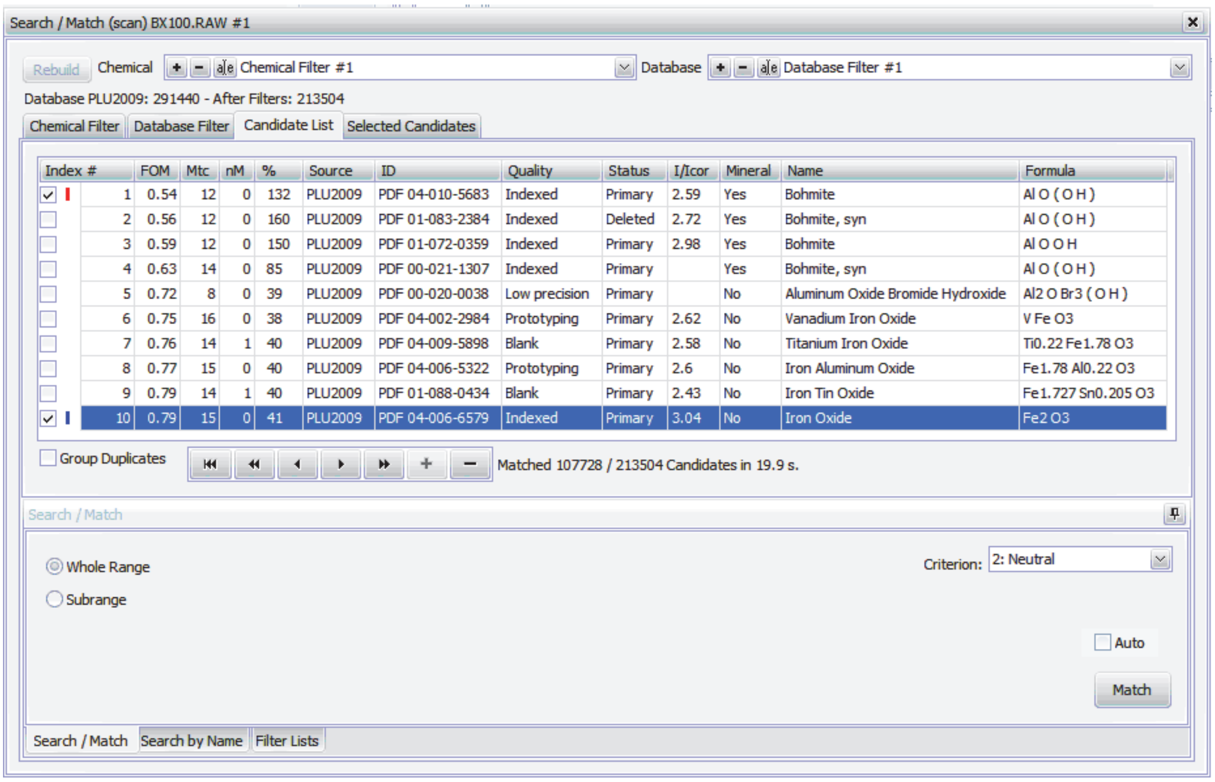
[1] The directory path to the EVA tutorial files is "C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials" under Windows XP and "C:\ProgramData\Bruker AXS\Tutorials" under Windows 7.
To access the folder with the explorer, select "Display hidden files and folders" in the Folders options.

Step 2: Performing the Search/Match Operation

Before the semi-quantitative phase analysis, all phases must be identified.

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” on page 1 or the EVA Manual.

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



Search / Match (scan) BX100.RAW #1

Chemical: Chemical Filter #1 Database: Database Filter #1

Database PLU2009: 291440 - After Filters: 213504

	Index #	FOM	Mtc	nM	%	Source	ID	Quality	Status	I/Icor	Mineral	Name	Formula
☑	1	0.54	12	0	132	PLU2009	PDF 04-010-5683	Indexed	Primary	2.59	Yes	Bohmite	Al O (O H)
☐	2	0.56	12	0	160	PLU2009	PDF 01-083-2384	Indexed	Deleted	2.72	Yes	Bohmite, syn	Al O (O H)
☐	3	0.59	12	0	150	PLU2009	PDF 01-072-0359	Indexed	Primary	2.98	Yes	Bohmite	Al O O H
☐	4	0.63	14	0	85	PLU2009	PDF 00-021-1307	Indexed	Primary		Yes	Bohmite, syn	Al O (O H)
☐	5	0.72	8	0	39	PLU2009	PDF 00-020-0038	Low precision	Primary		No	Aluminum Oxide Bromide Hydroxide	Al2 O Br3 (O H)
☐	6	0.75	16	0	38	PLU2009	PDF 04-002-2984	Prototyping	Primary	2.62	No	Vanadium Iron Oxide	V Fe O3
☐	7	0.76	14	1	40	PLU2009	PDF 04-009-5898	Blank	Primary	2.58	No	Titanium Iron Oxide	Ti0.22 Fe1.78 O3
☐	8	0.77	15	0	40	PLU2009	PDF 04-006-5322	Prototyping	Primary	2.6	No	Iron Aluminum Oxide	Fe1.78 Al0.22 O3
☐	9	0.79	14	1	40	PLU2009	PDF 01-088-0434	Blank	Primary	2.43	No	Iron Tin Oxide	Fe1.727 Sn0.205 O3
☑	10	0.79	15	0	41	PLU2009	PDF 04-006-6579	Indexed	Primary	3.04	No	Iron Oxide	Fe2 O3

☐ Group Duplicates

Matched 107728 / 213504 Candidates in 19.9 s.

Search / Match

● Whole Range
○ Subrange

Criterion: 2: Neutral

☐ Auto

Boehmite (PDF 04-010-5683) and Iron Oxide (PDF 04-006-6579) can be easily identified. The search results show several types of iron oxide, we select pure iron oxide.

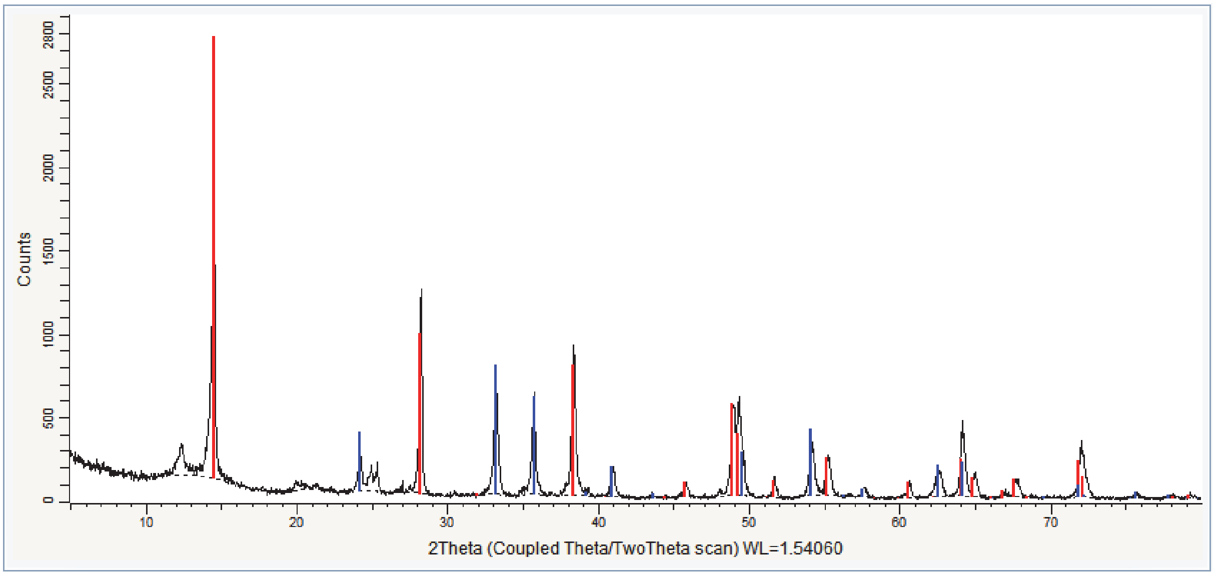
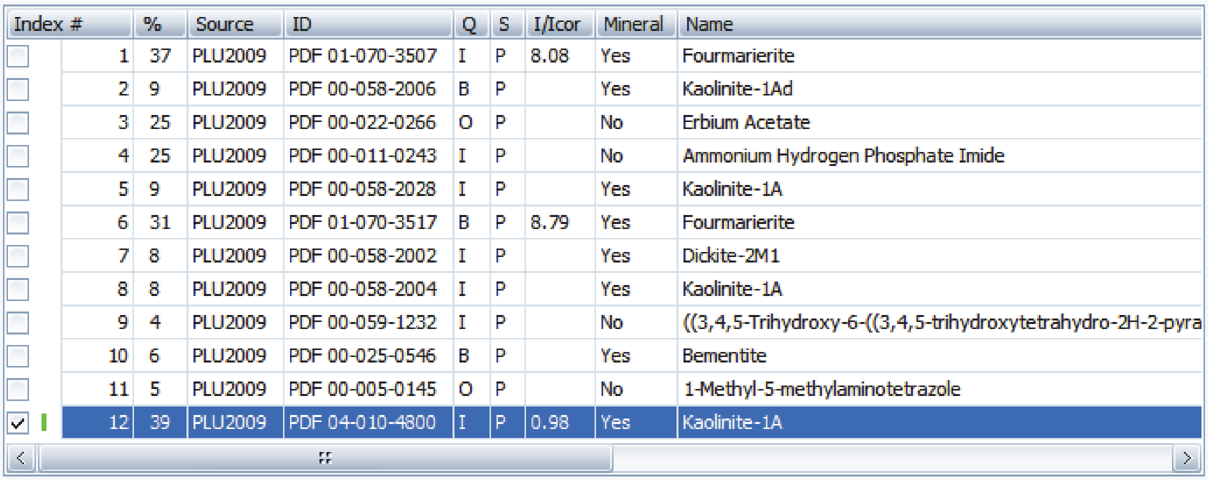


Fig. 107: Boehmite pattern in red and Iron Oxide pattern in blue

2. Remove the already explained regions by preparing a residual scan.
   Another run on the residual scan makes it possible to identify Kaolinite-1A. We select the pattern PDF 04-010-4800 which has an I/I_{cor} value and belongs to a structure database. Structure databases have calculated I/I_{cor} values which are generally more reliable than the measured I/I_{cor} values.



Index #		%	Source	ID	Q	S	I/Icor	Mineral	Name
☐	1	37	PLU2009	PDF 01-070-3507	I	P	8.08	Yes	Fourmarierite
☐	2	9	PLU2009	PDF 00-058-2006	B	P		Yes	Kaolinite-1Ad
☐	3	25	PLU2009	PDF 00-022-0266	O	P		No	Erbium Acetate
☐	4	25	PLU2009	PDF 00-011-0243	I	P		No	Ammonium Hydrogen Phosphate Imide
☐	5	9	PLU2009	PDF 00-058-2028	I	P		Yes	Kaolinite-1A
☐	6	31	PLU2009	PDF 01-070-3517	B	P	8.79	Yes	Fourmarierite
☐	7	8	PLU2009	PDF 00-058-2002	I	P		Yes	Dickite-2M1
☐	8	8	PLU2009	PDF 00-058-2004	I	P		Yes	Kaolinite-1A
☐	9	4	PLU2009	PDF 00-059-1232	I	P		No	((3,4,5-Trihydroxy-6-((3,4,5-trihydroxytetrahydro-2H-2-pyra
☐	10	6	PLU2009	PDF 00-025-0546	B	P		Yes	Bementite
☐	11	5	PLU2009	PDF 00-005-0145	O	P		No	1-Methyl-5-methylaminotetrazole
☑ 🟩	12	39	PLU2009	PDF 04-010-4800	I	P	0.98	Yes	Kaolinite-1A

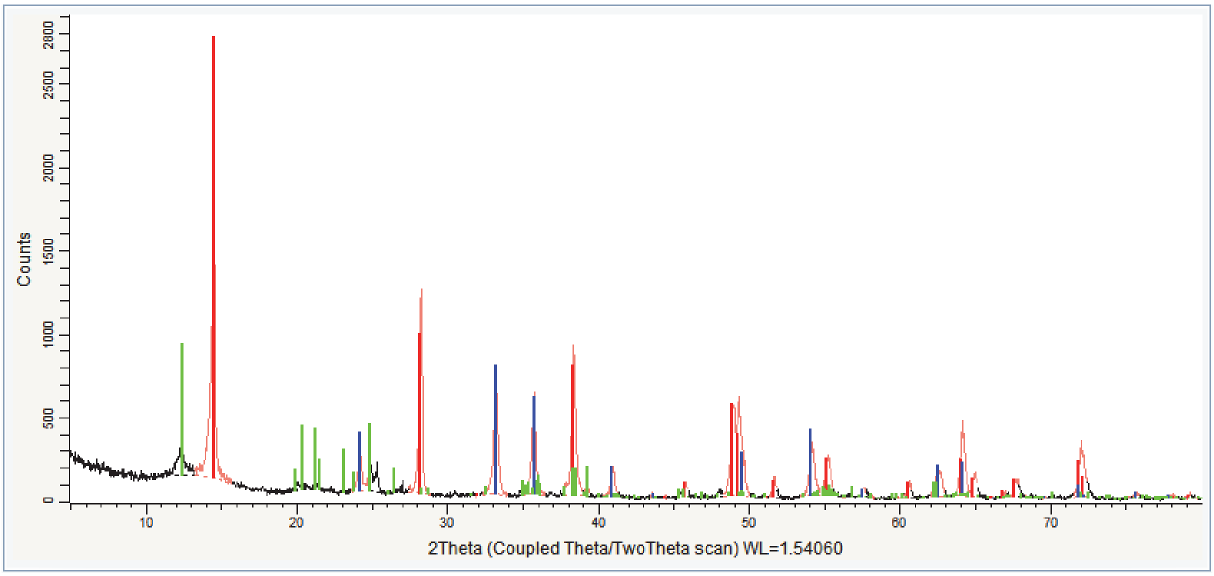
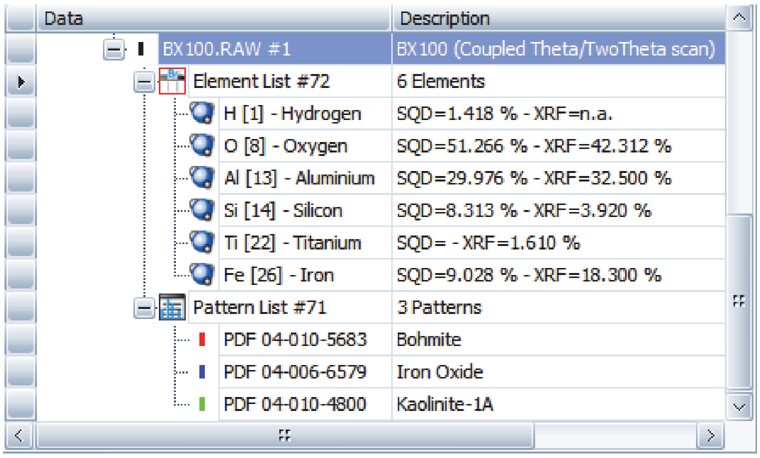


Fig. 108: Boehmite pattern in red, Iron Oxide pattern in blue and Kaolinite-1A pattern in green.

3. 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:

    - Select the scan BX100.RAW either in the data tree or in the graphical view.
    - 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. 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.



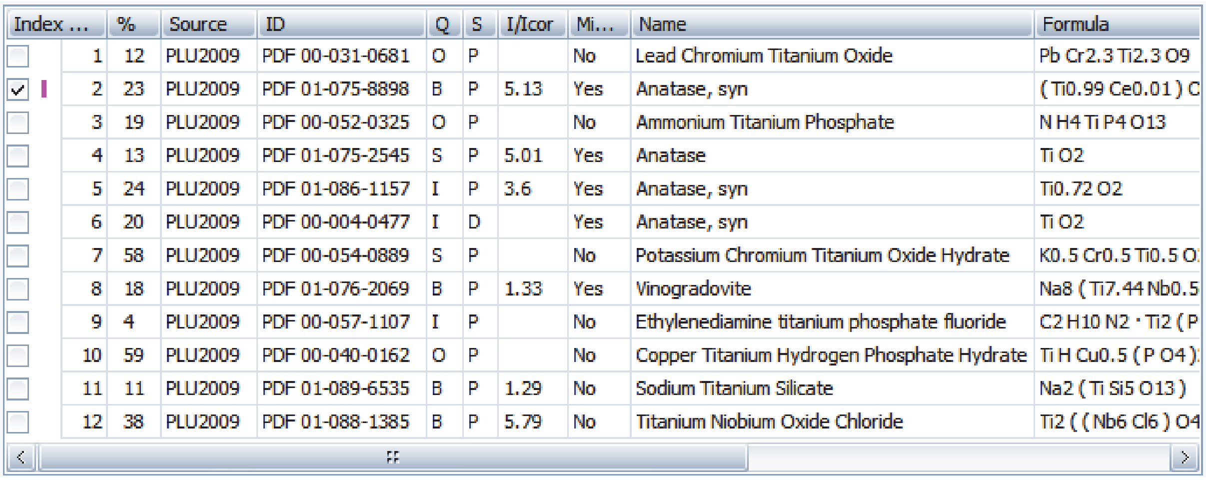
Data	Description
BX100.RAW #1	BX100 (Coupled Theta/TwoTheta scan)
Element List #72	6 Elements
H [1] - Hydrogen	SQD=1.418 % - XRF=n.a.
O [8] - Oxygen	SQD=51.266 % - XRF=42.312 %
Al [13] - Aluminium	SQD=29.976 % - XRF=32.500 %
Si [14] - Silicon	SQD=8.313 % - XRF=3.920 %
Ti [22] - Titanium	SQD= - XRF=1.610 %
Fe [26] - Iron	SQD=9.028 % - XRF=18.300 %
Pattern List #71	3 Patterns
PDF 04-010-5683	Bohmite
PDF 04-006-6579	Iron Oxide
PDF 04-010-4800	Kaolinite-1A

The chemical analysis indicates that the sample contains titanium.

4. Create a chemical filter from Titanium. To do so:

    - Select the Titanium in the data tree.
    - 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.

5. Another run using this new chemical filter makes it then possible to identify Anatase (PDF 01-075-8898).



	Index ...	%	Source	ID	Q	S	I/Icor	Mi...	Name	Formula
☐	1	12	PLU2009	PDF 00-031-0681	O	P		No	Lead Chromium Titanium Oxide	Pb Cr2.3 Ti2.3 O9
☑	2	23	PLU2009	PDF 01-075-8898	B	P	5.13	Yes	Anatase, syn	(Ti0.99 Ce0.01) C
☐	3	19	PLU2009	PDF 00-052-0325	O	P		No	Ammonium Titanium Phosphate	N H4 Ti P4 O13
☐	4	13	PLU2009	PDF 01-075-2545	S	P	5.01	Yes	Anatase	Ti O2
☐	5	24	PLU2009	PDF 01-086-1157	I	P	3.6	Yes	Anatase, syn	Ti0.72 O2
☐	6	20	PLU2009	PDF 00-004-0477	I	D		Yes	Anatase, syn	Ti O2
☐	7	58	PLU2009	PDF 00-054-0889	S	P		No	Potassium Chromium Titanium Oxide Hydrate	K0.5 Cr0.5 Ti0.5 O
☐	8	18	PLU2009	PDF 01-076-2069	B	P	1.33	Yes	Vinogradovite	Na8 (Ti7.44 Nb0.5
☐	9	4	PLU2009	PDF 00-057-1107	I	P		No	Ethylenediamine titanium phosphate fluoride	C2 H10 N2 · Ti2 (P
☐	10	59	PLU2009	PDF 00-040-0162	O	P		No	Copper Titanium Hydrogen Phosphate Hydrate	Ti H Cu0.5 (P O4)
☐	11	11	PLU2009	PDF 01-089-6535	B	P	1.29	No	Sodium Titanium Silicate	Na2 (Ti Si5 O13)
☐	12	38	PLU2009	PDF 01-088-1385	B	P	5.79	No	Titanium Niobium Oxide Chloride	Ti2 ((Nb6 Cl6) O4

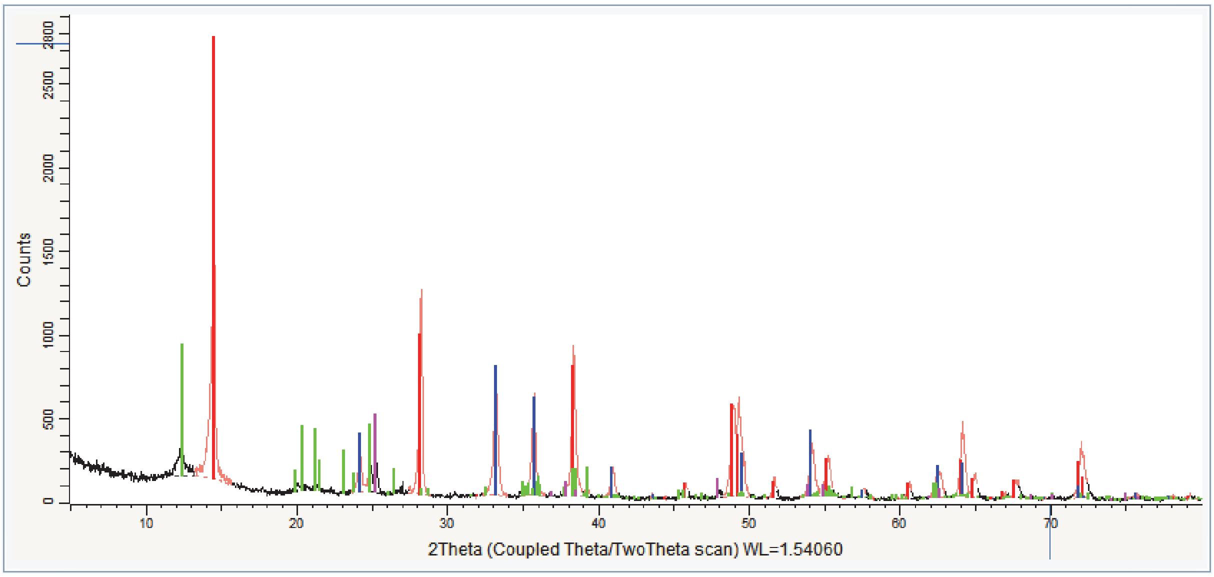


Fig. 109: Boehmite pattern in red, Iron Oxide pattern in blue, Kaolinite-1A pattern in green and Anatase pattern in pink.

Step 3: Performing the Semi-Quantitative Phase Analysis

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

1. The first phase identified in the list is Boehmite. 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. 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.

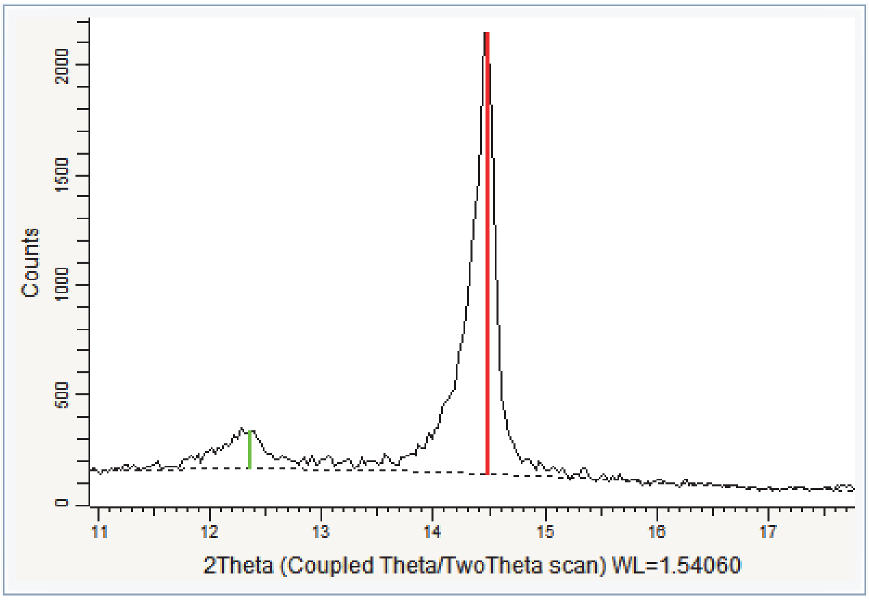
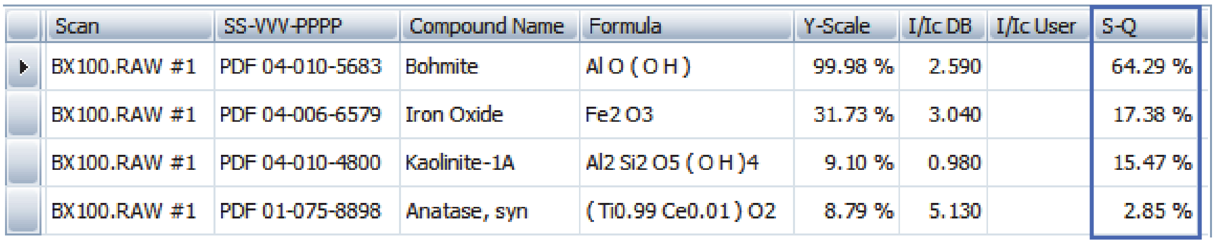


Fig. 110: Zoom on the peaks (2θ=38° to 48°)

2. Proceed the same way for the other phases.
3. Select the BX100 scan either in the data tree or in the 1D view.

4. The phases’ concentrations are listed in the **S-Q** column of the pattern column view.



Scan	SS-VVV-PPPP	Compound Name	Formula	Y-Scale	I/Ic DB	I/Ic User	S-Q
BX100.RAW #1	PDF 04-010-5683	Bohmite	Al O (O H)	99.98 %	2.590		64.29 %
BX100.RAW #1	PDF 04-006-6579	Iron Oxide	Fe2 O3	31.73 %	3.040		17.38 %
BX100.RAW #1	PDF 04-010-4800	Kaolinite-1A	Al2 Si2 O5 (O H)4	9.10 %	0.980		15.47 %
BX100.RAW #1	PDF 01-075-8898	Anatase, syn	(Ti0.99 Ce0.01) O2	8.79 %	5.130		2.85 %

Fig. 111: Semi-quantitative analysis results in the Pattern Column view

To display the results as a pie or bar chart:

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

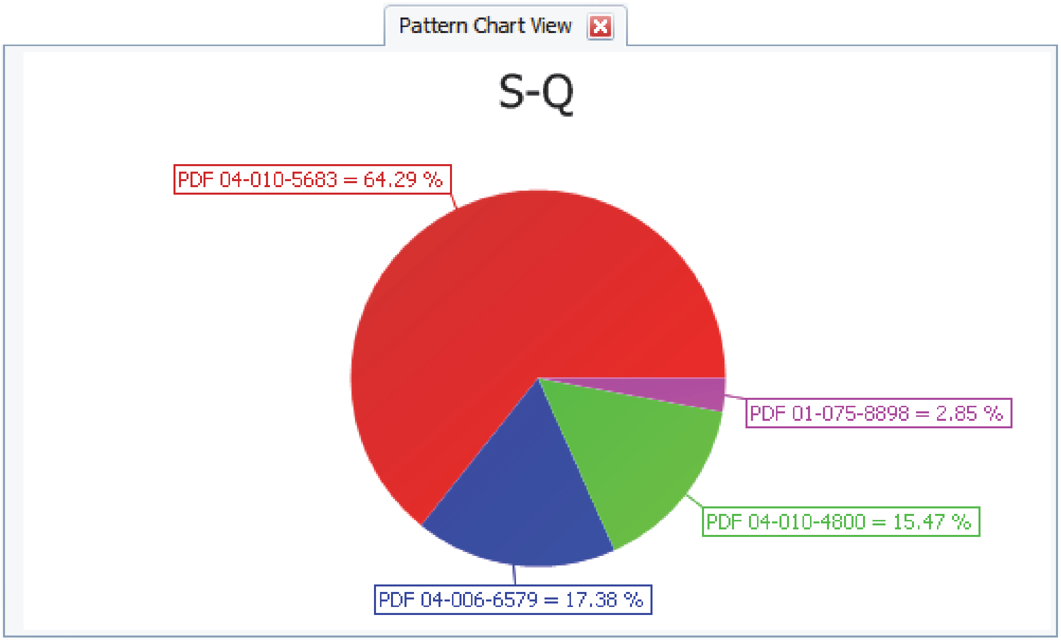
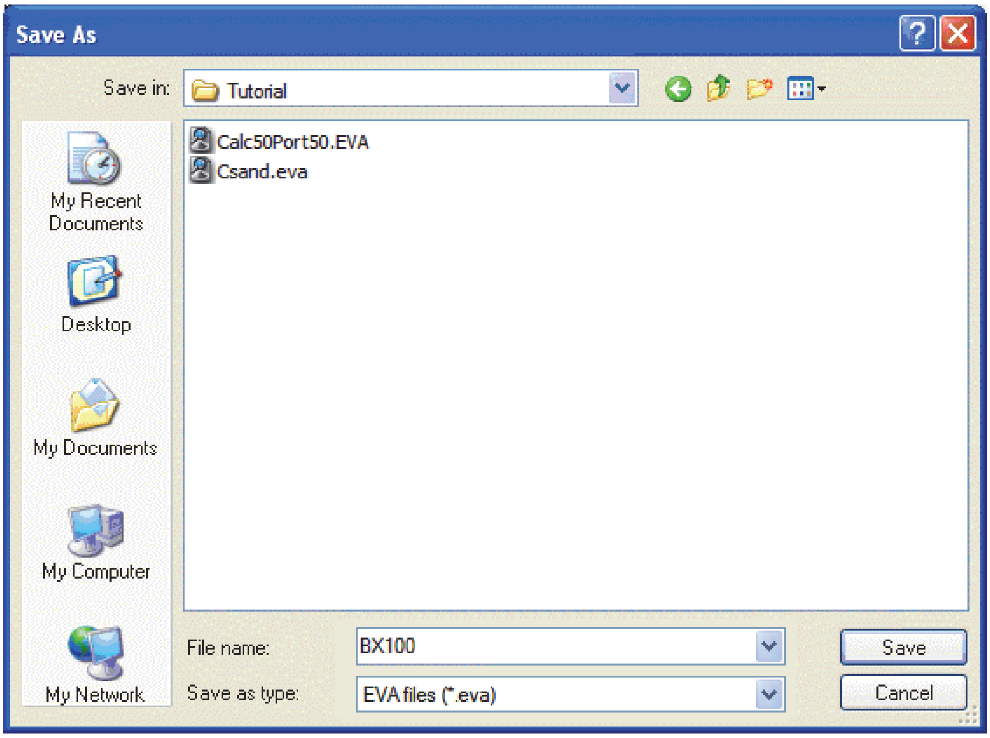


Fig. 112: Semi-quantitative analysis results as a pie chart

Step 4: Saving

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



Save in: Tutorial

Calc50Port50.EVA
Csand.eva

File name: BX100

Save as type: EVA files (*.eva)

Fig. 113: Saving BX100.EVA document

Using the d Multiplied By Tool

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. Saving.

NOTE

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

This tutorial was prepared using PDF 4+ 2009 as a reference database. You may have another reference database.

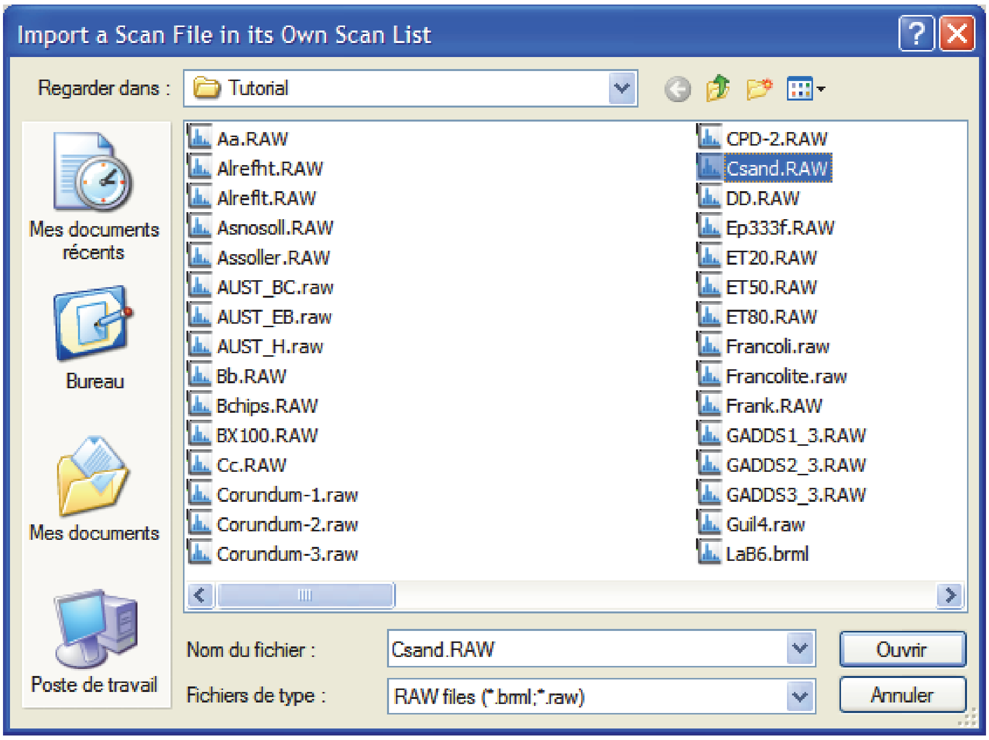
If you have no database, you cannot perform this part of the tutorial using the Search/Match.

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

New button

Import from file button

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 file** data command or the **Import from file** button. The Import from files dialog box will be displayed. Search the Tutorials/EVA[1] directory and select the Csand.RAW file.
3. Click **Open**. The scan Csand will be displayed in the graphical view of the EVA document.



Import a Scan File in its Own Scan List

Regarder dans : Tutorial

- Aa.RAW
- Alrefht.RAW
- Alrefit.RAW
- Asnosoll.RAW
- Assoller.RAW
- AUST_BC.raw
- AUST_EB.raw
- AUST_H.raw
- Bb.RAW
- Bchips.RAW
- BX100.RAW
- Cc.RAW
- Corundum-1.raw
- Corundum-2.raw
- Corundum-3.raw
- CPD-2.RAW
- Csand.RAW
- DD.RAW
- Ep333f.RAW
- ET20.RAW
- ET50.RAW
- ET80.RAW
- Francoli.raw
- Francolite.raw
- Frank.RAW
- GADDS1_3.RAW
- GADDS2_3.RAW
- GADDS3_3.RAW
- Guil4.raw
- LaB6.brml

Nom du fichier : Csand.RAW

Fichiers de type : RAW files (*.brml;*.raw)

Fig. 114: Import a Scan File dialog box

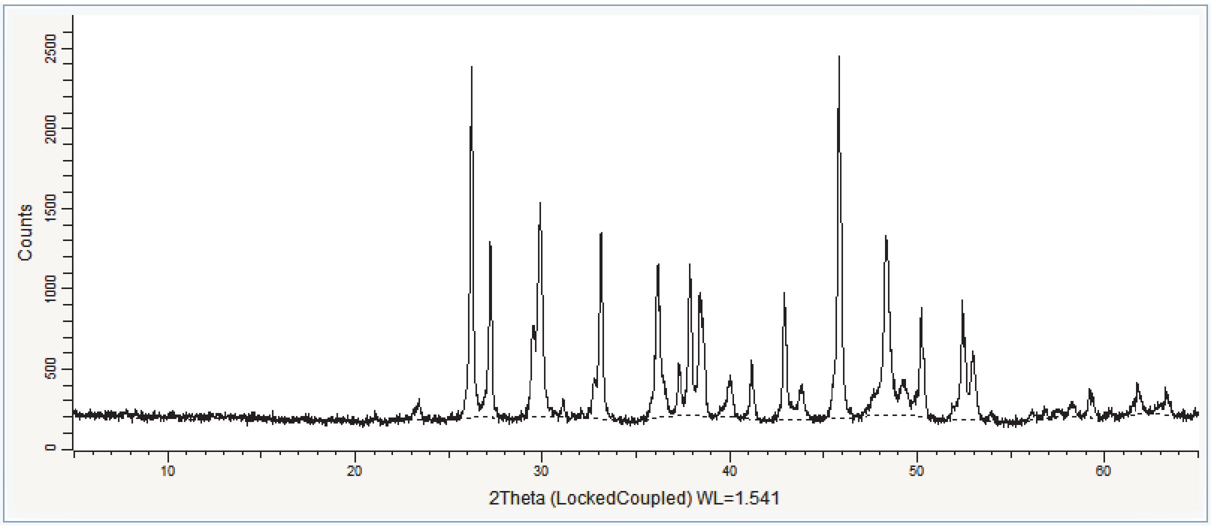


Fig. 115: Csand.RAW imported in the graphical view

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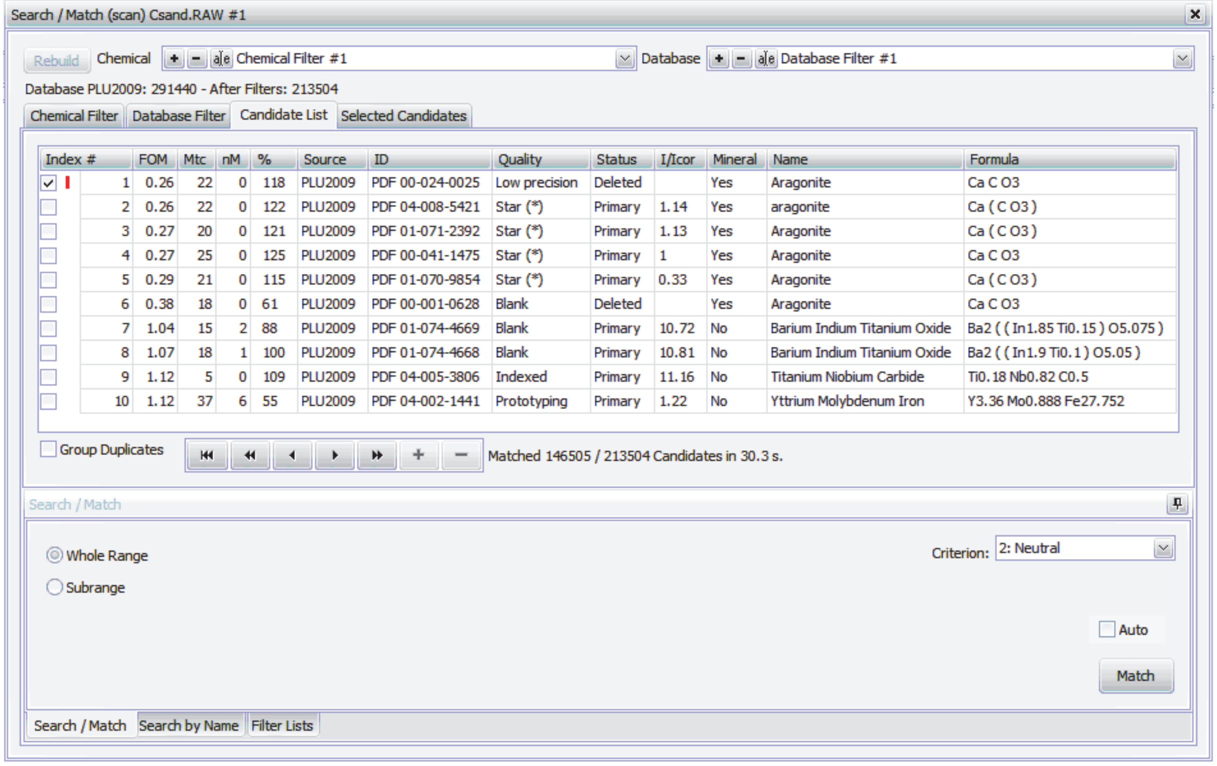
[1] The directory path to the EVA tutorial files is ″C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials″ under Windows XP and ″C:\ProgramData\Bruker AXS\Tutorials″ under Windows 7.
To access the folder with the explorer, select “Display hidden files and folders” in the Folders options.

Step 2: Performing the Search/Match Operation

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



Search / Match (scan) Csand.RAW #1

Chemical: Chemical Filter #1 Database: Database Filter #1

Database PLU2009: 291440 - After Filters: 213504

	Index #	FOM	Mtc	nM	%	Source	ID	Quality	Status	I/Icor	Mineral	Name	Formula
☑	1	0.26	22	0	118	PLU2009	PDF 00-024-0025	Low precision	Deleted		Yes	Aragonite	Ca C O3
☐	2	0.26	22	0	122	PLU2009	PDF 04-008-5421	Star (*)	Primary	1.14	Yes	aragonite	Ca (C O3)
☐	3	0.27	20	0	121	PLU2009	PDF 01-071-2392	Star (*)	Primary	1.13	Yes	Aragonite	Ca (C O3)
☐	4	0.27	25	0	125	PLU2009	PDF 00-041-1475	Star (*)	Primary	1	Yes	Aragonite	Ca C O3
☐	5	0.29	21	0	115	PLU2009	PDF 01-070-9854	Star (*)	Primary	0.33	Yes	Aragonite	Ca (C O3)
☐	6	0.38	18	0	61	PLU2009	PDF 00-001-0628	Blank	Deleted		Yes	Aragonite	Ca C O3
☐	7	1.04	15	2	88	PLU2009	PDF 01-074-4669	Blank	Primary	10.72	No	Barium Indium Titanium Oxide	Ba2 ((In1.85 Ti0.15) O5.075)
☐	8	1.07	18	1	100	PLU2009	PDF 01-074-4668	Blank	Primary	10.81	No	Barium Indium Titanium Oxide	Ba2 ((In1.9 Ti0.1) O5.05)
☐	9	1.12	5	0	109	PLU2009	PDF 04-005-3806	Indexed	Primary	11.16	No	Titanium Niobium Carbide	Ti0.18 Nb0.82 C0.5
☐	10	1.12	37	6	55	PLU2009	PDF 04-002-1441	Prototyping	Primary	1.22	No	Yttrium Molybdenum Iron	Y3.36 Mo0.888 Fe27.752

☐ Group Duplicates

Matched 146505 / 213504 Candidates in 30.3 s.

● Whole Range

○ Subrange

Criterion: 2: Neutral

☐ Auto

Aragonite (PDF 00-024-0025) can be easily identified.

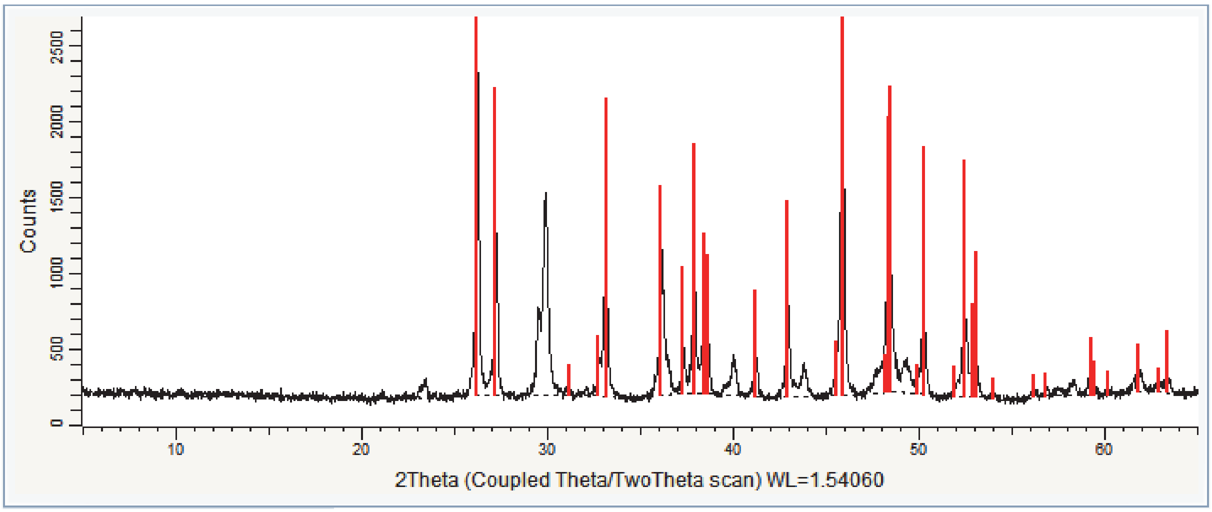
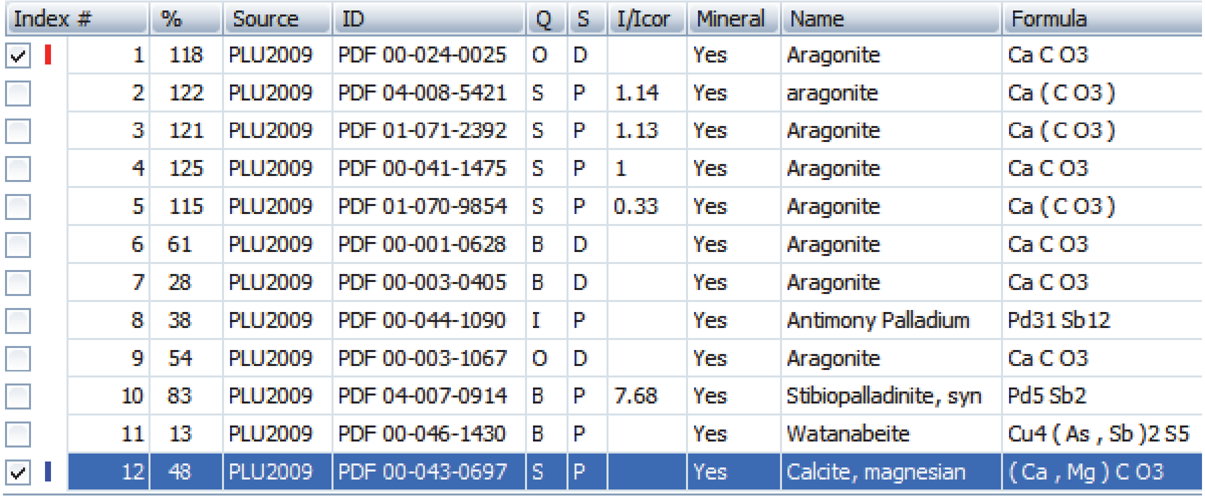


Fig. 116: Aragonite pattern in red

2. A run performed on the Mineral database makes it possible to find the Magnesian Calcite (PDF 00-043-0697).



Index #	%	Source	ID	Q	S	I/Icor	Mineral	Name	Formula
☑ 🟥 1	118	PLU2009	PDF 00-024-0025	O	D		Yes	Aragonite	Ca C O3
☐ 2	122	PLU2009	PDF 04-008-5421	S	P	1.14	Yes	aragonite	Ca (C O3)
☐ 3	121	PLU2009	PDF 01-071-2392	S	P	1.13	Yes	Aragonite	Ca (C O3)
☐ 4	125	PLU2009	PDF 00-041-1475	S	P	1	Yes	Aragonite	Ca C O3
☐ 5	115	PLU2009	PDF 01-070-9854	S	P	0.33	Yes	Aragonite	Ca (C O3)
☐ 6	61	PLU2009	PDF 00-001-0628	B	D		Yes	Aragonite	Ca C O3
☐ 7	28	PLU2009	PDF 00-003-0405	B	D		Yes	Aragonite	Ca C O3
☐ 8	38	PLU2009	PDF 00-044-1090	I	P		Yes	Antimony Palladium	Pd31 Sb12
☐ 9	54	PLU2009	PDF 00-003-1067	O	D		Yes	Aragonite	Ca C O3
☐ 10	83	PLU2009	PDF 04-007-0914	B	P	7.68	Yes	Stibiopalladinite, syn	Pd5 Sb2
☐ 11	13	PLU2009	PDF 00-046-1430	B	P		Yes	Watanabeite	Cu4 (As , Sb)2 S5
☑ 🟦 12	48	PLU2009	PDF 00-043-0697	S	P		Yes	Calcite, magnesian	(Ca , Mg) C O3

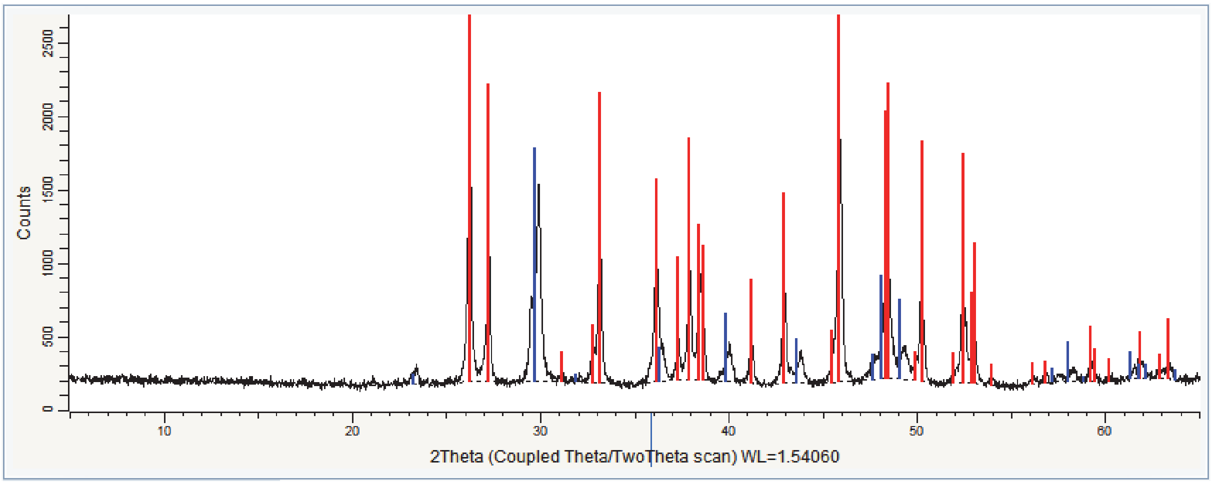
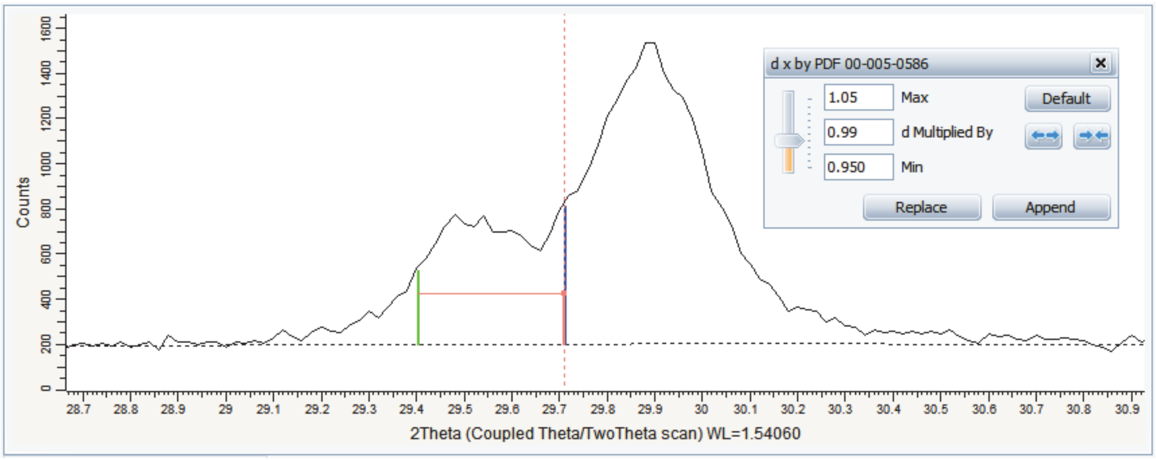


Fig. 117: Aragonite pattern in red and Magnesian calcite in blue

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.
4. Click **d x by** in the Data Command panel
   — or —
   Right-click the pattern, then click **d x by** on the context menu.

   The **d x by** dialog box will be displayed.
5. 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.


d x by PDF 00-005-0586

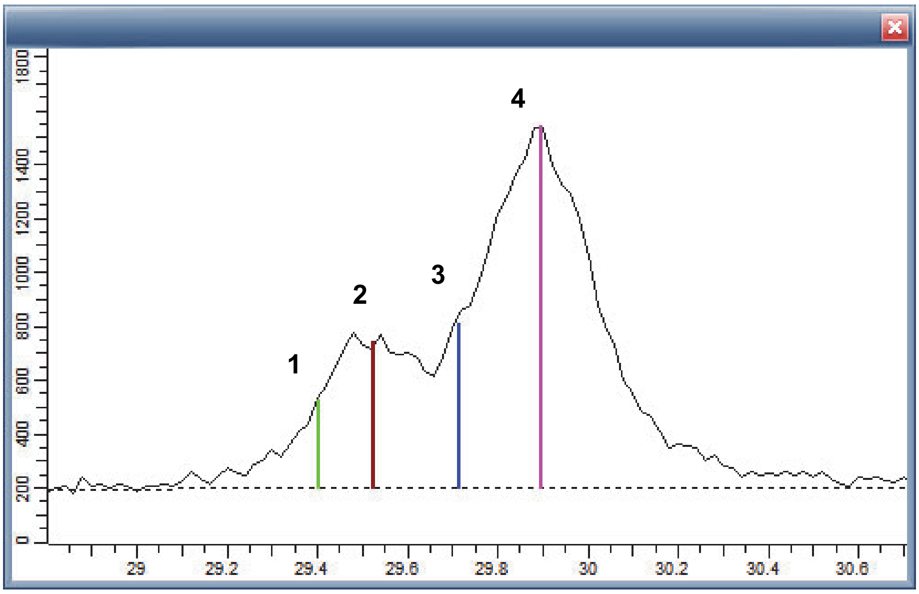
1.05 Max

0.99 d Multiplied By

0.950 Min

Fig. 118: 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

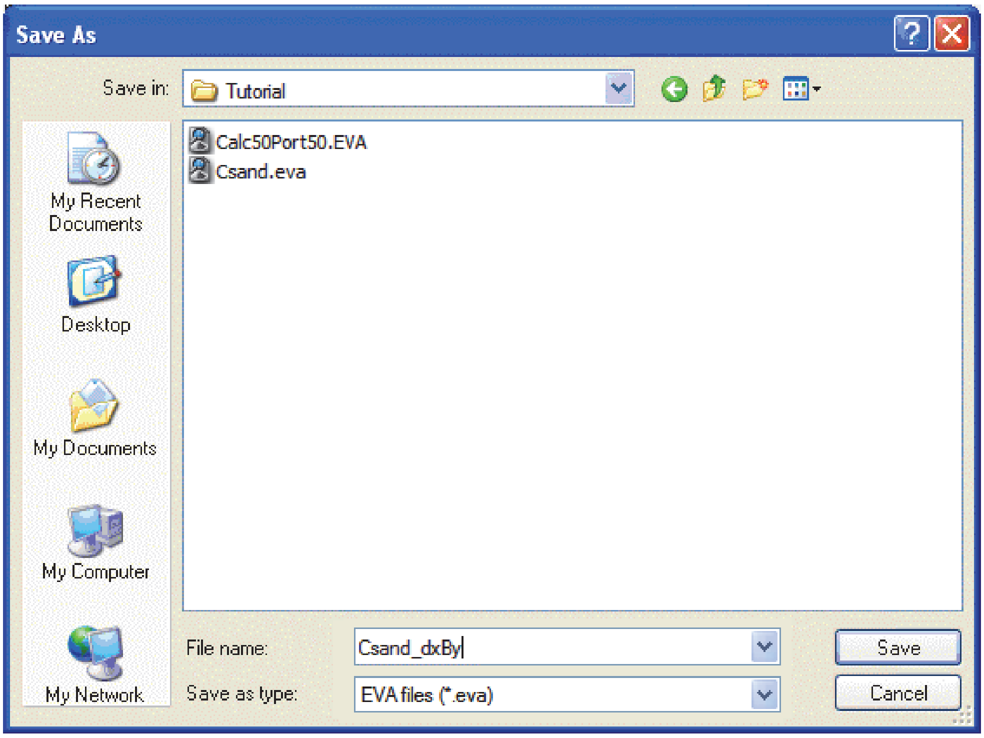
2 Calcite pattern 00-005-0586 multiplied by 0.996.

3 Magnesian Calcite pattern 00-043-0687

4 Calcite pattern 00-005-0586 multiplied by 0.984.

Step 4: Saving

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



Save in: Tutorial

File name: Csand_dxBy

Save as type: EVA files (*.eva)

Fig. 119: Saving Csand_dxBy.EVA document

Using the Tune Cell Tool

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 $Ca_{10}(PO_4)_6F_2$ is that P is partly replaced by C.

The replacement of P^{5+} (ionic radius 0.35) by the smaller C^{4+} (0.16) is expressed by deformation of the PO_4-tetraeder, with shorter P-O-distances and the reduction of a_o cell parameter[1].

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.

NOTE

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

This tutorial was prepared using PDF 4+ 2009 as a reference database. You may have another reference database.

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

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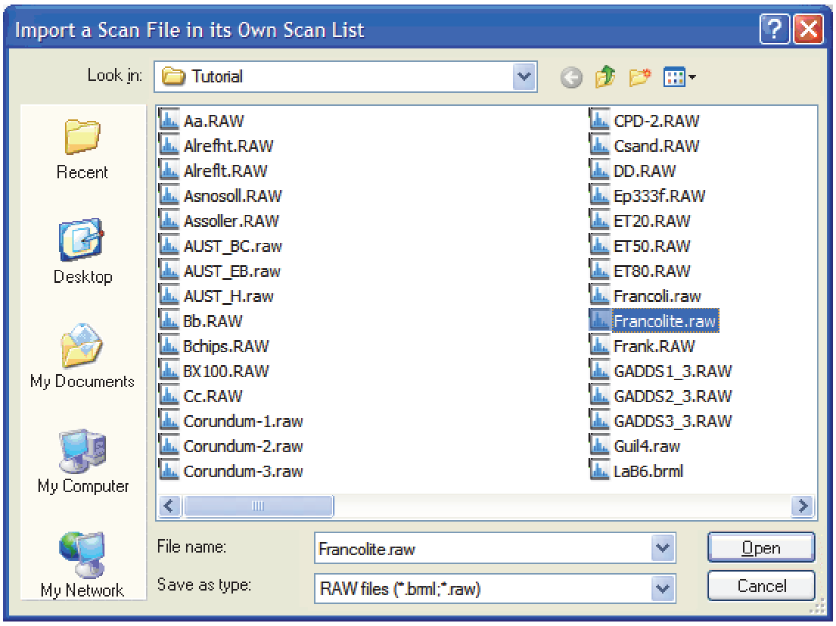
[1] X-Ray Powder Diffraction Study of Francolite by the Rietveld Method, B. Perdikatsis, Materials Science Forum Vols. 79-82 (1991), pp. 809-814.

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

New button

Import from file button

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 file** data command or the **Import from file** button. The Import from files dialog box will be displayed. Search the Tutorials/EVA[1] directory and select the Francolite.RAW file.
3. Click **Open**. The scan Francolite will be displayed in the graphical view of the EVA document.



File name: Francolite.raw

Save as type: RAW files (*.brml;*.raw)

Fig. 120: Import a Scan File dialog box

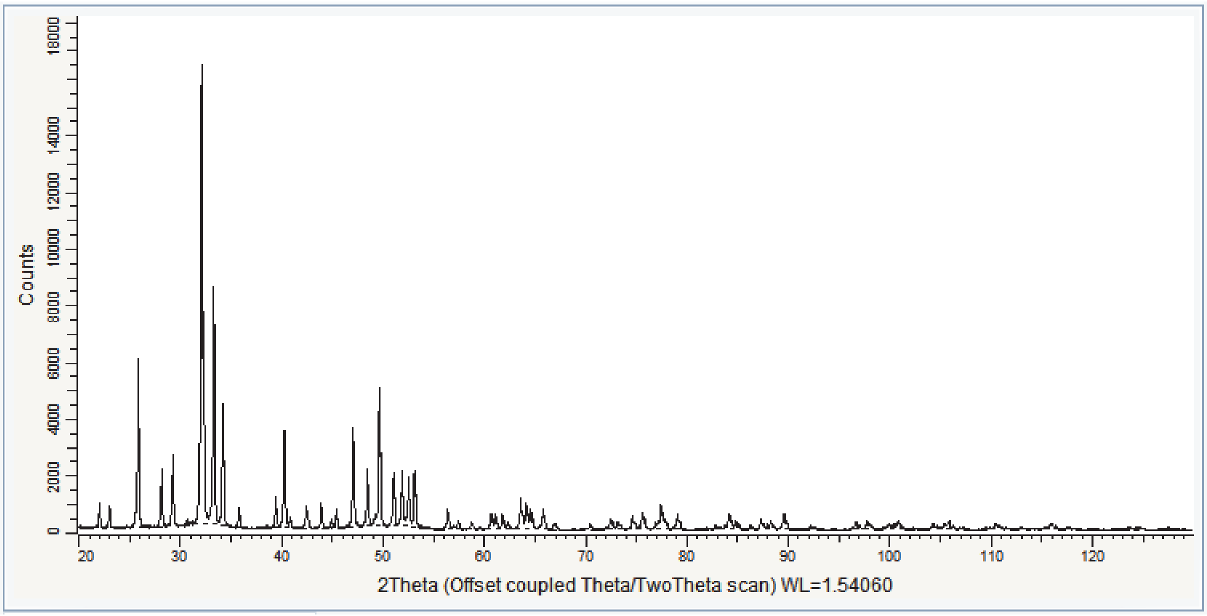


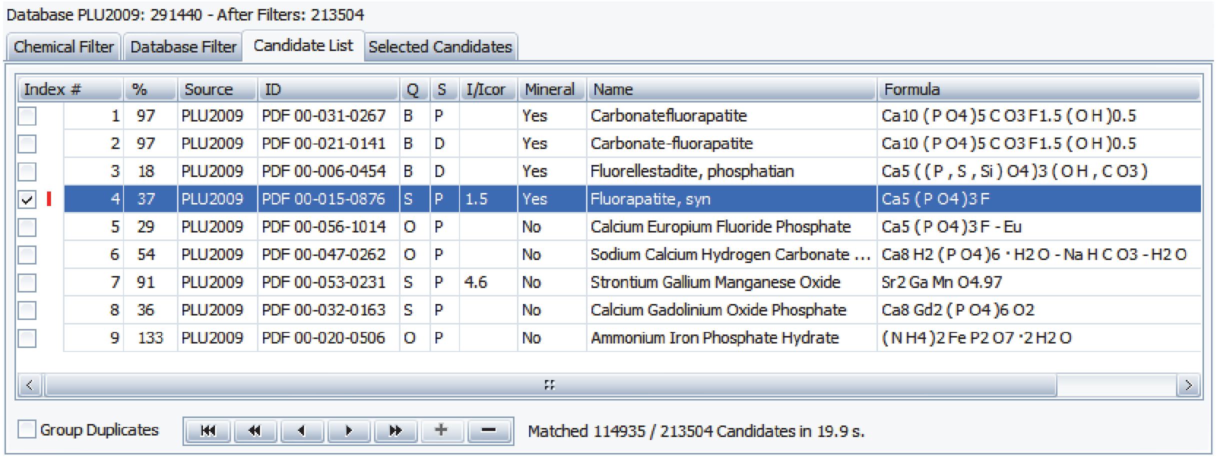
Fig. 121: Francolite.RAW imported in the graphical view

---

[1] 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.

Step 2: Performing the Search/Match Operation

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



Database PLU2009: 291440 - After Filters: 213504

	Index #	%	Source	ID	Q	S	I/Icor	Mineral	Name	Formula
☐	1	97	PLU2009	PDF 00-031-0267	B	P		Yes	Carbonatefluorapatite	Ca10 (P O4)5 C O3 F1.5 (O H)0.5
☐	2	97	PLU2009	PDF 00-021-0141	B	D		Yes	Carbonate-fluorapatite	Ca10 (P O4)5 C O3 F1.5 (O H)0.5
☐	3	18	PLU2009	PDF 00-006-0454	B	D		Yes	Fluorellestadite, phosphatian	Ca5 ((P, S, Si) O4)3 (O H, C O3)
☑	4	37	PLU2009	PDF 00-015-0876	S	P	1.5	Yes	Fluorapatite, syn	Ca5 (P O4)3 F
☐	5	29	PLU2009	PDF 00-056-1014	O	P		No	Calcium Europium Fluoride Phosphate	Ca5 (P O4)3 F - Eu
☐	6	54	PLU2009	PDF 00-047-0262	O	P		No	Sodium Calcium Hydrogen Carbonate ...	Ca8 H2 (P O4)6 · H2 O - Na H C O3 - H2 O
☐	7	91	PLU2009	PDF 00-053-0231	S	P	4.6	No	Strontium Gallium Manganese Oxide	Sr2 Ga Mn O4.97
☐	8	36	PLU2009	PDF 00-032-0163	S	P		No	Calcium Gadolinium Oxide Phosphate	Ca8 Gd2 (P O4)6 O2
☐	9	133	PLU2009	PDF 00-020-0506	O	P		No	Ammonium Iron Phosphate Hydrate	(N H4)2 Fe P2 O7 ·2 H2 O

☐ Group Duplicates

Matched 114935 / 213504 Candidates in 19.9 s.

Carbonatefluoroapatite is easily identified but we select Fluorapatite (PDF 00-015-0876) for the need of the example.

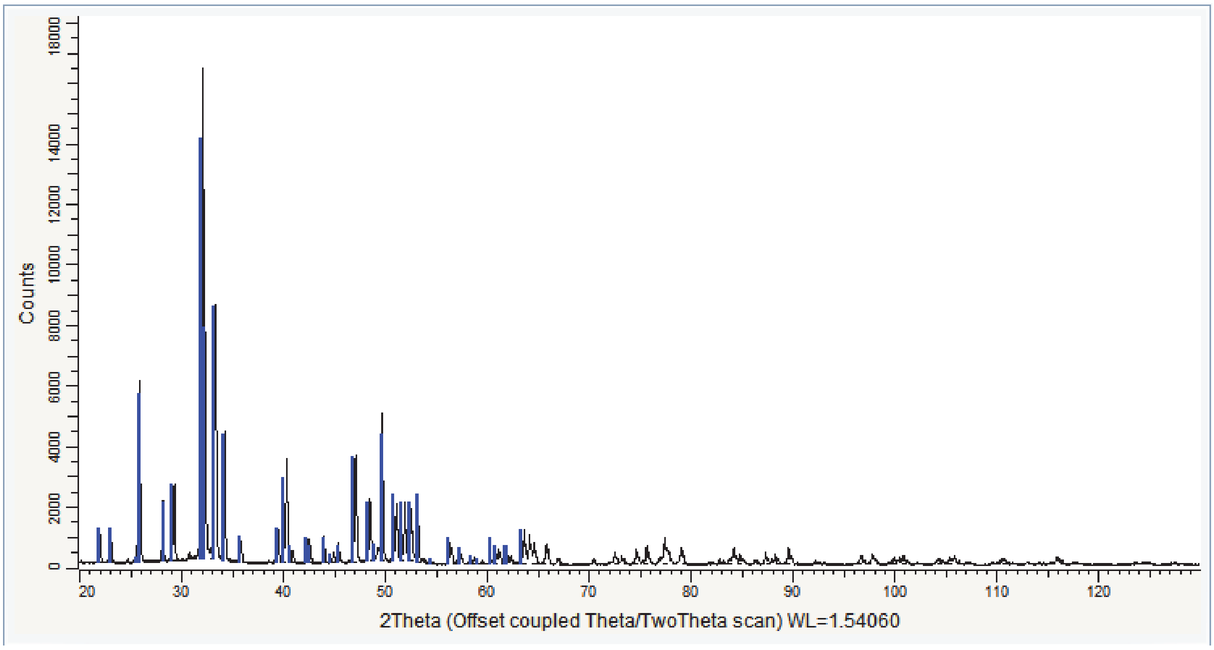
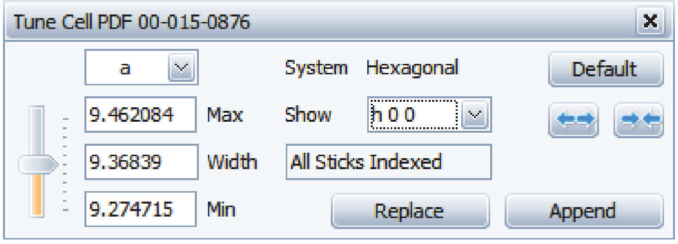


Fig. 122: Fluorapatite pattern in blue

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 —
   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 **h00** in the **Show** drop-down list to see lines which position depend only on *a*.



Tune Cell PDF 00-015-0876

a

System Hexagonal

9.462084 Max

Show h 0 0

9.36839 Width

All Sticks Indexed

9.274715 Min

4. Zoom in on one of the (h00)-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.

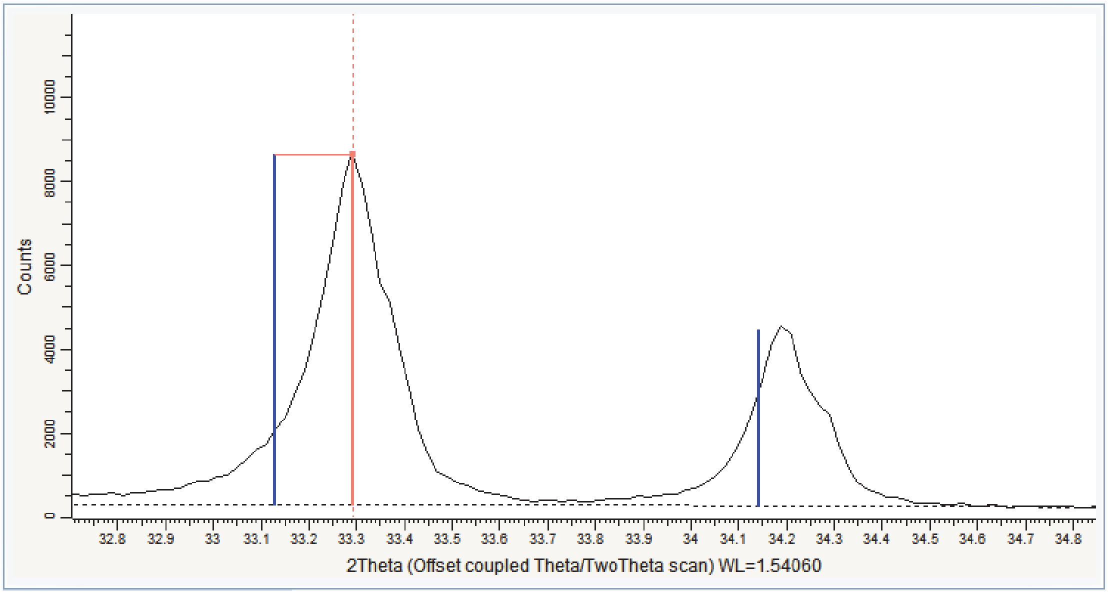
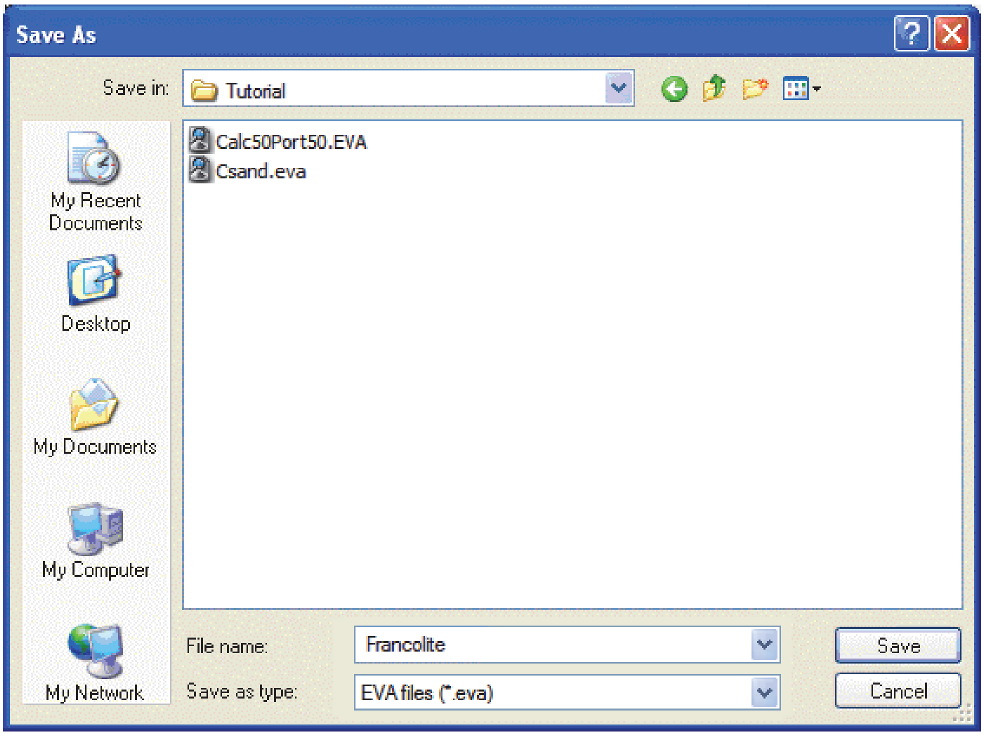


Fig. 123: (300) stick (located at 2theta=33.129°) of the pattern PDF 00-015-0876 shifted to fit the corresponding peak.

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.

Step 4: Saving

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



Save in: Tutorial

Calc50Port50.EVA

Csand.eva

File name: Francolite

Save as type: EVA files (*.eva)

Fig. 124: Saving Francolite.EVA document

Displaying a Pattern with Another Wavelength

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.

NOTE

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

This tutorial was prepared using PDF 4+ 2009 as a reference database. You may have another reference database.

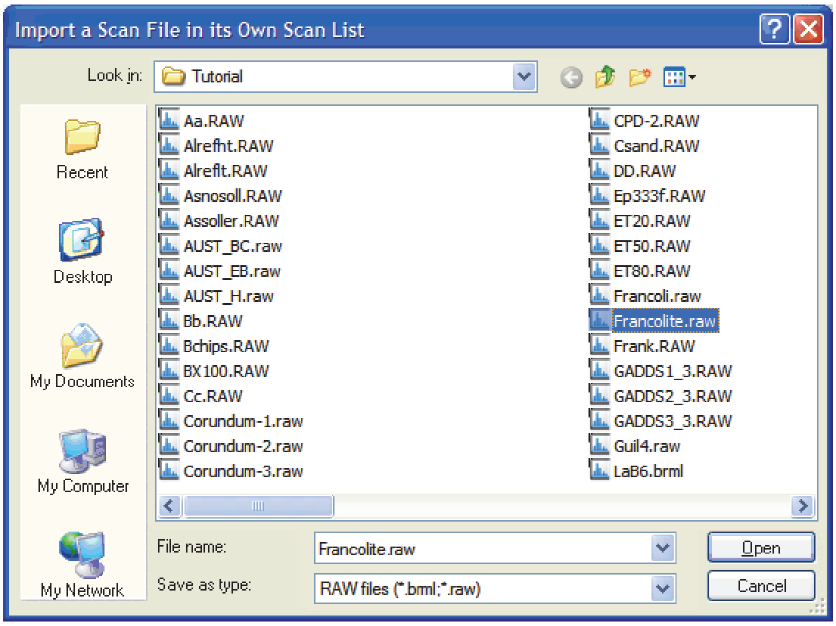
If you have no database, you cannot perform this part of the tutorial using the Search/Match.

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

New button

Import from file button

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 file** data command or the **Import from file** button. The Import from files dialog box will be displayed. Search the Tutorials/EVA[1] directory and select the Francolite.RAW file.
3. Click **Open**. The scan Francolite will be displayed in the graphical view of the EVA document.



Import a Scan File in its Own Scan List

Look in: Tutorial

Aa.RAW
Alrefht.RAW
Alrefit.RAW
Asnosoll.RAW
Assoller.RAW
AUST_BC.raw
AUST_EB.raw
AUST_H.raw
Bb.RAW
Bchips.RAW
BX100.RAW
Cc.RAW
Corundum-1.raw
Corundum-2.raw
Corundum-3.raw
CPD-2.RAW
Csand.RAW
DD.RAW
Ep333f.RAW
ET20.RAW
ET50.RAW
ET80.RAW
Francoli.raw
Francolite.raw
Frank.RAW
GADDS1_3.RAW
GADDS2_3.RAW
GADDS3_3.RAW
Guil4.raw
LaB6.brml

File name: Francolite.raw

Save as type: RAW files (*.brml;*.raw)

Fig. 125: Import a Scan File dialog box

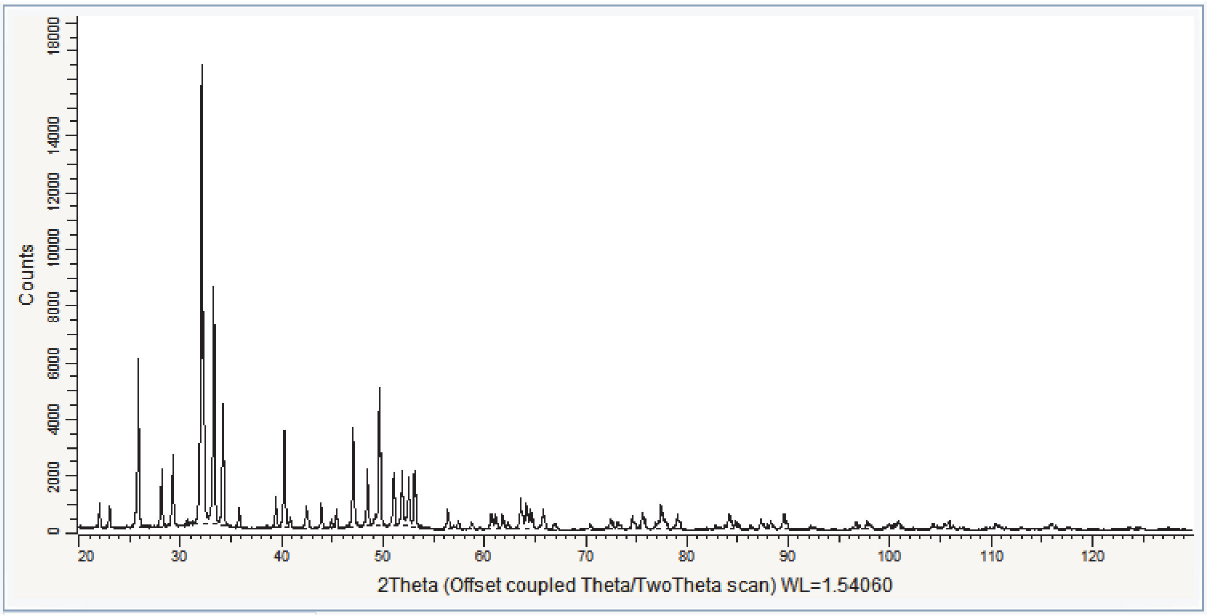


Fig. 126: Francolite.RAW imported in the graphical view

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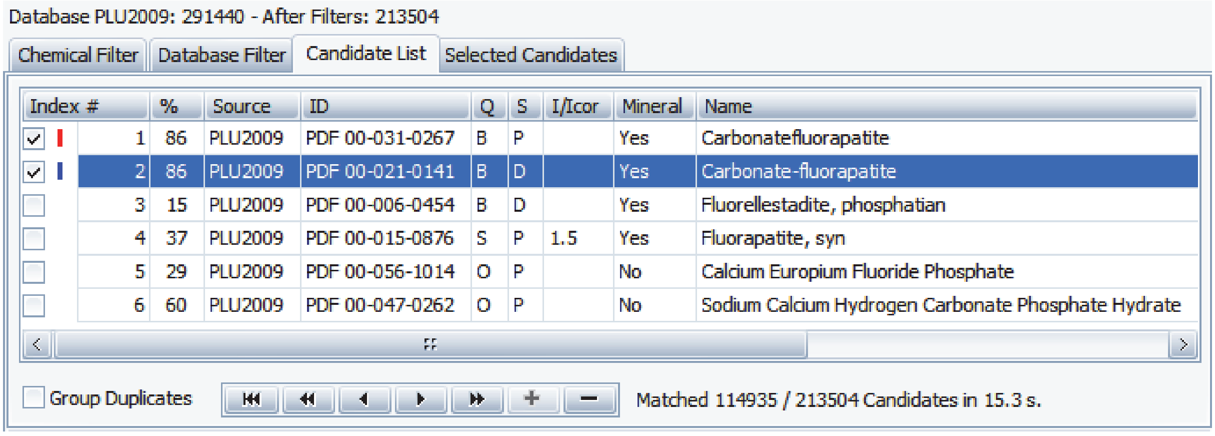
[1] The directory path to the EVA tutorial files is "C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials" under Windows XP and "C:\ProgramData\Bruker AXS\Tutorials" under Windows 7.
To access the folder with the explorer, select "Display hidden files and folders" in the Folders options.

Step 2: Performing the Search/Match Operation

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


Database PLU2009: 291440 - After Filters: 213504

Index #	%	Source	ID	Q	S	I/Icor	Mineral	Name
☑ 1	86	PLU2009	PDF 00-031-0267	B	P		Yes	Carbonatefluorapatite
☑ 2	86	PLU2009	PDF 00-021-0141	B	D		Yes	Carbonate-fluorapatite
☐ 3	15	PLU2009	PDF 00-006-0454	B	D		Yes	Fluorellestadite, phosphatian
☐ 4	37	PLU2009	PDF 00-015-0876	S	P	1.5	Yes	Fluorapatite, syn
☐ 5	29	PLU2009	PDF 00-056-1014	O	P		No	Calcium Europium Fluoride Phosphate
☐ 6	60	PLU2009	PDF 00-047-0262	O	P		No	Sodium Calcium Hydrogen Carbonate Phosphate Hydrate

☐ Group Duplicates

Matched 114935 / 213504 Candidates in 15.3 s.

Carbonatefluoroapatite is easily identified. Select both patterns PDF 00-031-0267 and PDF 00-021-0141. It will allow viewing the change.

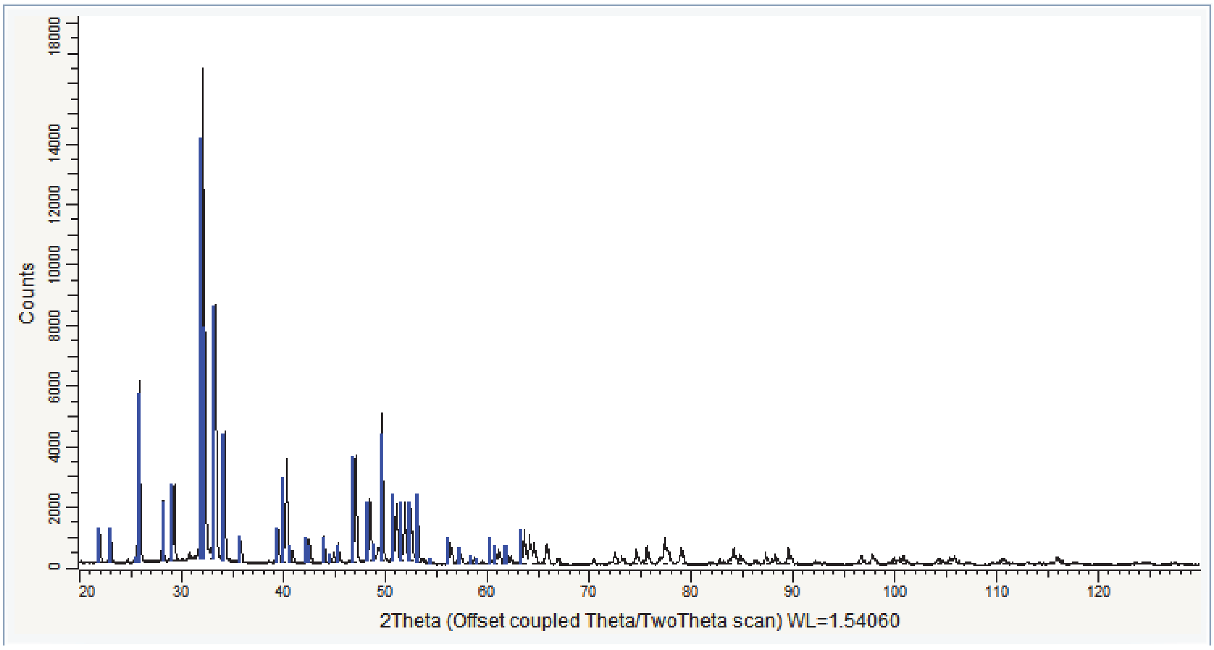


Fig. 127: Carbonatefluorapatite pattern in blue. The two patterns are superposed.

Step 3: Changing the Wavelength

1. Select the pattern PDF 00-021-0141 in the data tree.
2. In the pattern property table, clear the **Scan WL** check box to be able to enter another wavelength.

   We want to check if there is a pollution of the X-ray tube. The WLα_1 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 WLα_1 radiation.
3. In the **Wavelength** drop-down list below, select the WLα_1 wavelength. The pattern PDF 00-021-0141 will be displayed with this new wavelength.
4. Zoom in from 2Theta=20° to 2Theta=55°.

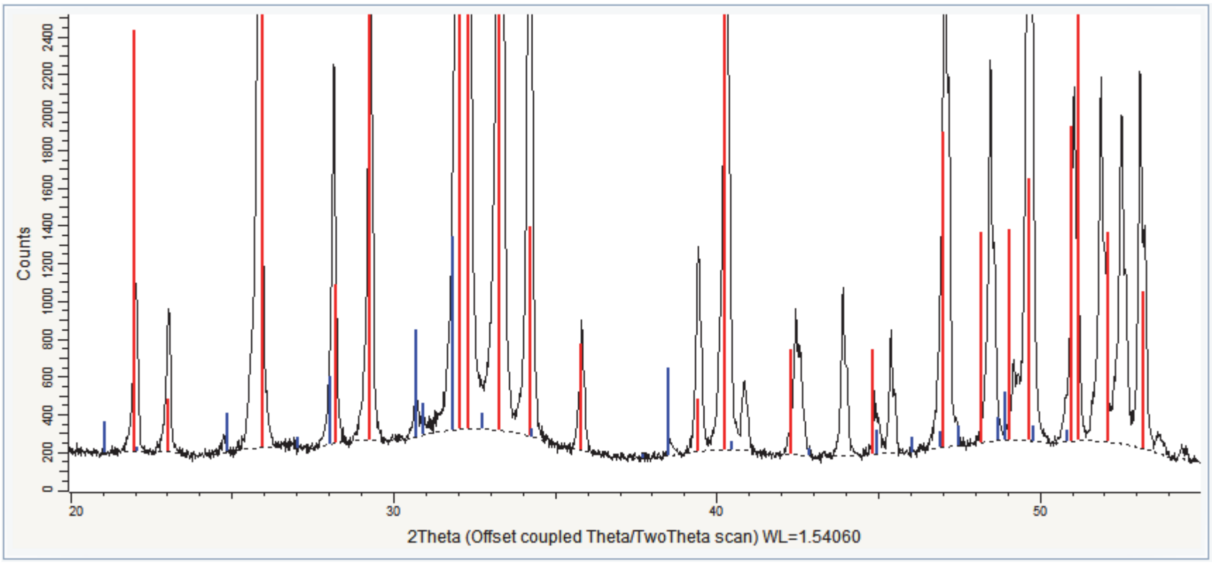


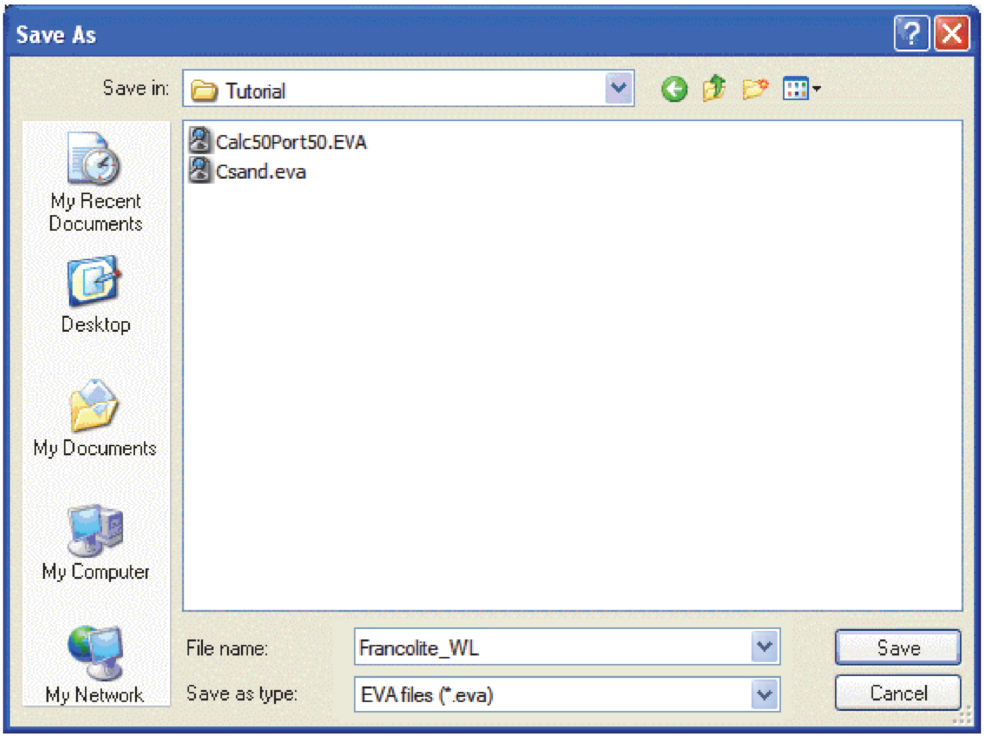
Fig. 128: Carbonatefluorapatite pattern displayed with the WLα_1 wavelength in blue and original pattern in red. Zoom on the 20-55° 2Theta range.

5. 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.

Step 4: Saving

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



Save in: Tutorial

File name: Francolite_WL

Save as type: EVA files (*.eva)

Fig. 129: Saving Francolite_WL.EVA document

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:

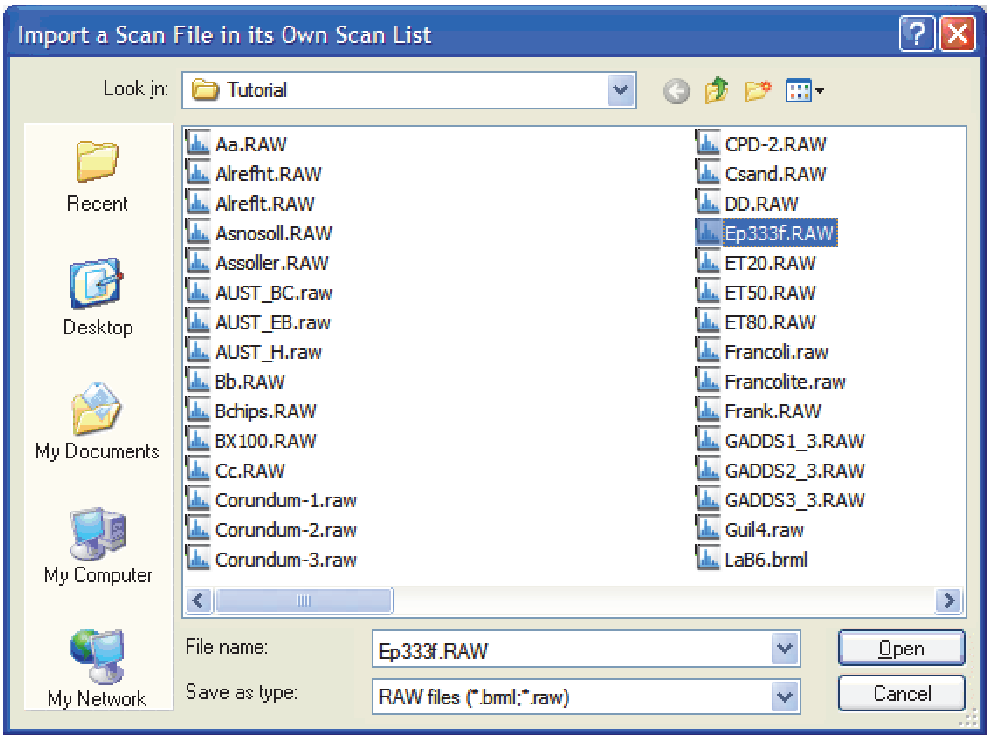
1. Creating a new EVA document and importing Ep333f.RAW.
2. Creating and working with the waterfall view.
3. Saving the EVA document containing the scan.

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

New button

Import from file button

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 file** data command or the **Import from file** button. The Import from files dialog box will be displayed.
3. Search the Tutorials/EVA[1] directory and select the Ep333f.RAW file.
4. Click **Open**. The scan Ep333f will be displayed in the graphical view of the EVA document.



File name: Ep333f.RAW

Save as type: RAW files (*.brml;*.raw)

Fig. 130: Import a Scan File dialog box

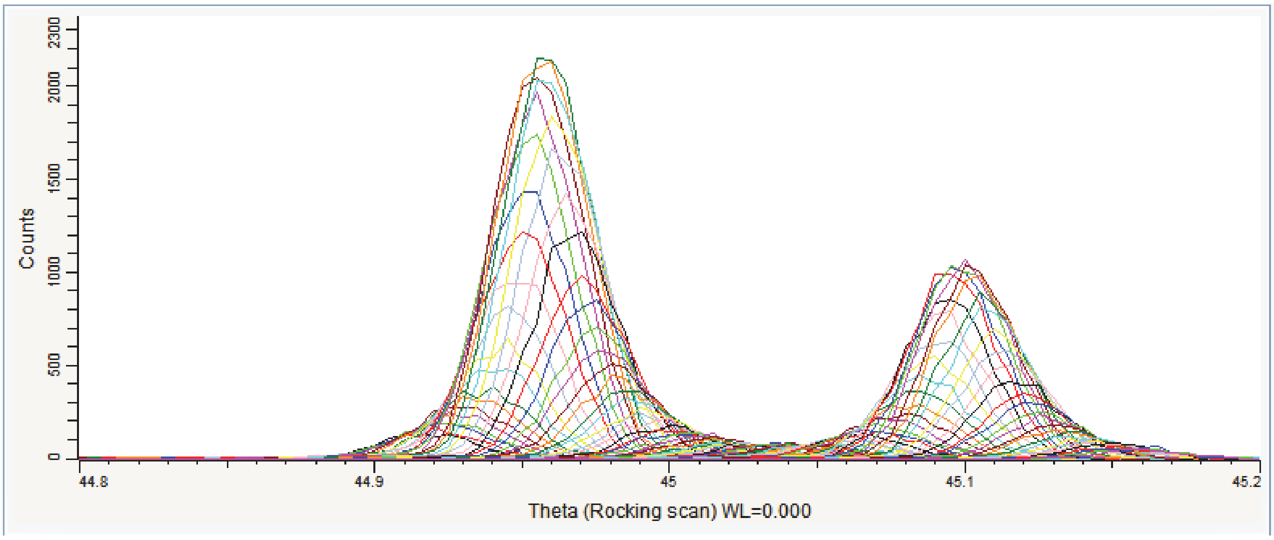


Fig. 131: Ep333f.RAW file imported in the graphical view

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[1] 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.

Step 2: Creating and Working with the Waterfall View.

1. Select the **Waterfall display** check box in the Theta View property panel: the scans will be displayed as a waterfall.

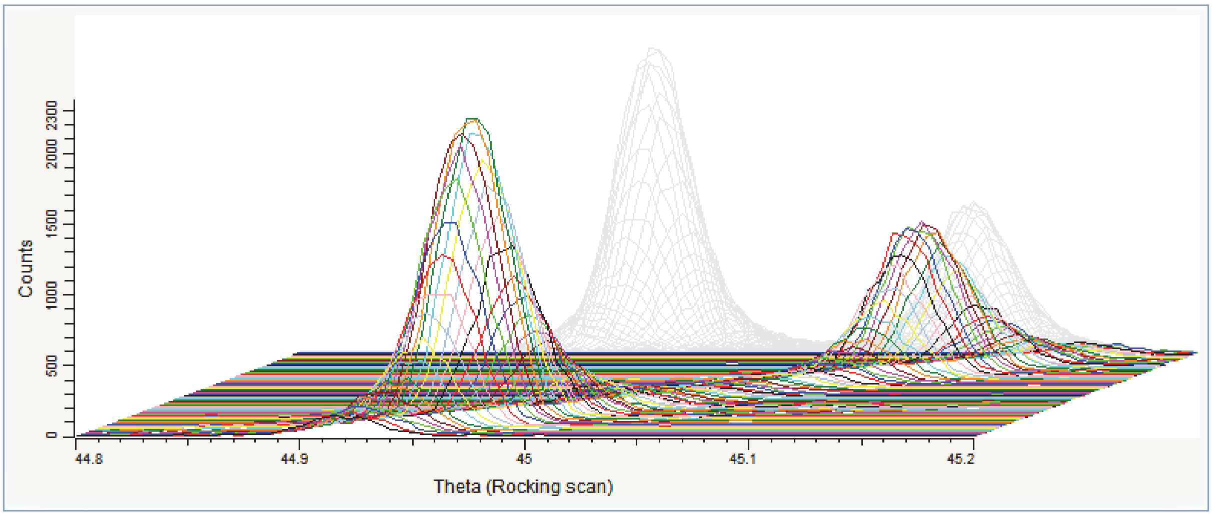


Fig. 132: Waterfall display

2. Change the perspective of the display.

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

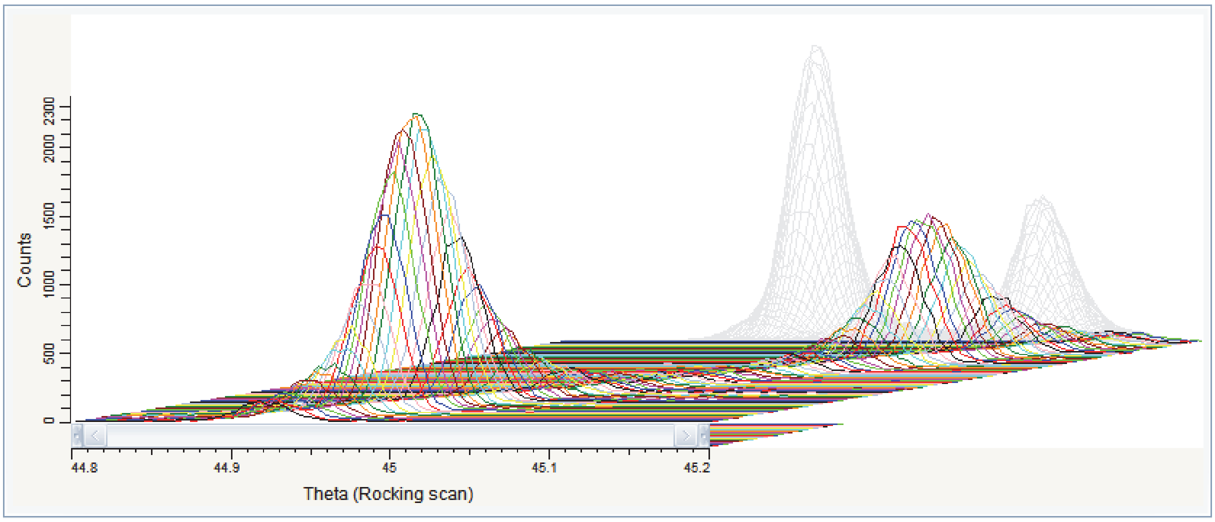


Fig. 133: Perspective horizontally modified

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

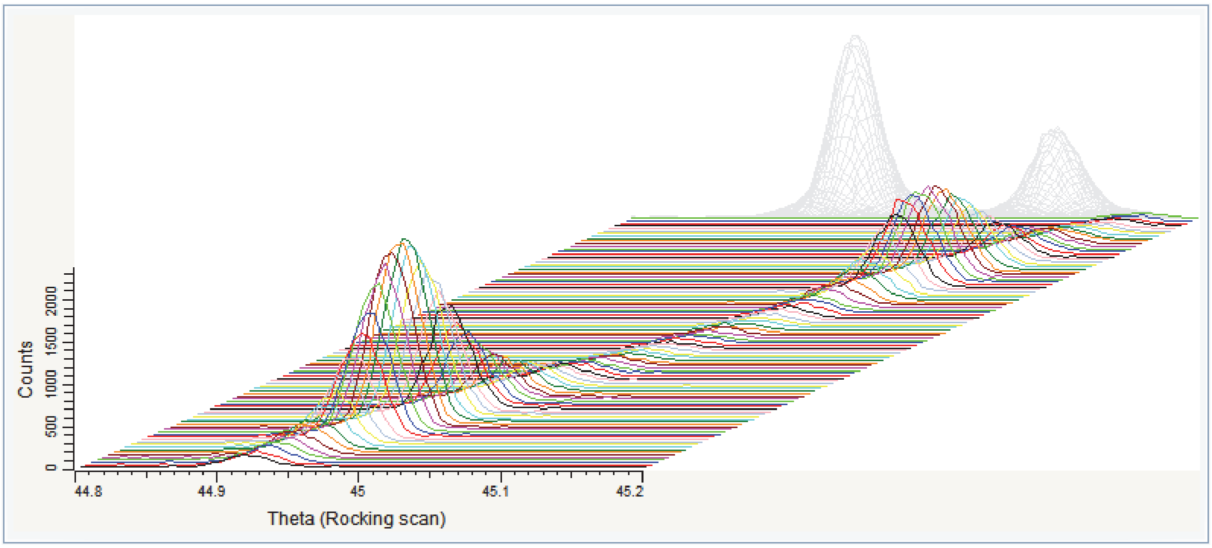


Fig. 134: Perspective horizontally and vertically modified

3. 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.

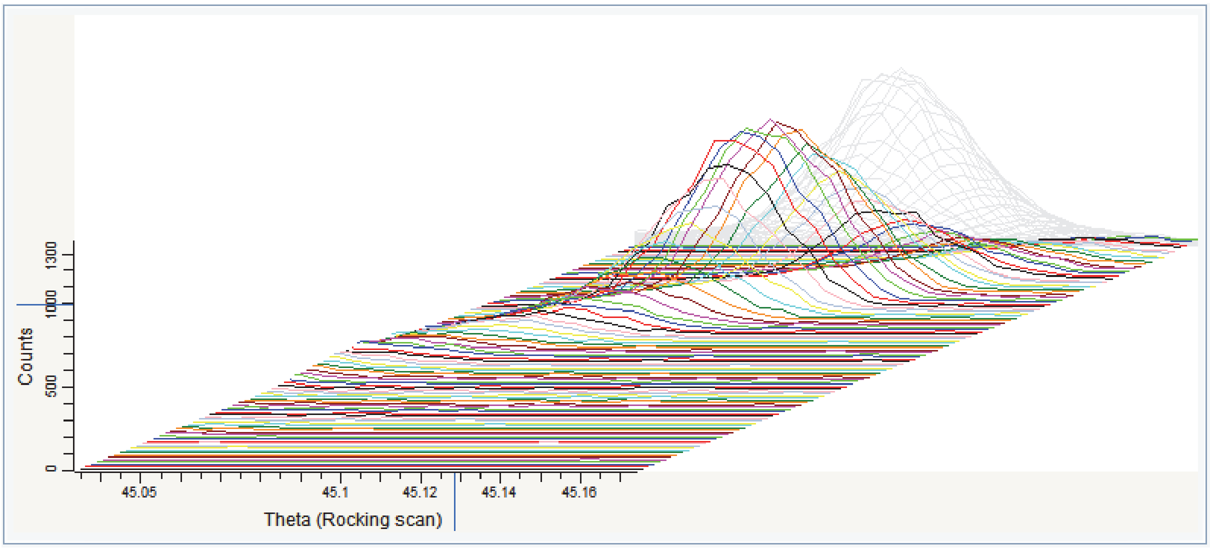
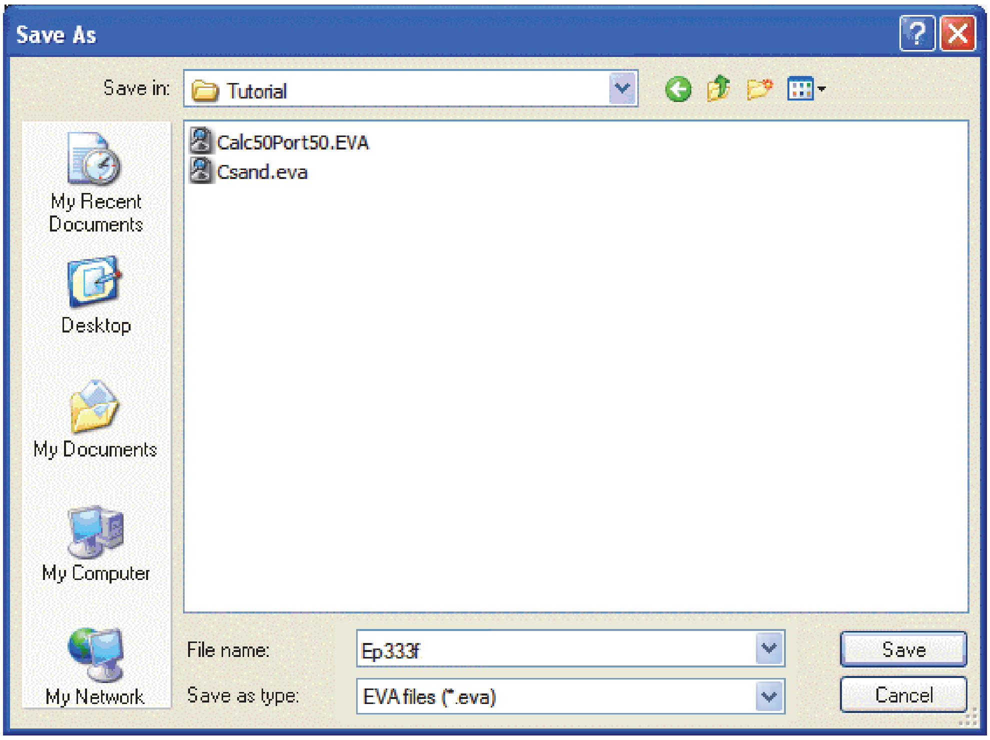


Fig. 135: Zoom on the right peak

Step 3: Saving

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



Save in: Tutorial

File name: Ep333f

Save as type: EVA files (*.eva)

Fig. 136: Saving Ep333f.EVA document

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:

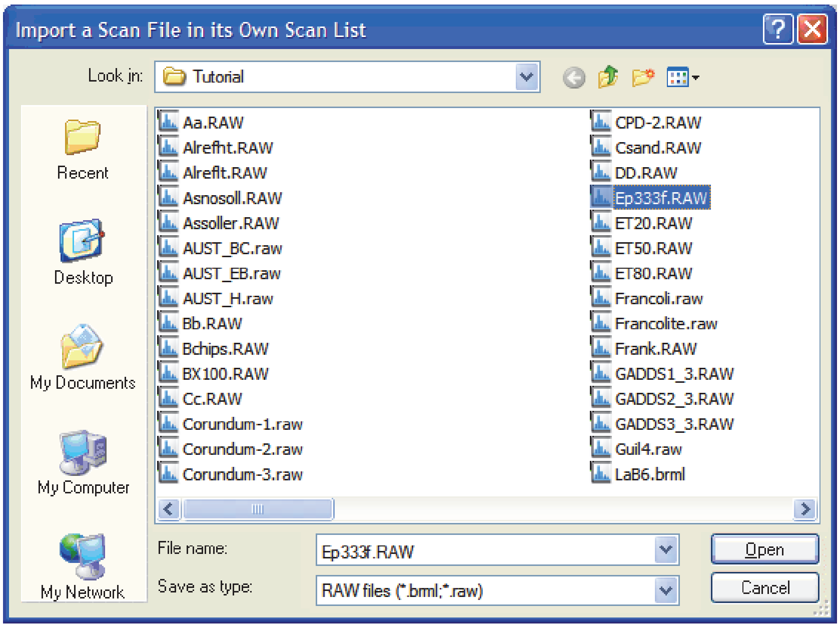
1. Creating a new EVA document and importing Ep333f.RAW.
2. Creating and working with the 2D view.
3. Saving the EVA document containing the scan.

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

New button

Import from file button

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 file** data command or the **Import from file** button. The Import from files dialog box will be displayed.
3. Search the Tutorials/EVA[1] directory and select the Ep333f.RAW file.
4. Click **Open**. The scan Ep333f will be displayed in the graphical view of the EVA document.



Import a Scan File in its Own Scan List

Look in: Tutorial

Aa.RAW
Alrefht.RAW
Alrefit.RAW
Asnosoll.RAW
Assoller.RAW
AUST_BC.raw
AUST_EB.raw
AUST_H.raw
Bb.RAW
Bchips.RAW
BX100.RAW
Cc.RAW
Corundum-1.raw
Corundum-2.raw
Corundum-3.raw
CPD-2.RAW
Csand.RAW
DD.RAW
Ep333f.RAW
ET20.RAW
ET50.RAW
ET80.RAW
Francoli.raw
Francolite.raw
Frank.RAW
GADDS1_3.RAW
GADDS2_3.RAW
GADDS3_3.RAW
Guil4.raw
LaB6.brml

File name: Ep333f.RAW

Save as type: RAW files (*.brml;*.raw)

Fig. 137: Import a Scan File dialog box

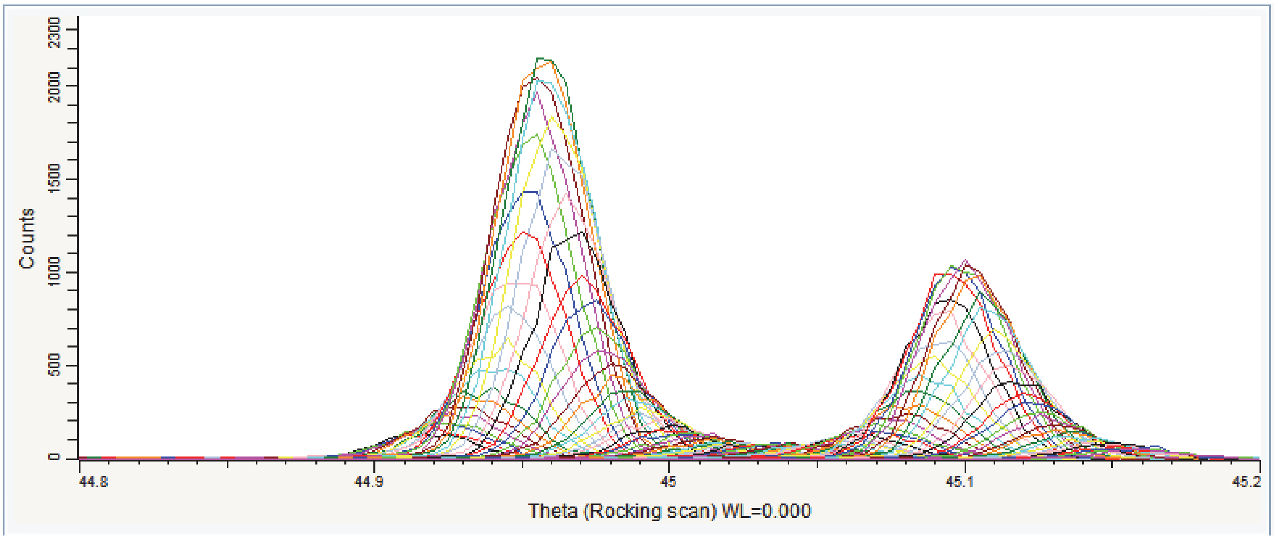


Fig. 138: Ep333f.RAW file imported in the graphical view

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[1] 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.

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

Case #1: 2D view with intensity map

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 —
Right-click the scan list in the data tree to display the context menu. Click **Create** and then **2D View** on the related submenu.

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

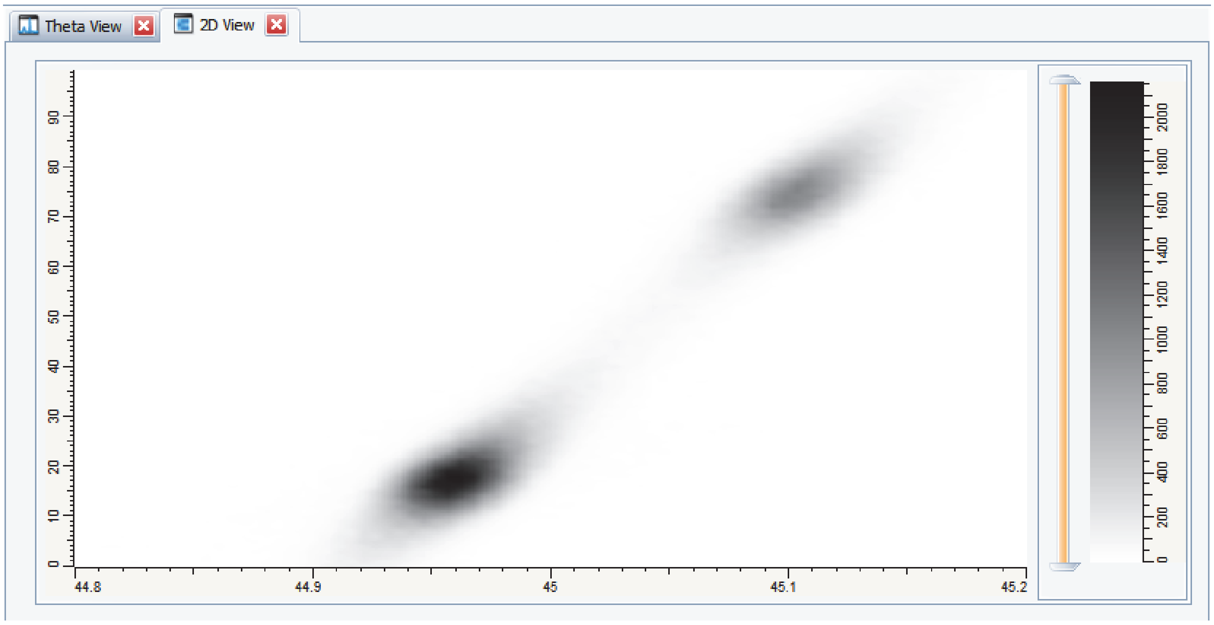


Fig. 139: 2D view with intensity map

4. 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.

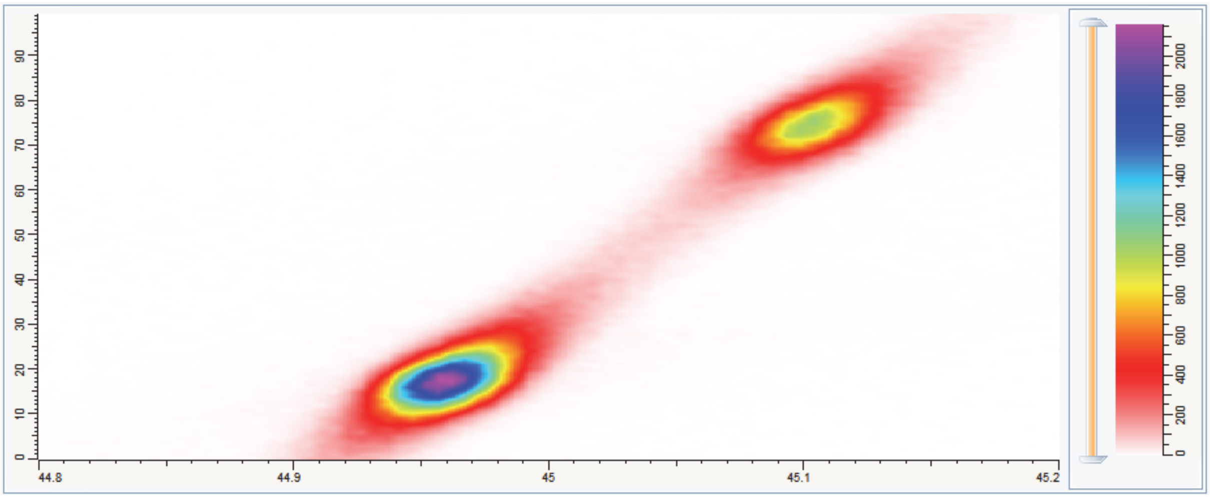


Fig. 140: 2D view with colored intensity map

Case #2: 2D view with levels

1. Make certain the list of scans is selected; if not, select it in the data tree.
2. 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.

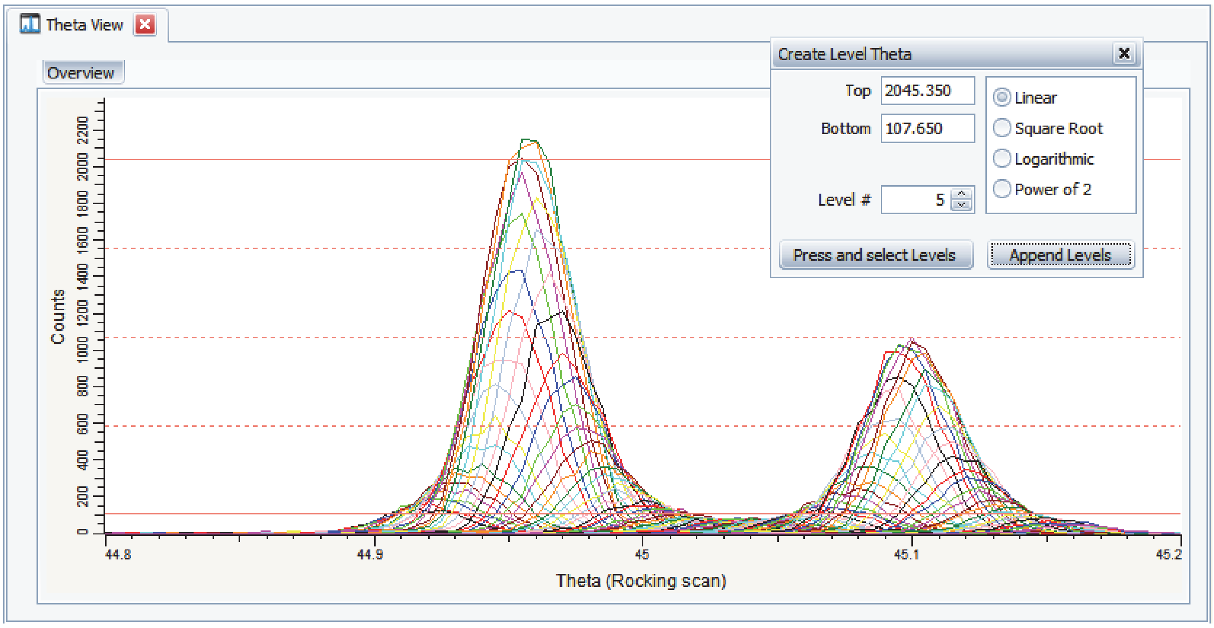

Create Level Theta
Top 2045.350
Bottom 107.650
Level # 5
● Linear
○ Square Root
○ Logarithmic
○ Power of 2

Fig. 141: Creating levels: Create Level dialog box and ghost levels in the graphical view

3. 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.

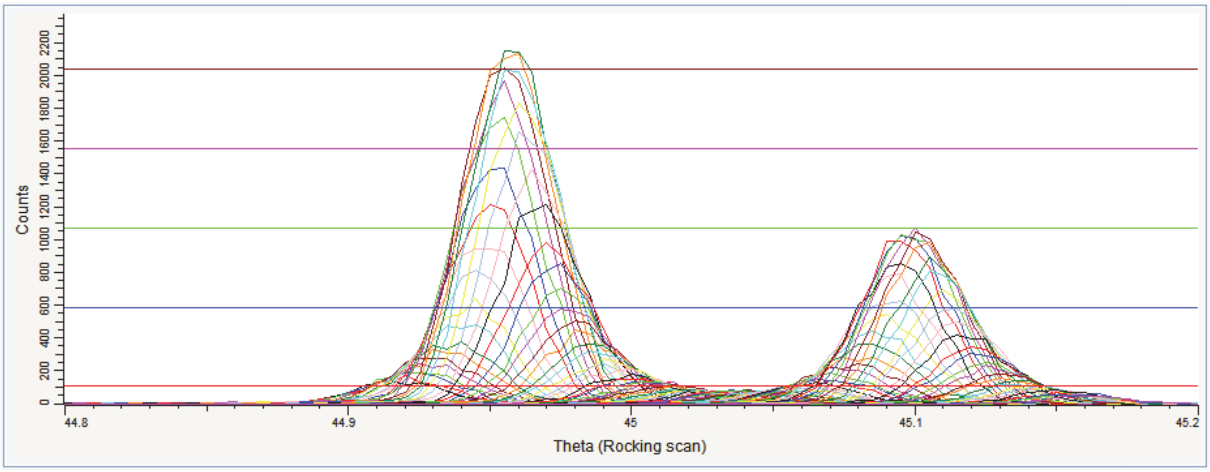


Fig. 142: Creating levels: levels displayed in the graphical view

4. Click **2D View** in the Create list of the Data Command panel
   — 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.

5. 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.

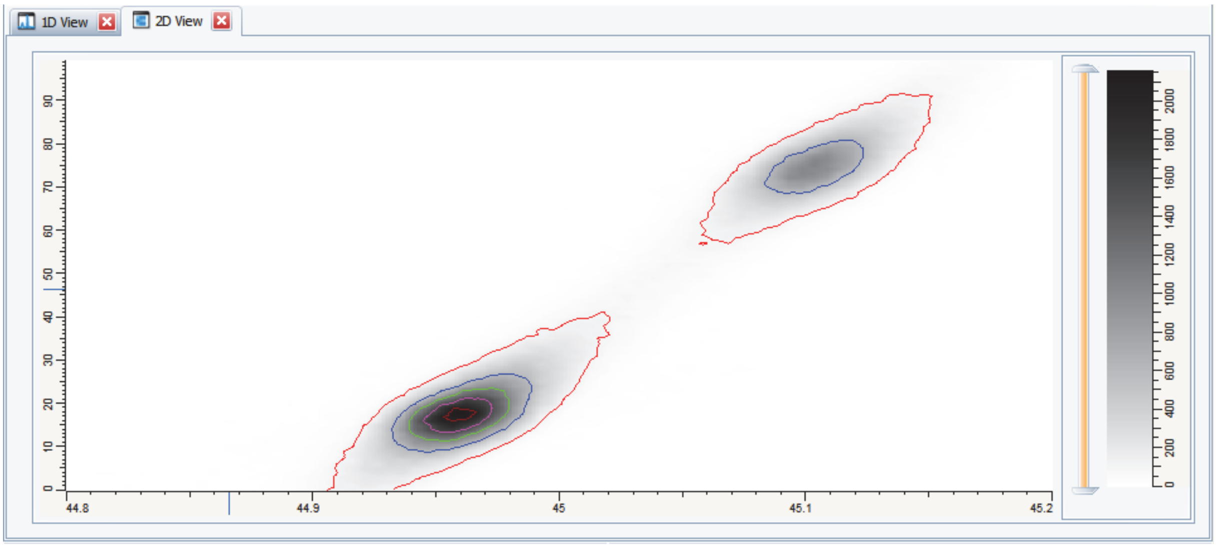
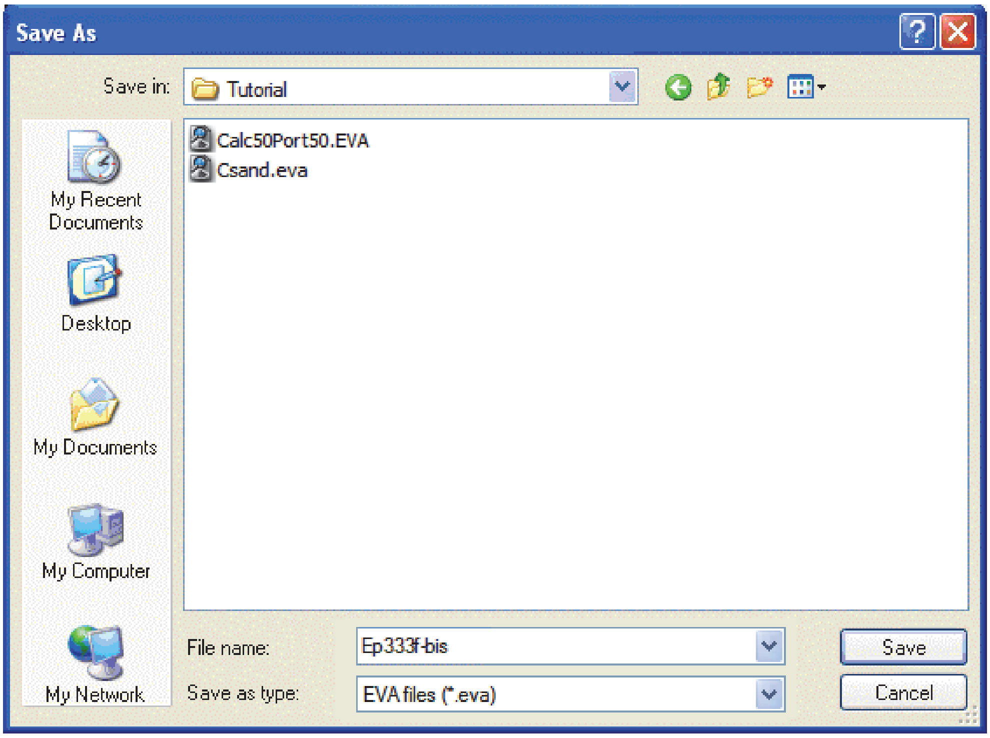


Fig. 143: 2D view with intensity map and levels

Step 3: Saving

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



Save in: Tutorial

Calc50Port50.EVA
Csand.eva

File name: Ep333f-bis

Save as type: EVA files (*.eva)

Fig. 144: Saving Ep333f-bis.EVA document

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:

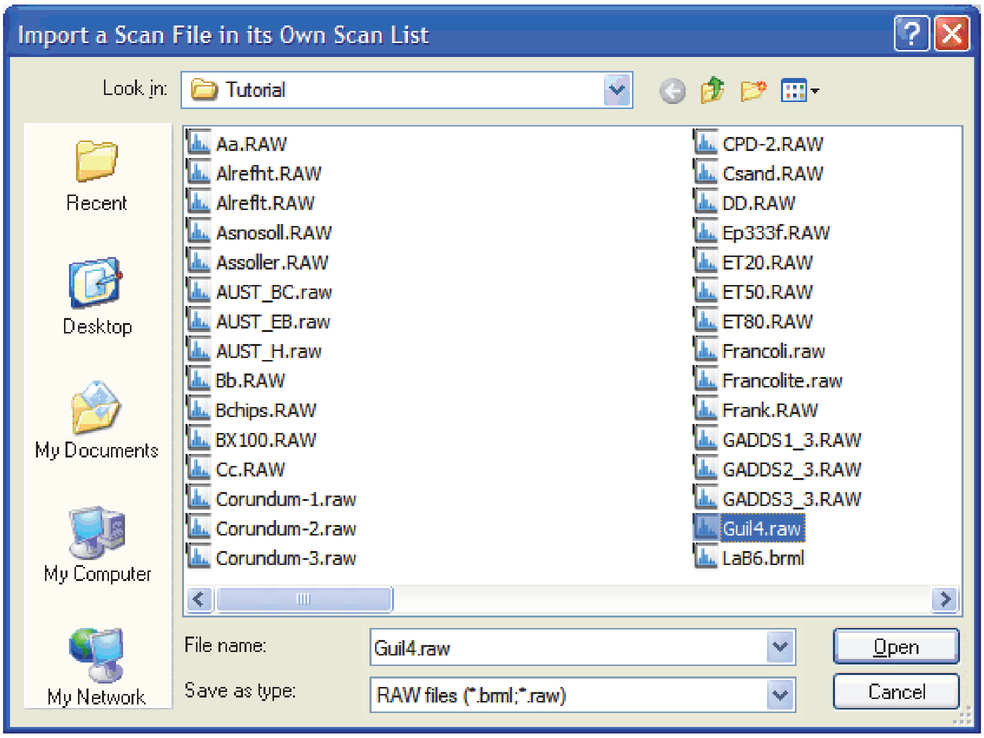
1. Creating a new EVA document and importing Guil4.RAW.
2. Creating the 2D view with levels.
3. Sorting the scans on the Y-axis by temperature.
4. Saving the EVA document containing the scan.

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

New button

Import from file button

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 file** data command or the **Import from file** button. The Import from files dialog box will be displayed.
3. Search the Tutorials/EVA[1] directory and select the Guil4.RAW file.
4. Click **Open**. The scan Guil4 will be displayed in the graphical view of the EVA document.



File name: Guil4.raw

Save as type: RAW files (*.brml;*.raw)

Fig. 145: Import a Scan File dialog box

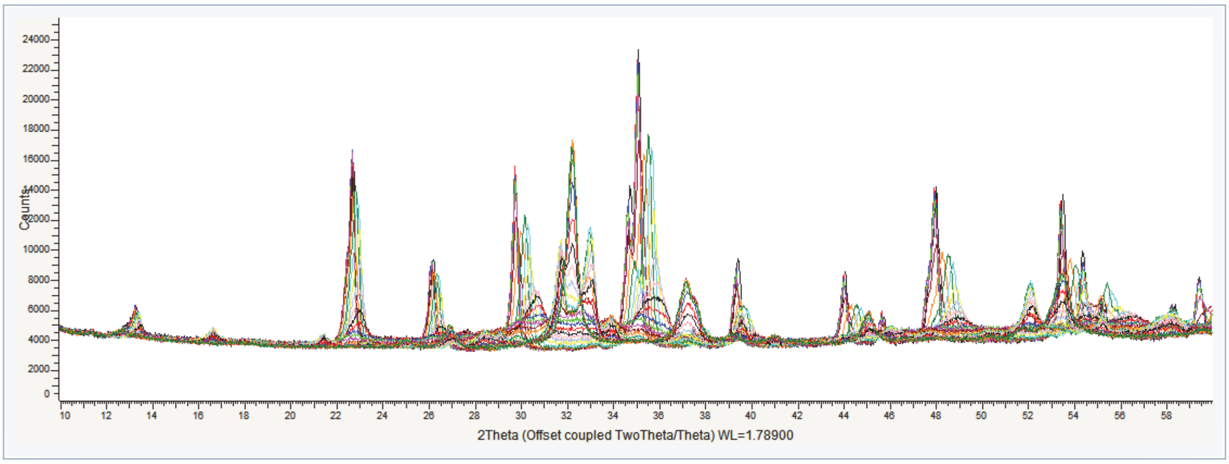


Fig. 146: Guil4.RAW file imported in the graphical view

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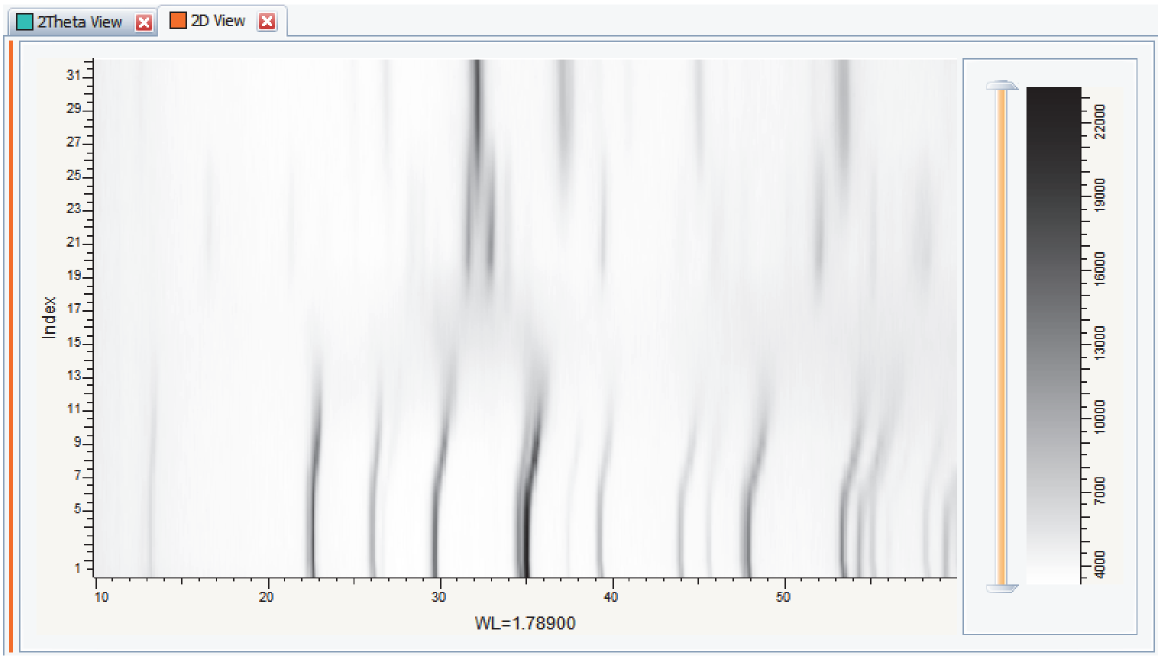
[1] The directory path to the EVA tutorial files is "C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials" under Windows XP and "C:\ProgramData\Bruker AXS\Tutorials" under Windows 7.
To access the folder with the explorer, select "Display hidden files and folders" in the Folders options.

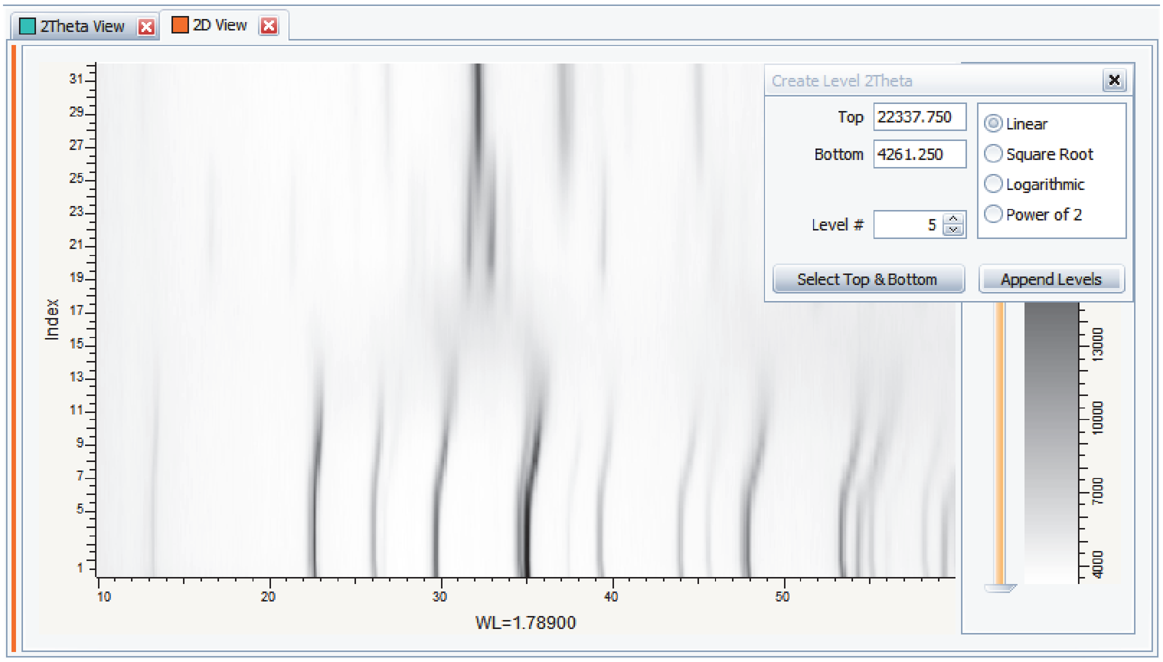
Step 2: Creating the 2D View with Levels

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 —
   Right-click the scan list in the data tree to display the context menu. Click **Create** and then **2D View** on the related submenu.
3. The 2D View will be displayed in a new tab.



4. 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.


Create Level 2Theta

Top 22337.750

Bottom 4261.250

Level # 5

◉ Linear
○ Square Root
○ Logarithmic
○ Power of 2

Fig. 147: Creating levels: Create Level dialog box

5. 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.
6. The Intensity map and the Levels are displayed by default. Leave the **Intensity map** and the **Levels** check boxes selected.

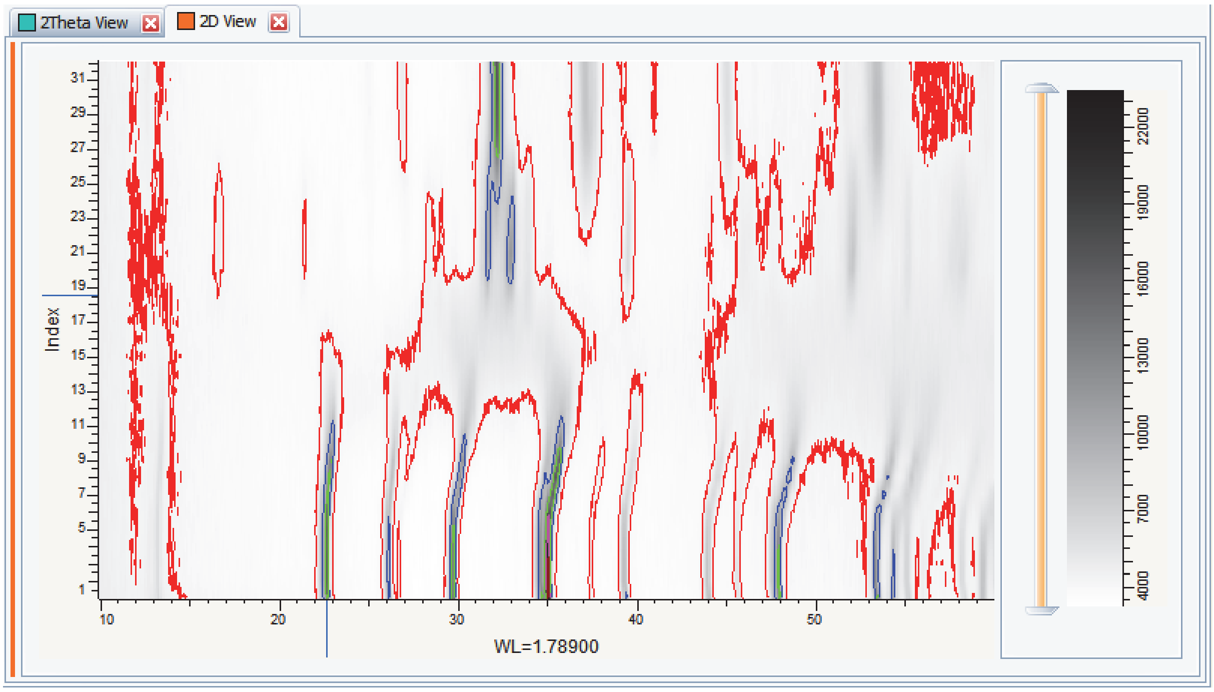


Fig. 148: 2D view with intensity map and levels, scans sorted by index on the Y-axis

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.

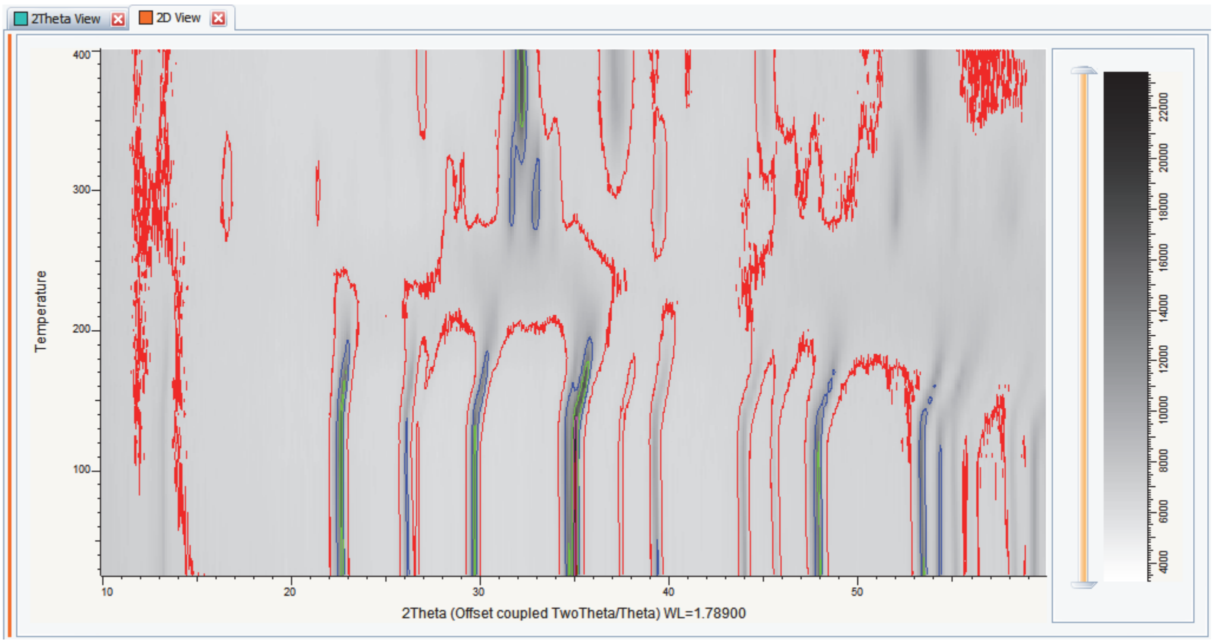
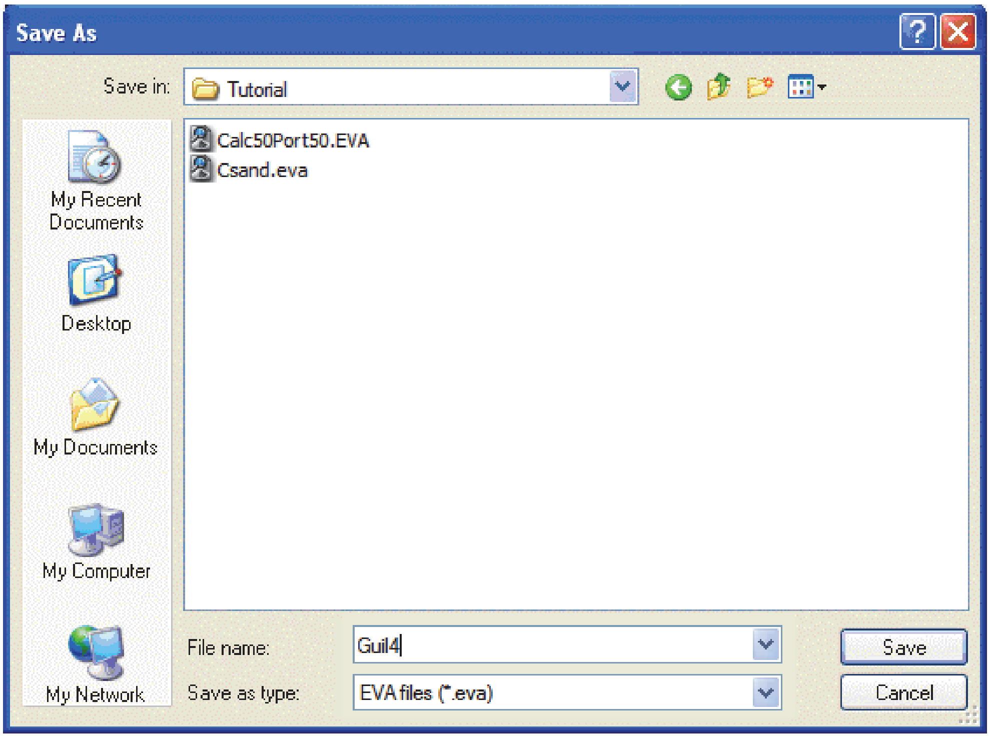


Fig. 149: 2D view with intensity map and levels, scans sorted by temperature on the Y-axis

Step 4: Saving

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



File name: Guil4

Save as type: EVA files (*.eva)

Fig. 150: Saving Guil4.EVA document

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:

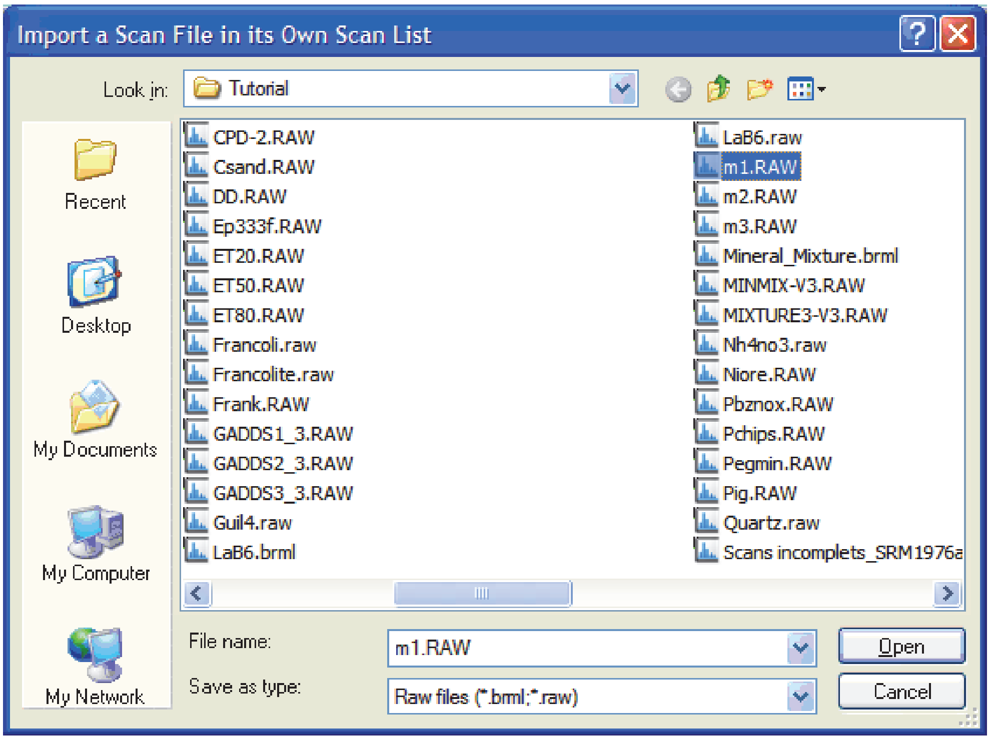
1. Creating a new EVA document and importing m1.RAW.
2. Creating and managing the PIP and VIP views.
3. Saving the EVA document containing the scan.

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

New button

Import from file button

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 file** data command or the **Import from file** button. The Import from files dialog box will be displayed.
3. Search the Tutorials/EVA[1] directory and select the m1.RAW file.
4. Click **Open**. The scan m1 will be displayed in the graphical view of the EVA document.



Look in: Tutorial

File name: m1.RAW

Save as type: Raw files (*.brml;*.raw)

Fig. 151: Import a Scan File dialog box

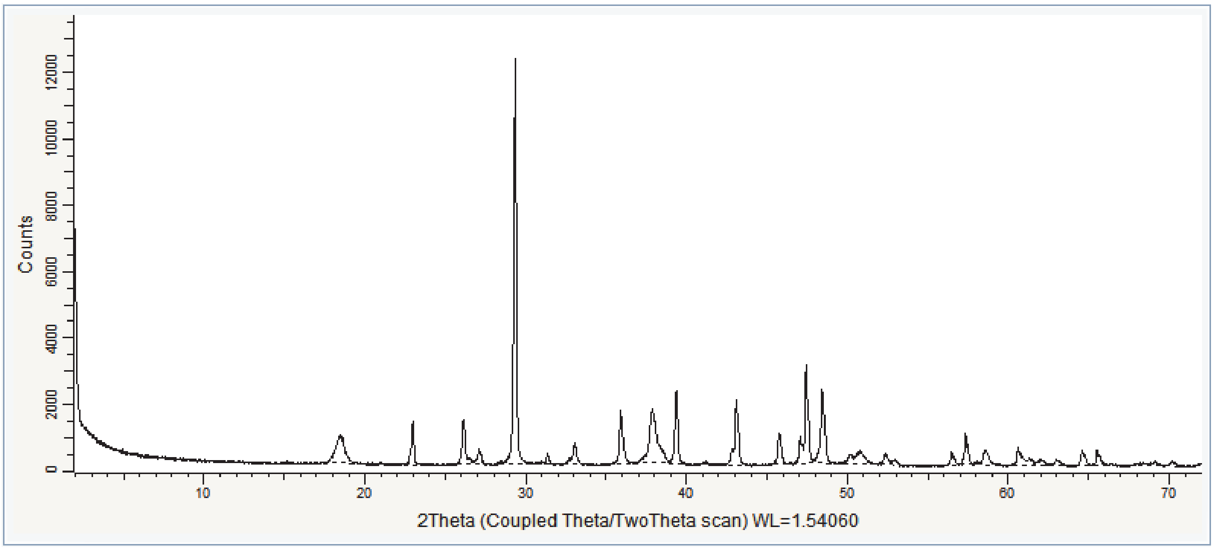


Fig. 152: m1.RAW file imported in the graphical view

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[1] 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.

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

Case #1: Creating a PIP view

PIP mode button

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.

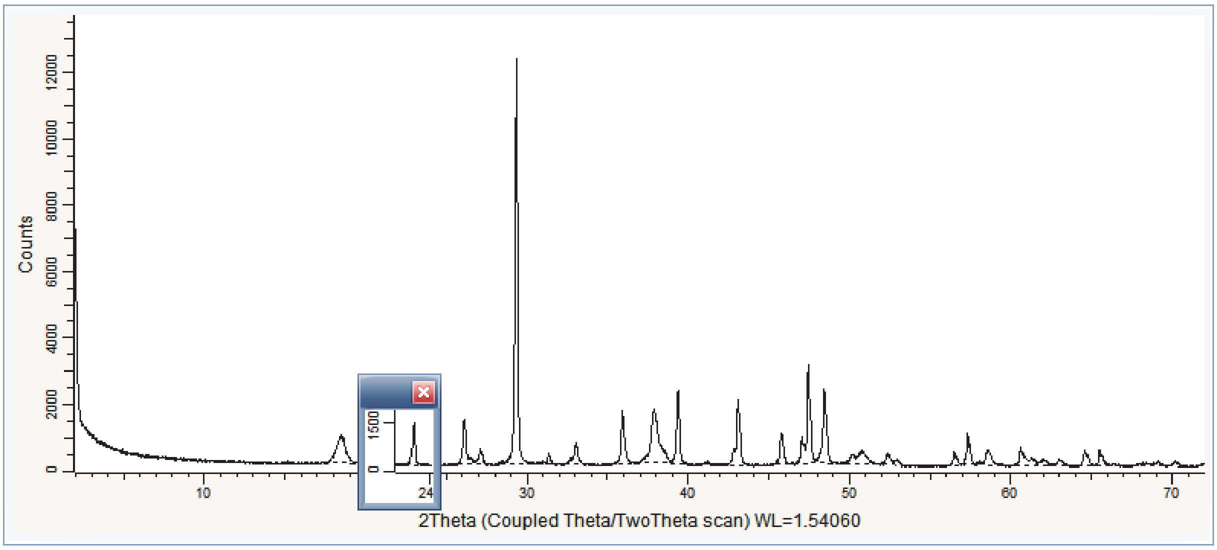


Fig. 153: Creating a PIP view

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

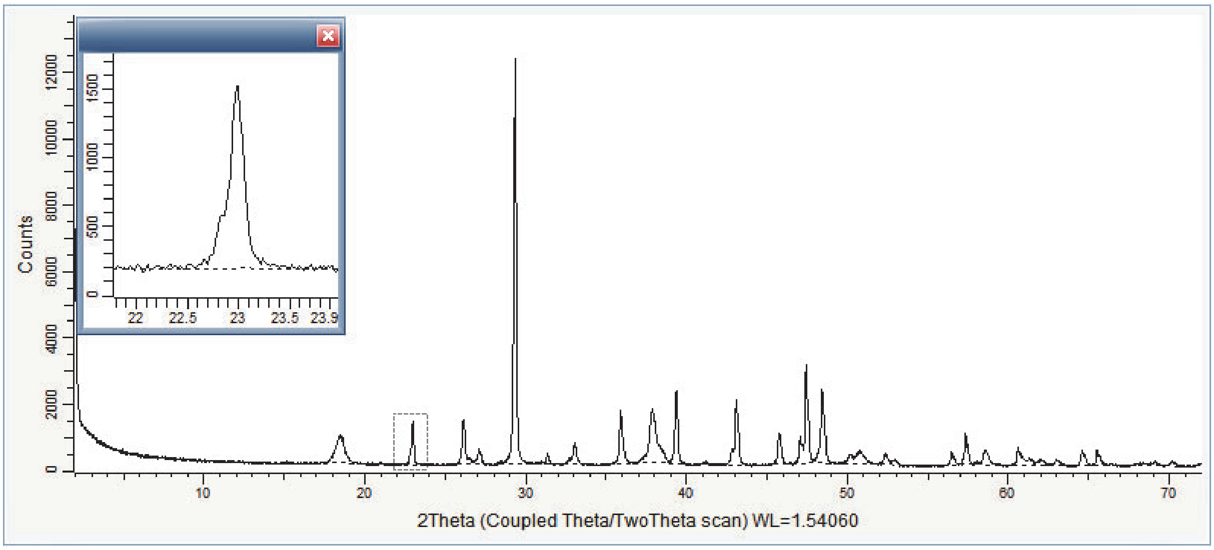


Fig. 154: Moving and resizing the PIP view

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.

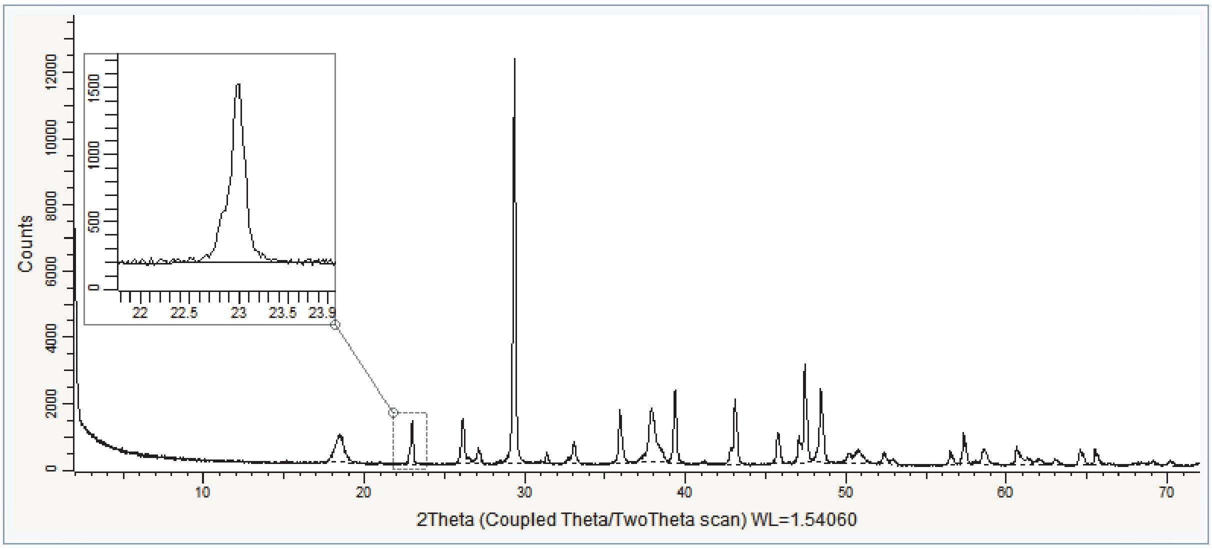


Fig. 155: PIP view inserted and linked to the original zone

<u>Case #2: Creating a VIP view</u>

1. Zoom in on the zone between the 2θ angles 37° and 47°.

VIP mode button

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.

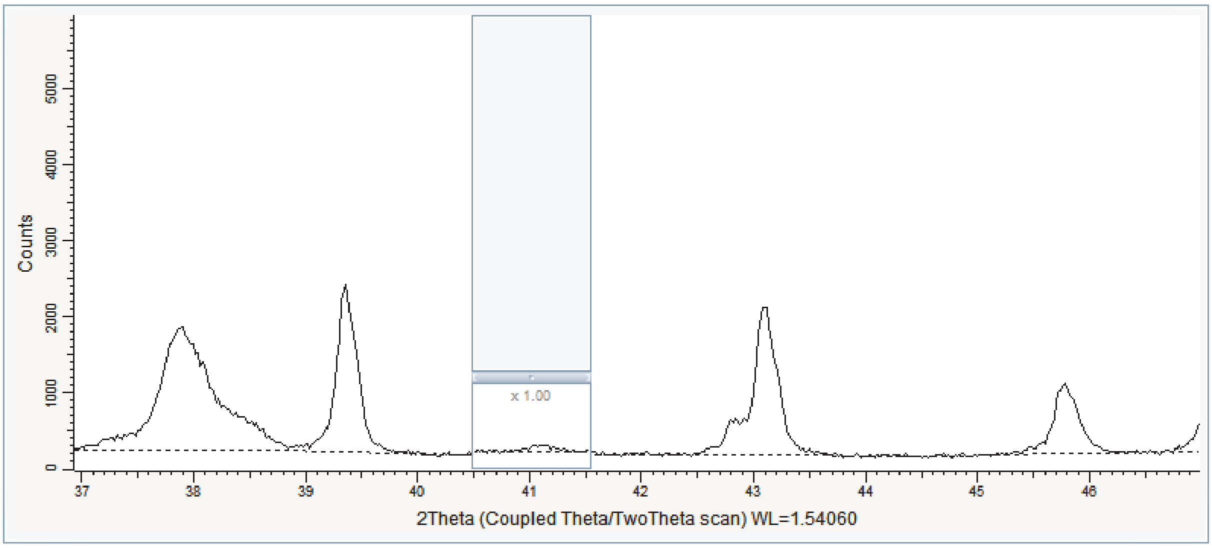


Fig. 156: Creating a VIP view

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

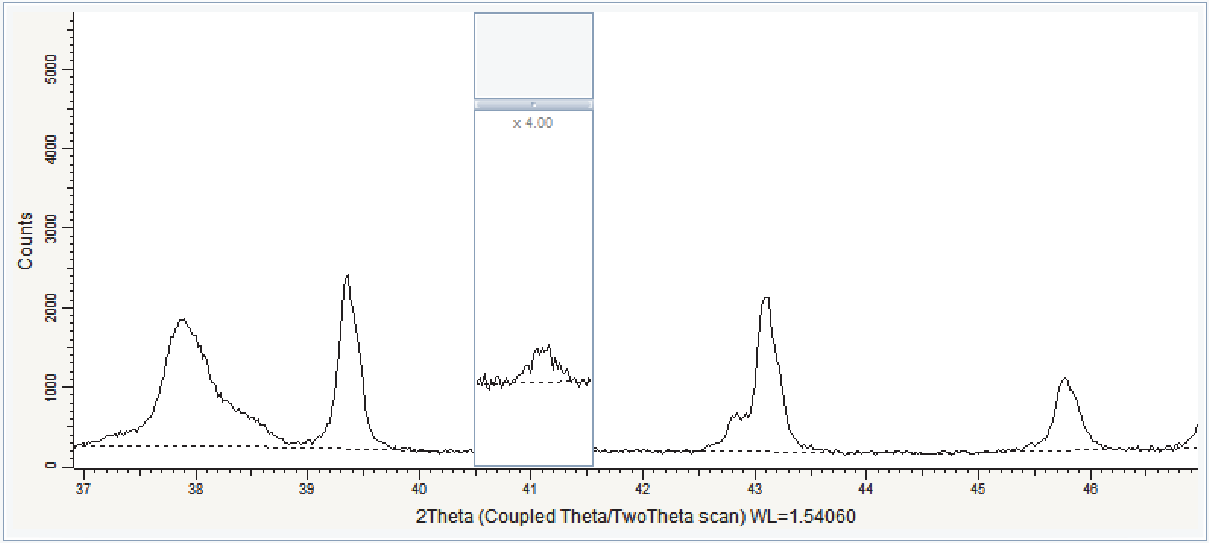


Fig. 157: Changing the scale

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

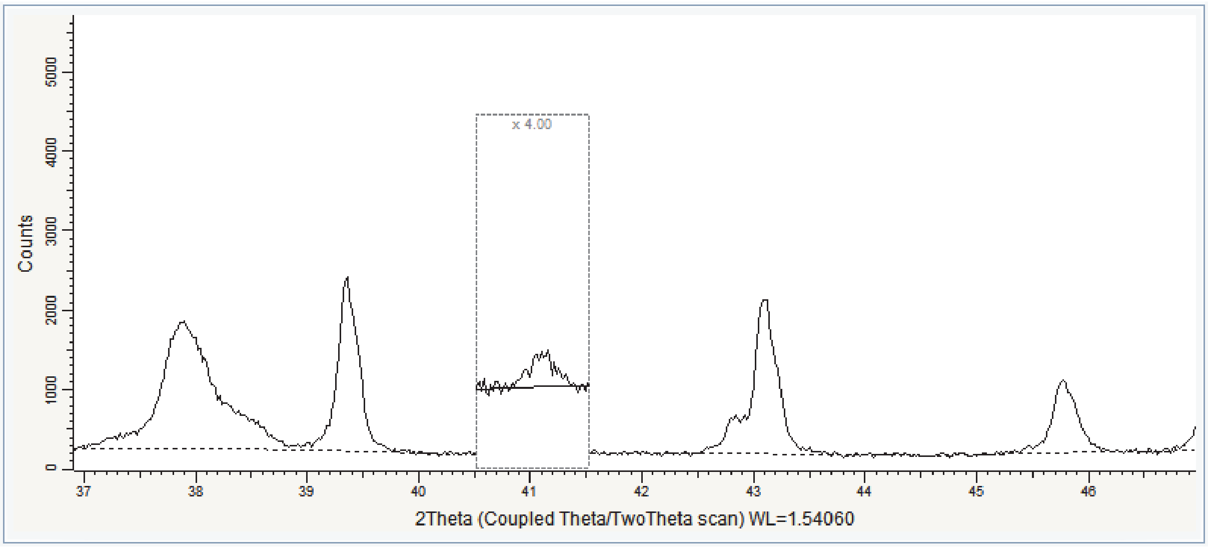
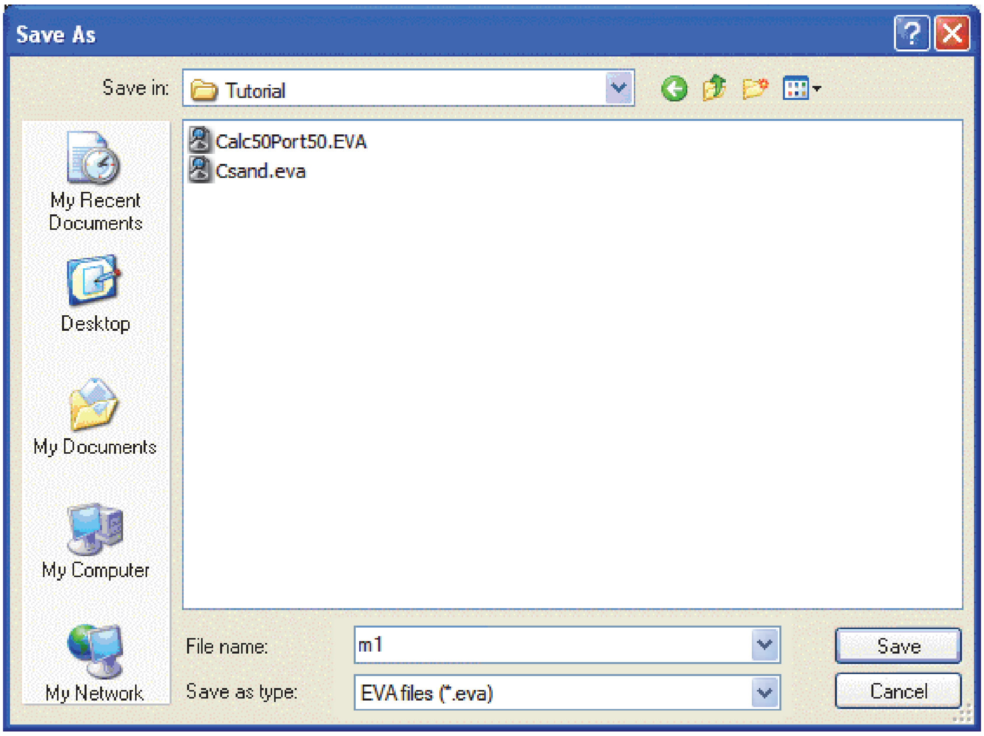


Fig. 158: VIP view inserted in the graphical view

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

Step 3: Saving

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



File name: m1

Fig. 159: Saving m1.EVA document

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=…**
3. The peak is displayed in the graphical view and added to the peak list in the data tree.

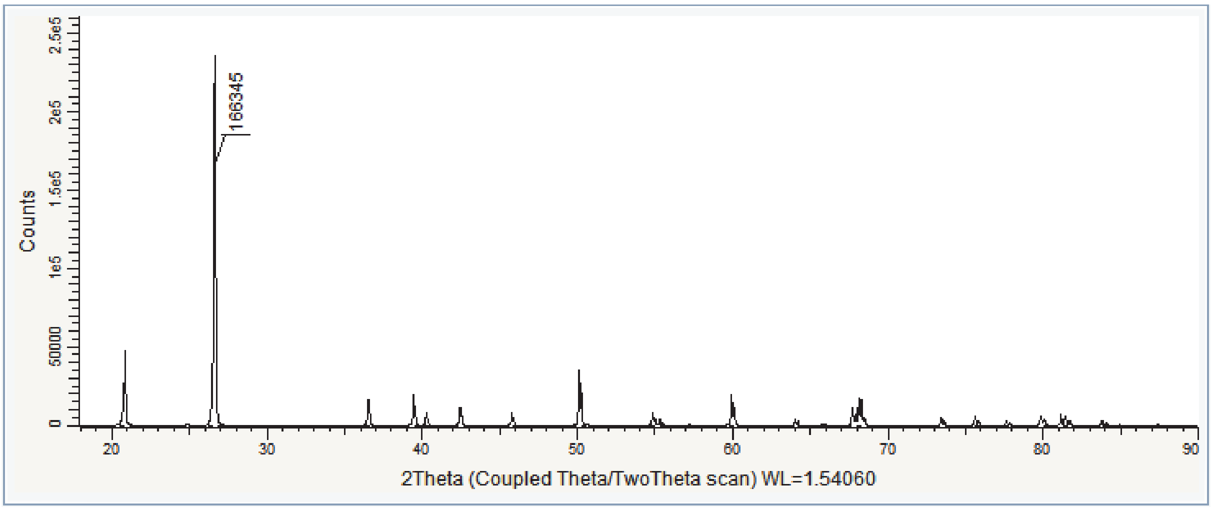


Fig. 160: Peak inserted manually in the graphical view

4. Select the peak in the data tree if necessary.
5. 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.

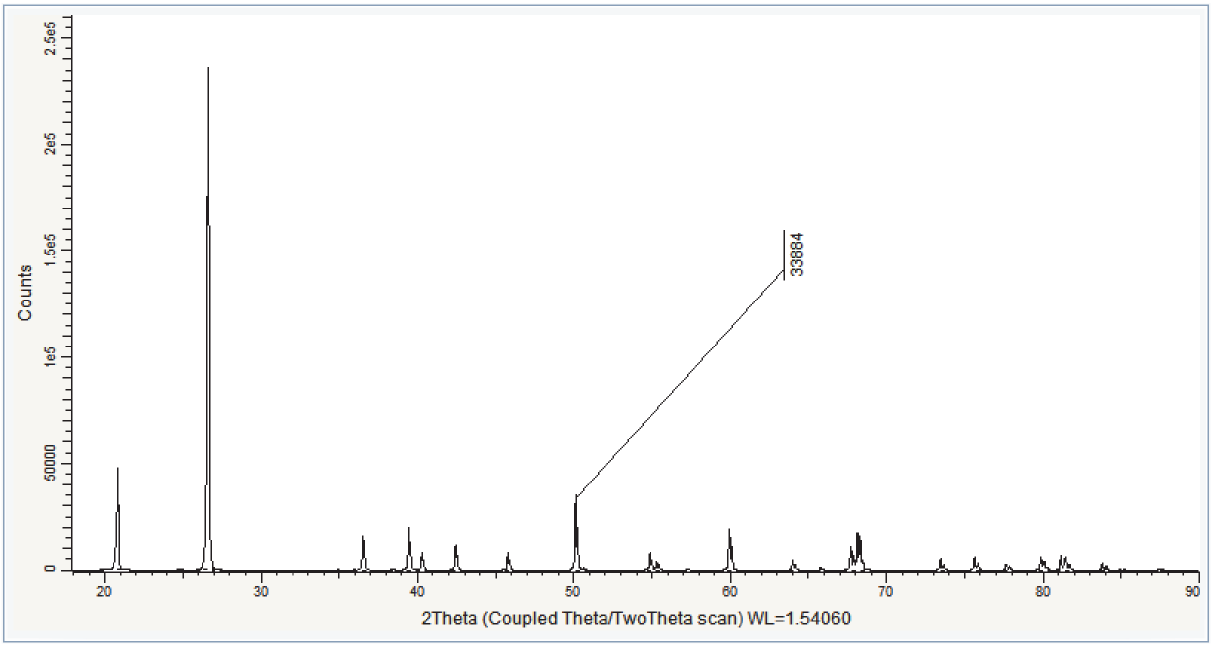


Fig. 161: Anchor and text position changed

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

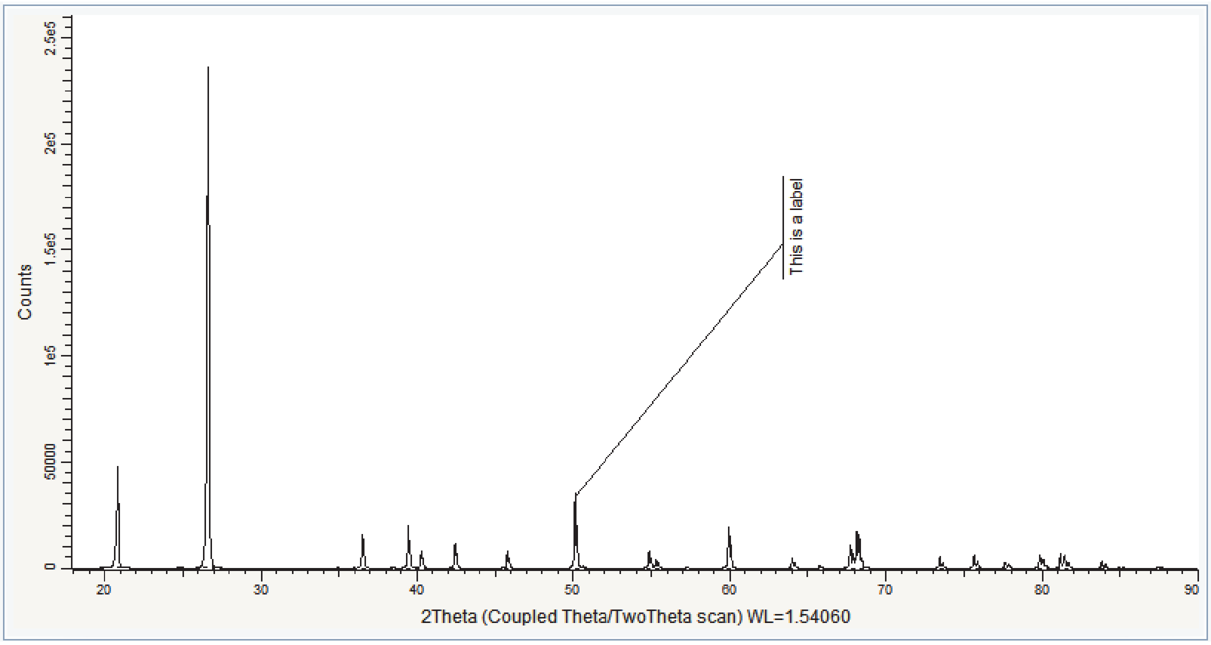


Fig. 162: Anchor and text position changed

7. Customize the resulting “label” if necessary:

- 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).
- 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).
- 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).
- 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).
- 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).
- 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).

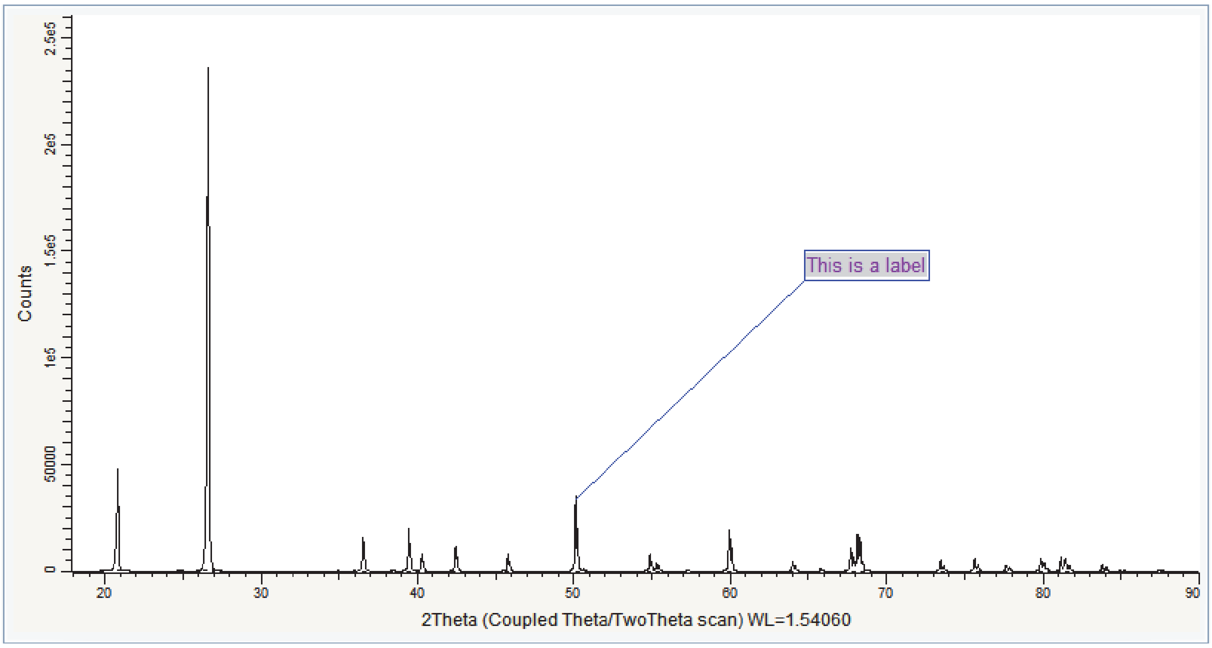


Fig. 163: Label customized according to the procedure previously described

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:

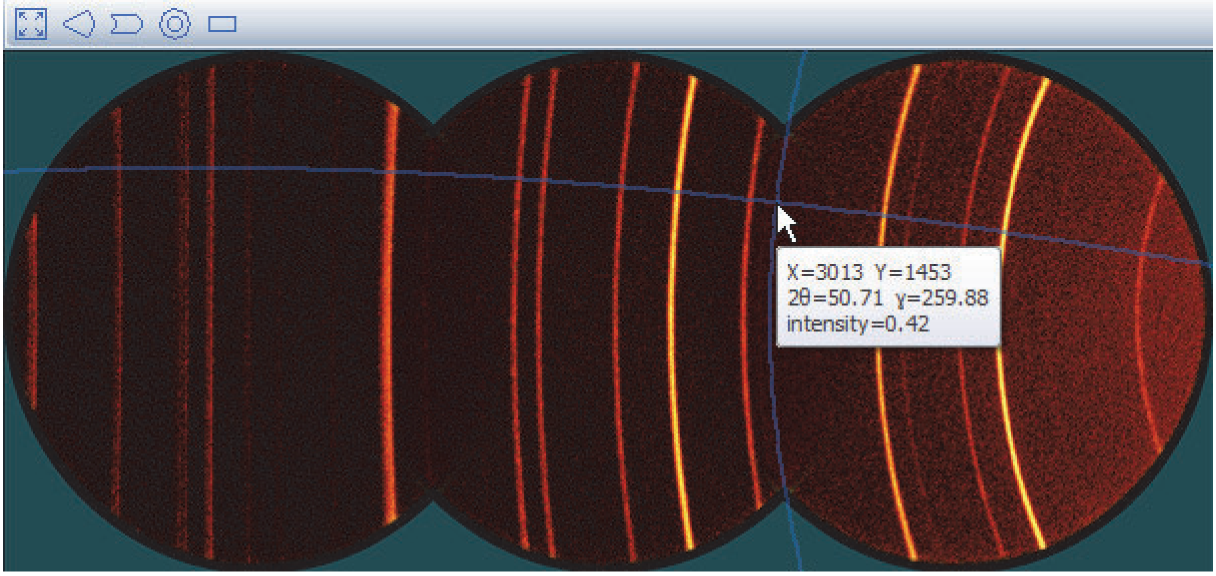
1. Creating a new EVA document and importing Cor standard.brml.
2. Selecting the integration cursor and drawing the integration area.
3. Displaying the Cursors Preview tool and integrate.

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

New button

Import from file button

1. Click **New** on the **File** menu or use the toolbar button. The EVA document will be empty.
2. Click the **Import From File** data command or the **Import From File** button. The Import From File dialog box will be displayed.
3. Search the “Tutorials\EVA”[1] 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.



X=3013 Y=1453
2θ=50.71 γ=259.88
intensity=0.42

Fig. 164: 2D Frame View after loading a measurement with three mergeable frames

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[1] 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.

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

Slice Cursor button

1. Click on the **Slice Cursor** button.
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.

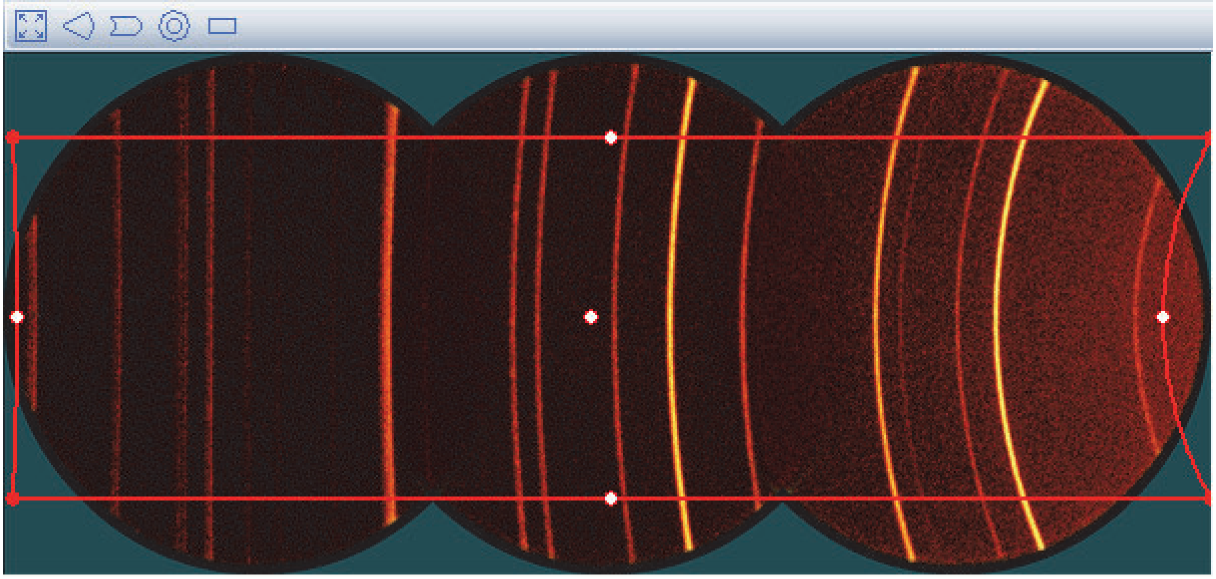


Fig. 165: Slice Cursor prepared for the subsequent integration

Step 3: Displaying the Cursors Preview Tool and Integration

1. Click on the **Cursors Preview** command in the command bar or the context menu of the slice cursor.
2. If the preview is satisfactory, click on the Integrate button to create the final integrated scan. The scan is created in a separate scan list.

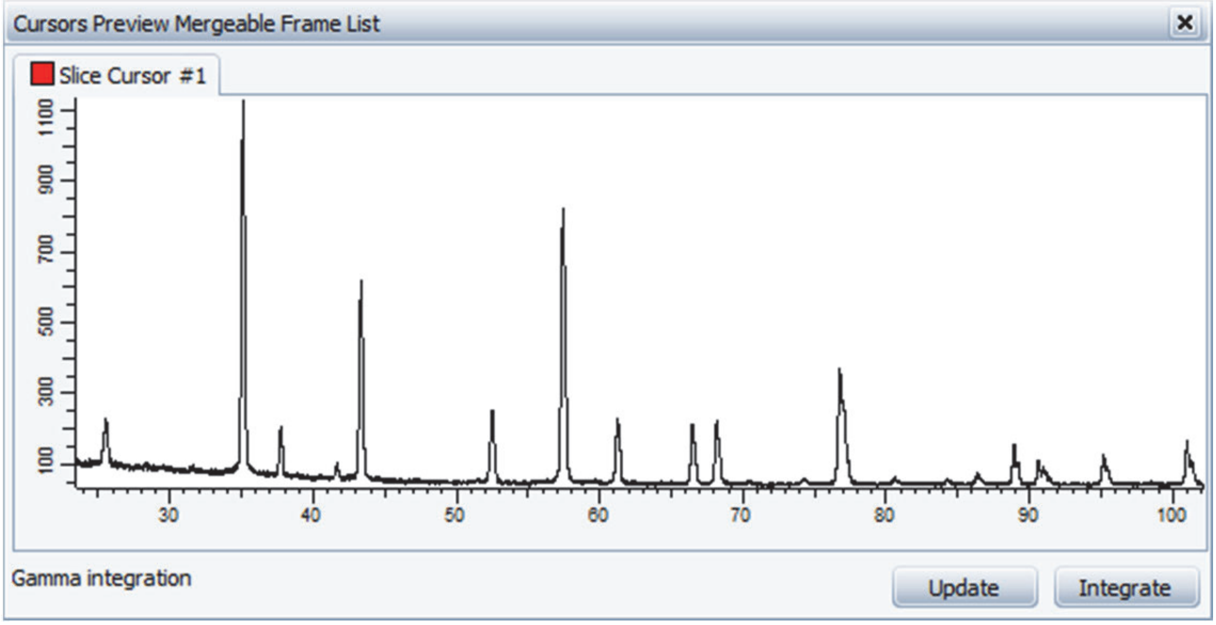


Fig. 166: The Cursors Preview Tool with the preview of the integration result

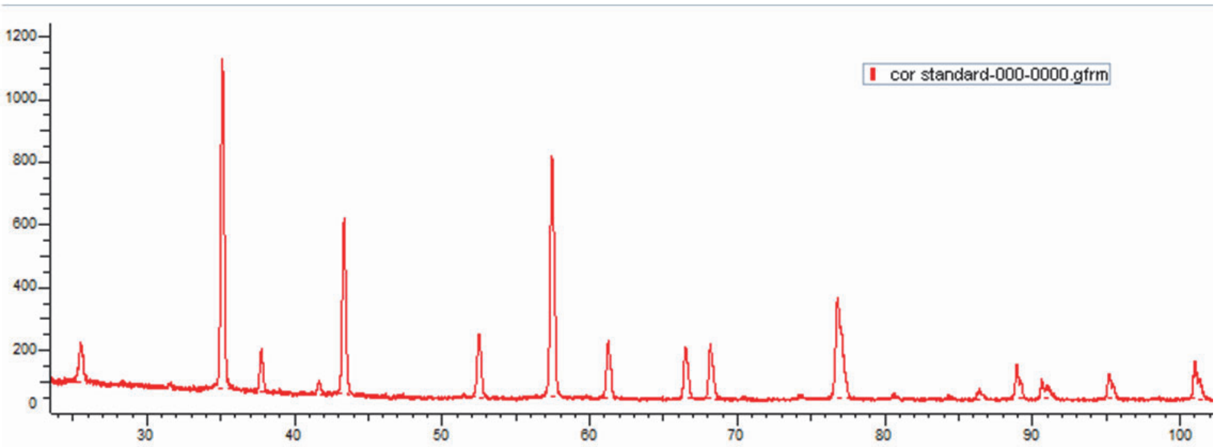


Fig. 167: The resulting integrated scan

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.

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

New button

Import from file button

1. Click **New** on the **File** menu or use the dedicated button in the toolbar. The EVA document will be empty.
2. Click the **Import From File** data command or the **Import From File** button. The Import From File 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.

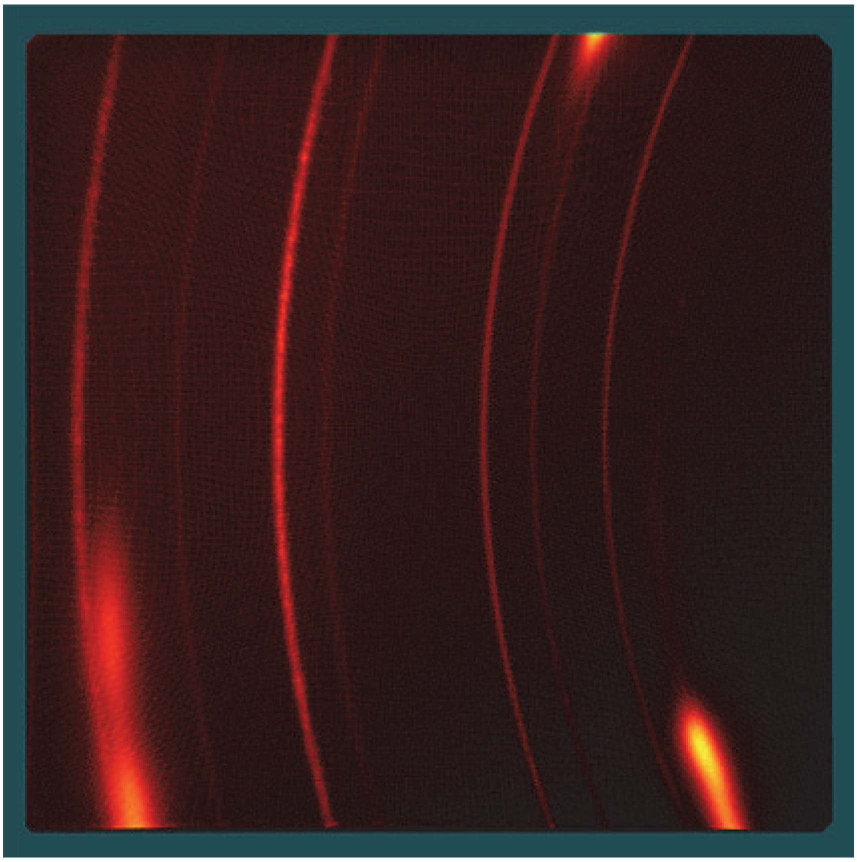


Fig. 168: 2D Frame View after loading a measurement with stackable frames

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

Ring Cursor button

1. Click on the **Ring Cursor** button.
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.

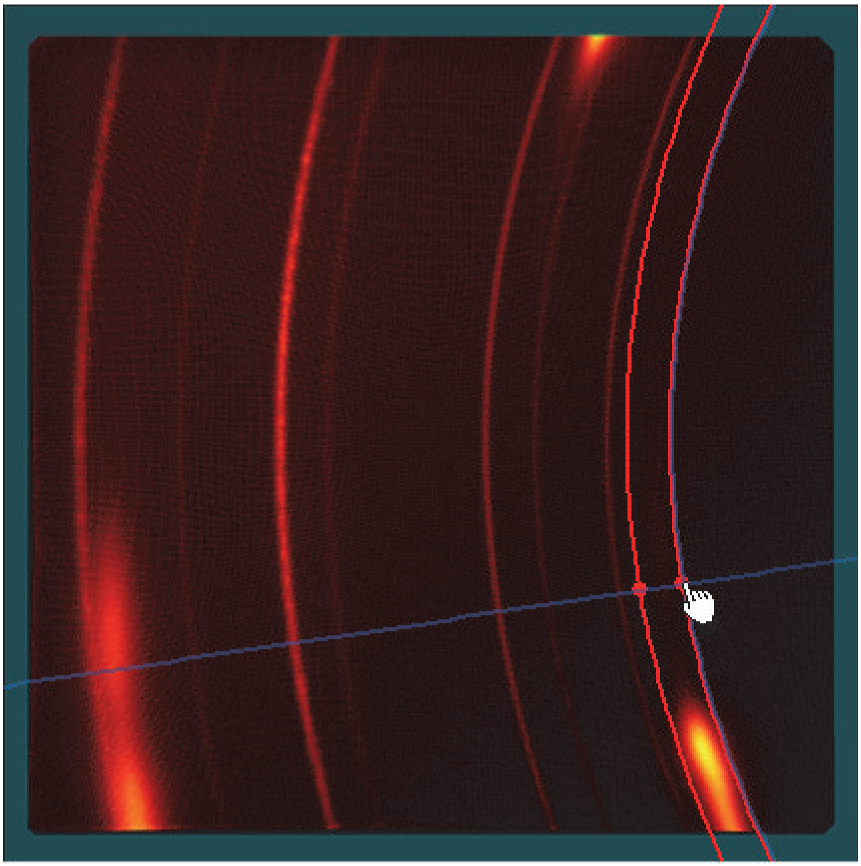
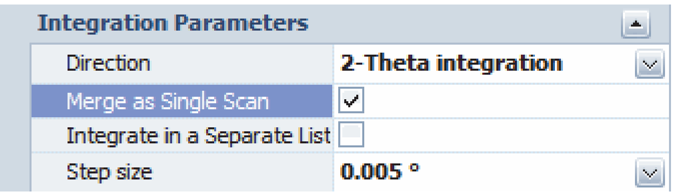


Fig. 169: Ring Cursor prepared for the subsequent integration

Step 3: Displaying the Cursors Preview Tool and Integrate

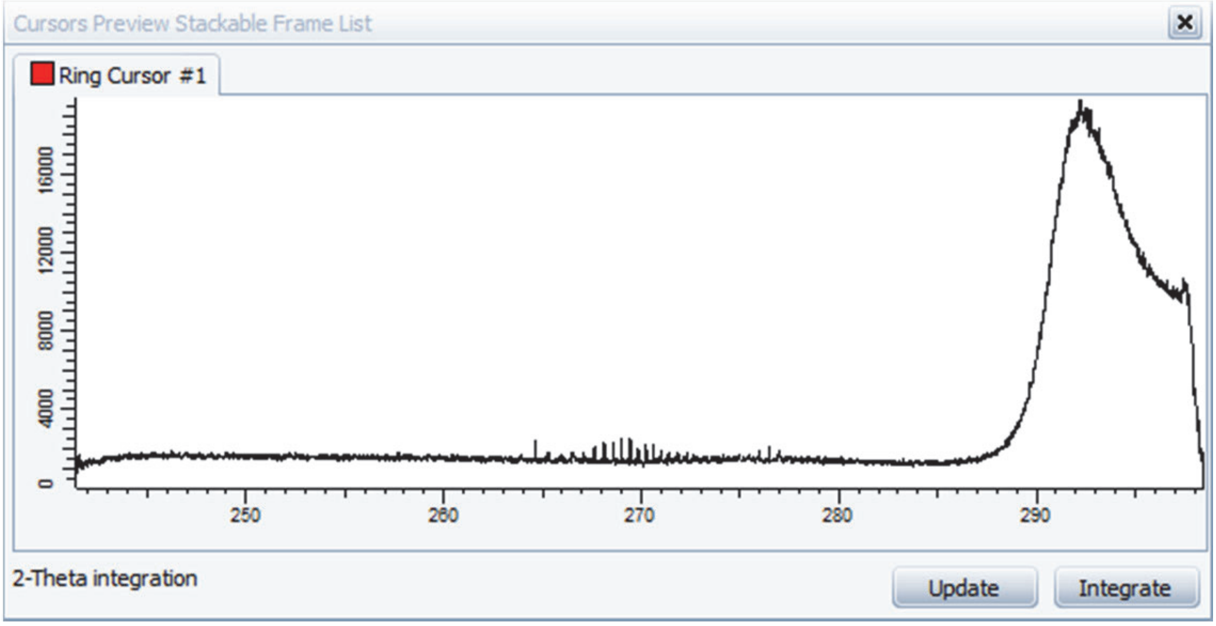
1. Change the direction of the integration in the cursor's properties to "2-Theta integration". Select "Merge as Single Scan".
2. Click on the **Cursors Preview** command in the command bar or the context menu of the ring cursor.
3. If the preview is satisfactory, click on the Integrate button to create the final integrated scan. The scan will be created in a separate scan list.



Integration Parameters

Direction	2-Theta integration
Merge as Single Scan	☑
Integrate in a Separate List	☐
Step size	0.005 °

Fig. 170: The integration parameters of the ring cursor



2-Theta integration

Fig. 171: The Cursors Preview Tool with the preview of the integration result

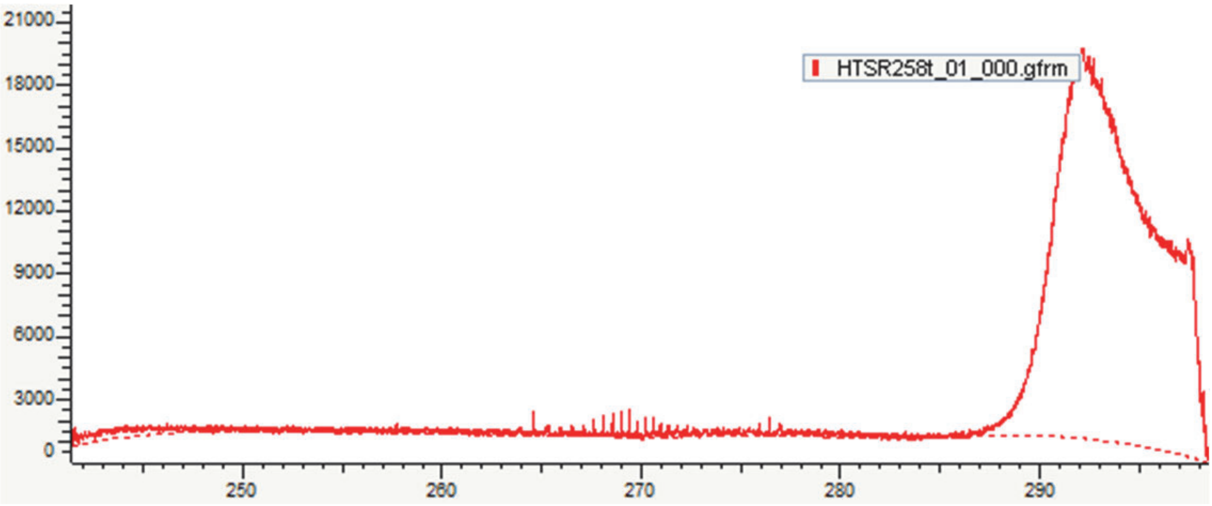


Fig. 172: The resulting integrated scan

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.

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

New button

Import from file button

1. Click **New** on the **File** menu or use the toolbar button. The EVA document will be empty.
2. Click the **Import From File** data command or the **Import From File** button. The Import From File 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.

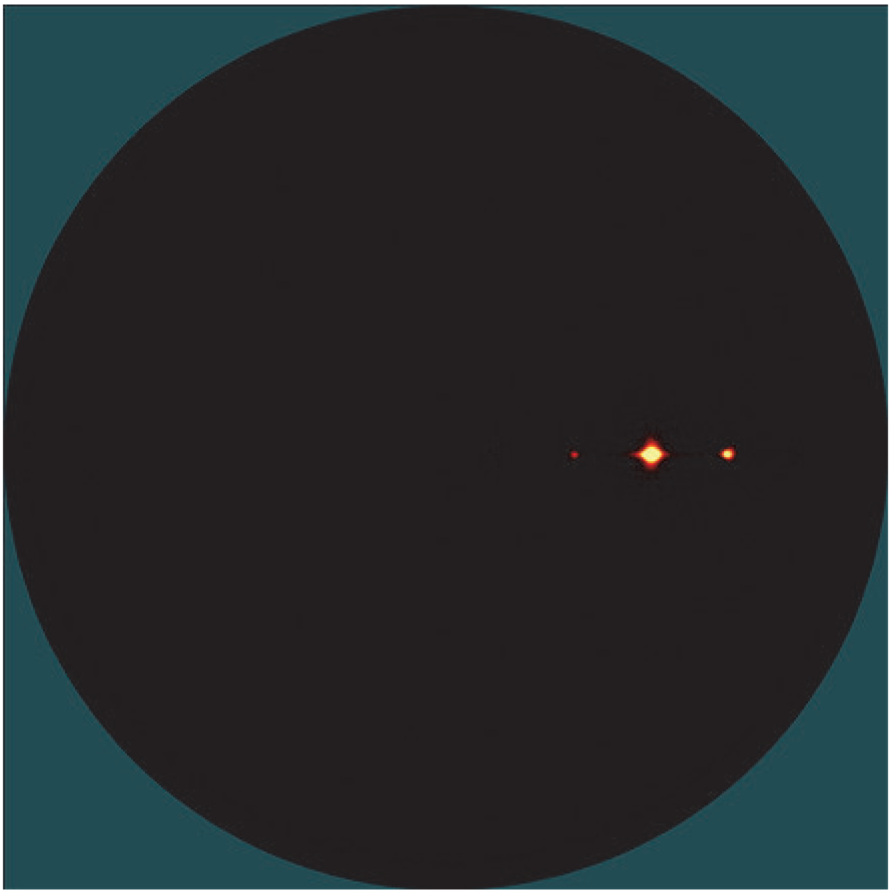


Fig. 173: 2D Frame View after loading a measurement with stackable frames

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

Area Cursor button

1. Zoom into the frame view by clicking and dragging the mouse to make the bright spots clearly visible.
2. Click on the **Area Cursor** button.
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.

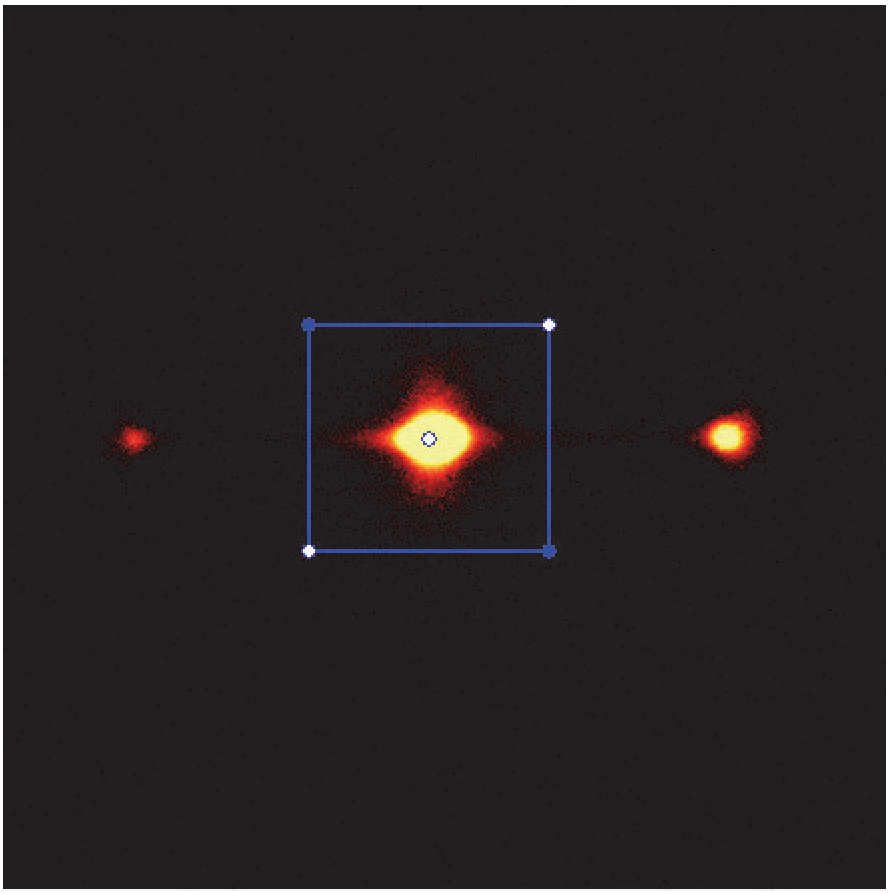
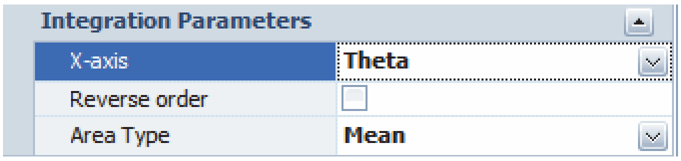


Fig. 174: Ring Cursor prepared for the subsequent integration

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 on the **Cursors Preview** command in the command bar or the context menu of the slice cursor.
3. If the preview is satisfactory, click on the Integrate button to create the final integrated scan. The scan will be created in a separate scan list.



Integration Parameters

X-axis	**Theta**
Reverse order	☐
Area Type	**Mean**

Fig. 175: The integration parameters of the ring cursor

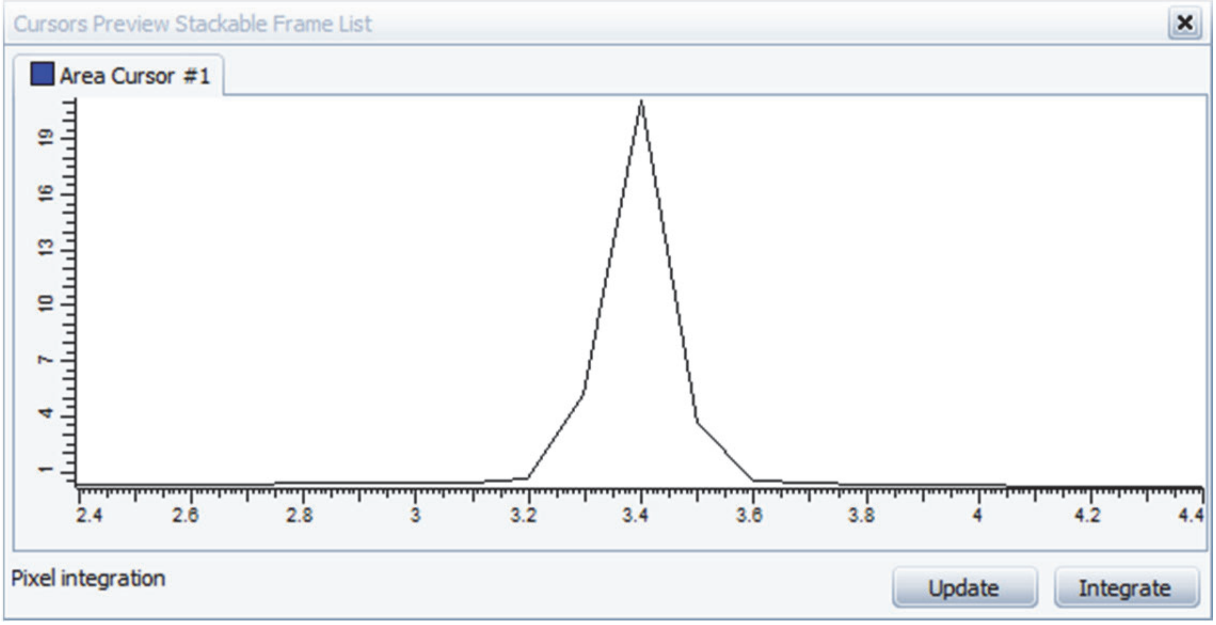


Fig. 176: The Cursors Preview Tool with the preview of the integration result

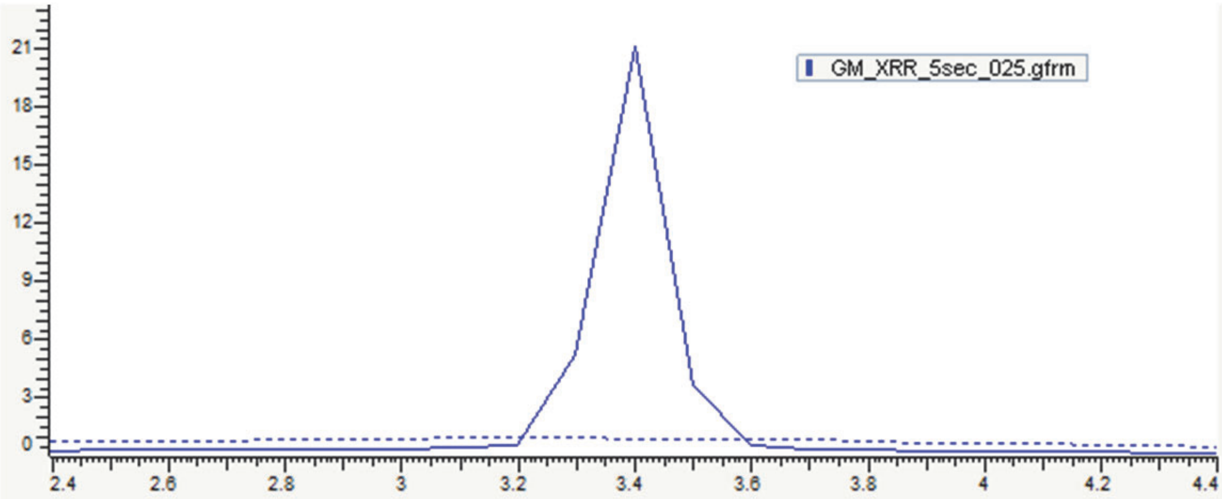


Fig. 177: The resulting integrated scan

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:

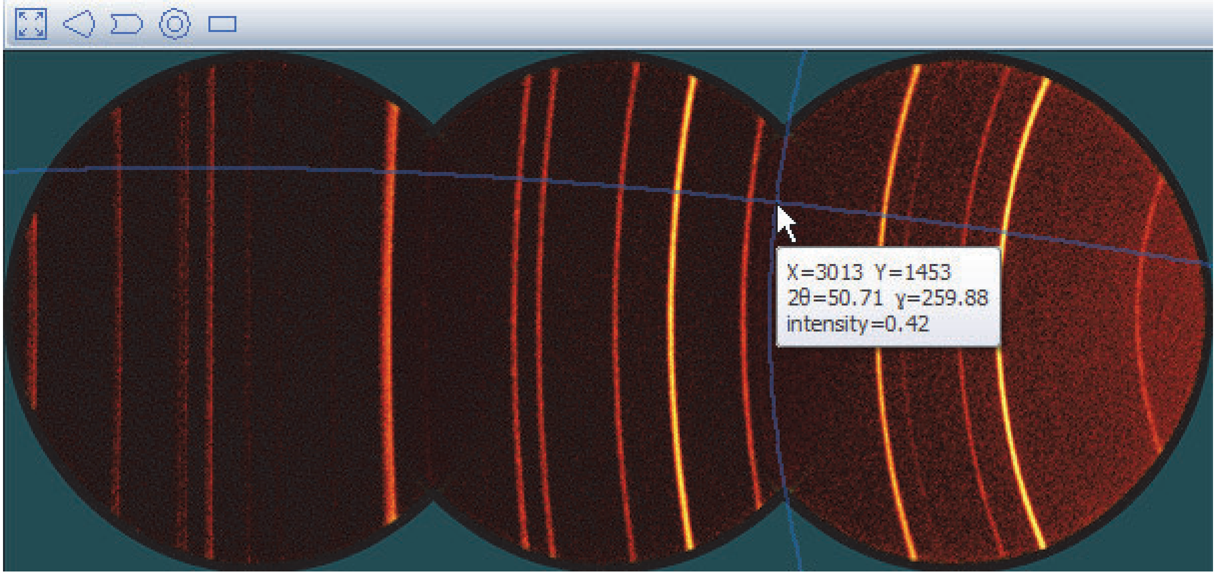
1. Creating a new EVA document and importing Cor standard.brml.
2. Check the integration with the Full Frame cursor.
3. Changing the default mask to exclude non-exposed areas.
4. Selecting the integration cursor and integrate.

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

New button

Import from file button

1. Click **New** on the **File** menu or use the toolbar button. The EVA document will be empty.
2. Click the **Import From File** data command or the **Import From File** button. The Import From File 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.



```
X=3013 Y=1453
2θ=50.71 γ=259.88
intensity=0.42
```

Fig. 178: 2D Frame View exhibiting non-exposed areas around the frames

Step 2: Check the Integration with the Full Frame Cursor

Full Frame Cursor button

1. Click on the **Full Frame Cursor** button in the command bar. The whole merged frame is marked for integration.
2. Click the **Integrate Cursor** command in the command bar or the context menu of the cursor to create the integrated scan. 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.

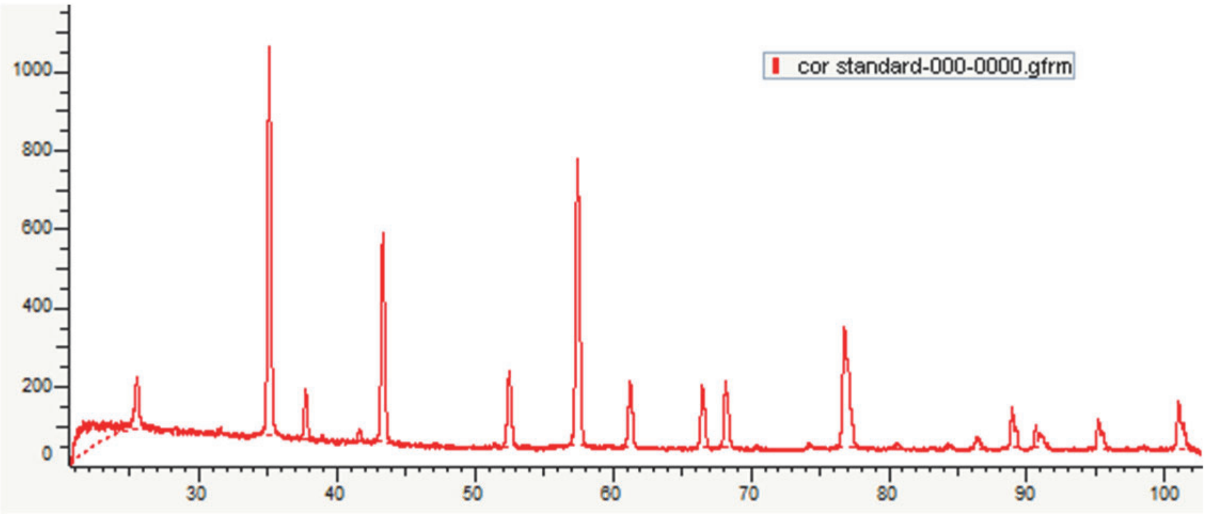
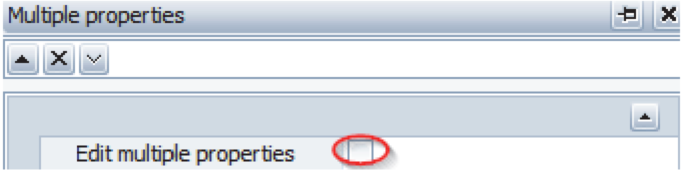


Fig. 179: Integrated scan with intensity drop at low angles due to mask misalignment

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

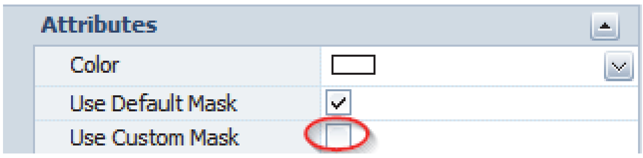
1. Click on the **Edit Multiple Properties** check mark to display the combined properties for all three frames.



Multiple properties

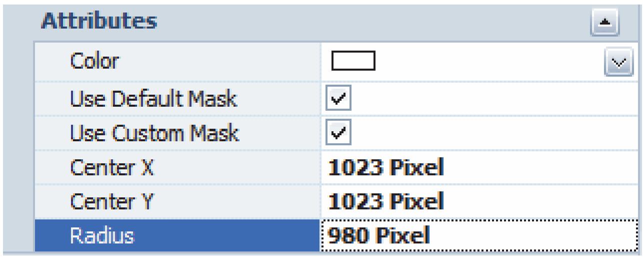
Edit multiple properties ☐

2. Click the **Use Custom Mask** check mark to display the mask properties:



Attributes	
Color	▭
Use Default Mask	☑
Use Custom Mask	☐

3. Change the Radius to 980 pixel:



Attributes	
Color	▭
Use Default Mask	☑
Use Custom Mask	☑
Center X	1023 Pixel
Center Y	1023 Pixel
Radius	980 Pixel

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

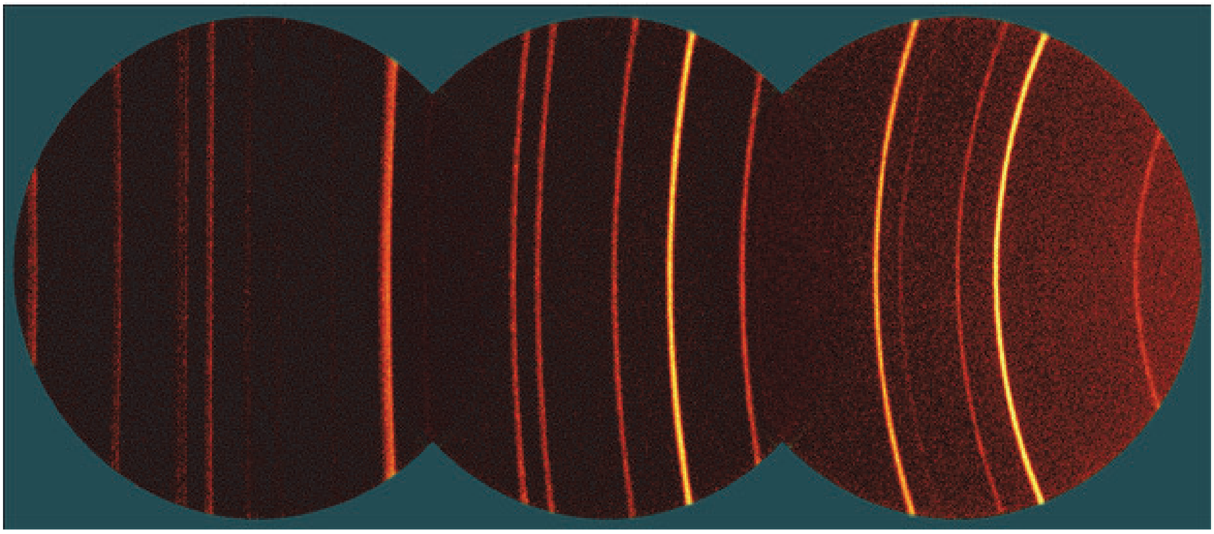


Fig. 180: 2D Frame View with an adjusted default mask

Step 4: Selecting the Integration Cursor and Integration

Full Frame Cursor button

1. Click on the **Full Frame Cursor** button in the command bar. The whole merged frame is marked for integration.
2. Click the **Integrate Cursor** command in the command bar or the context menu of the cursor to create the integrated scan. The scan is created in a separate scan list.

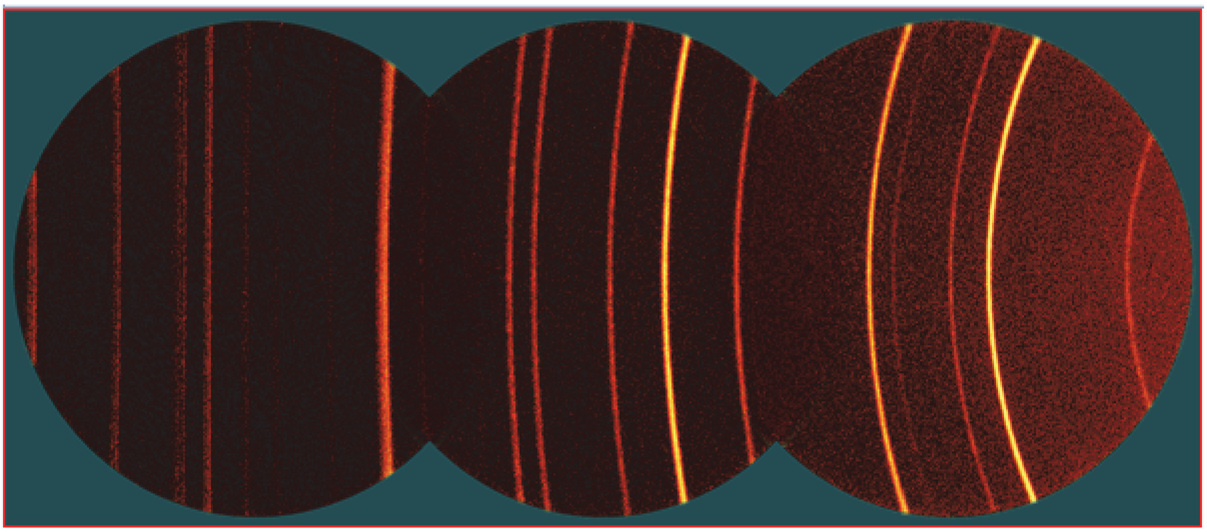


Fig. 181: 2D Frame View with the full frame cursor drawn along its edges

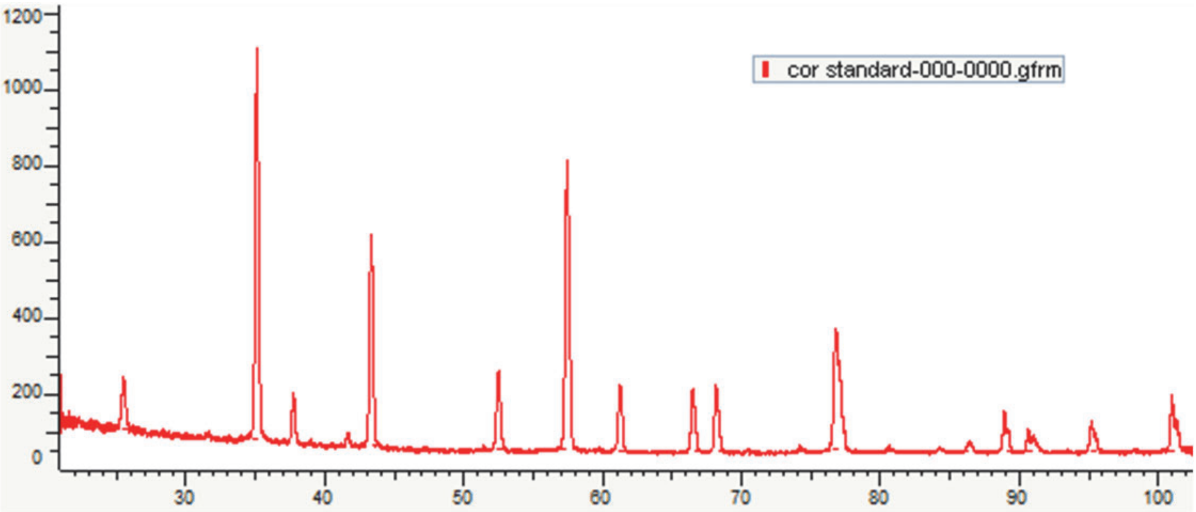


Fig. 182: The resulting integrated scan

Using Printing Options

This chapter will describe how to use some printing options.

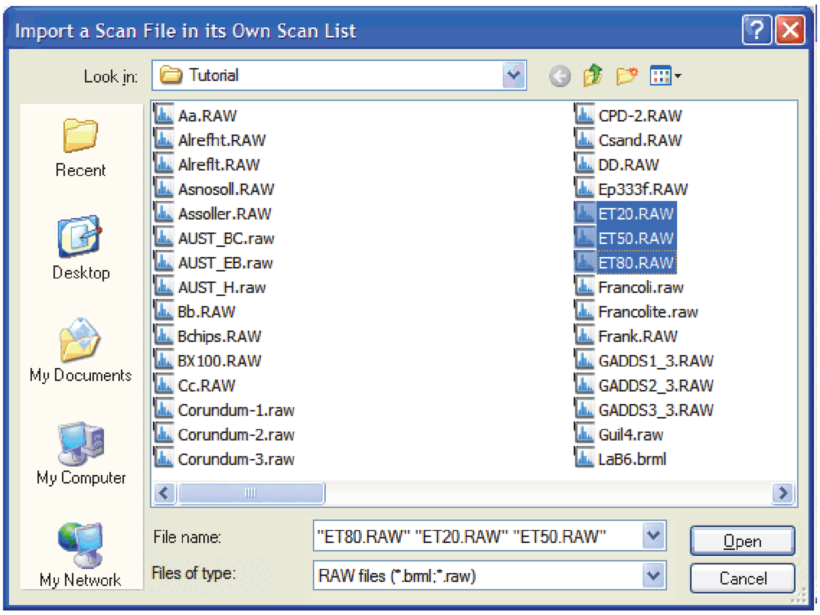
Vertical Table

“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.

New button

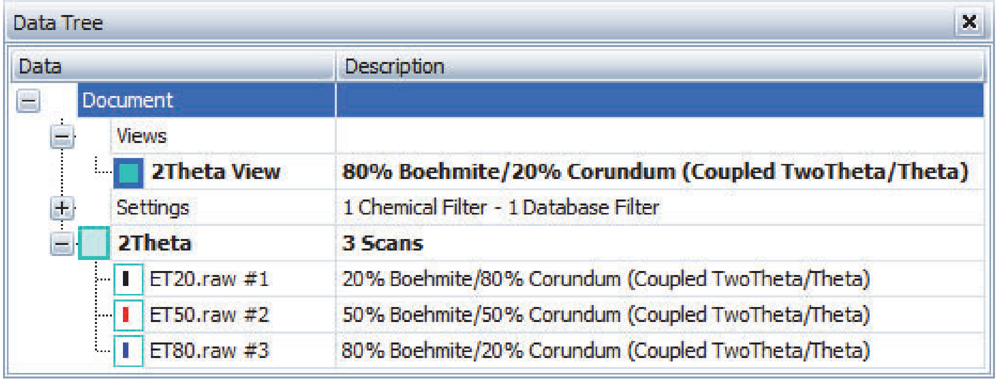
Import from file button

1. Click **New** on the **File** menu or use the button in the toolbar. The EVA document will be empty.
2. Click the **Import from file** data command or the **Import from file** button. The Import from files dialog box will be displayed.
3. Search the Tutorials/EVA[1] directory and select the ET20.RAW, ET50.RAW and ET80.RAW files.
4. Click **Open**. The scans will be displayed in the graphical view of the EVA document and added to the data tree.



File name: "ET80.RAW" "ET20.RAW" "ET50.RAW"
Files of type: RAW files (*.brml;*.raw)

Fig. 183: Import a Scan File dialog box



Data	Description
Document	
Views	
2Theta View	80% Boehmite/20% Corundum (Coupled TwoTheta/Theta)
Settings	1 Chemical Filter - 1 Database Filter
2Theta	3 Scans
ET20.raw #1	20% Boehmite/80% Corundum (Coupled TwoTheta/Theta)
ET50.raw #2	50% Boehmite/50% Corundum (Coupled TwoTheta/Theta)
ET80.raw #3	80% Boehmite/20% Corundum (Coupled TwoTheta/Theta)

Fig. 183: ET20.RAW, ET50.RAW and ET80.RAW added to the data tree

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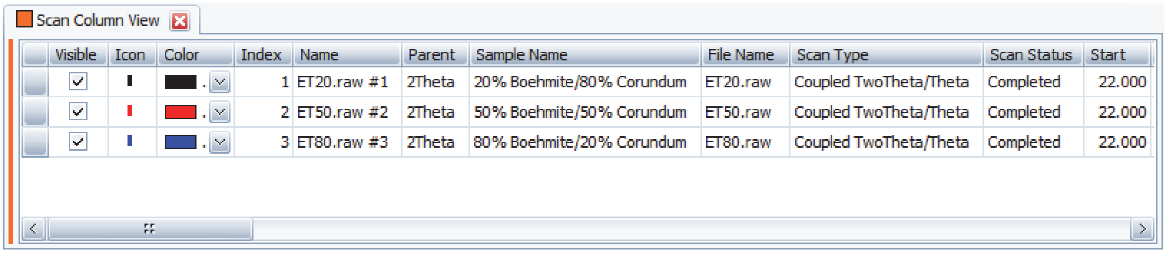
[1] The directory path to the EVA tutorial files is ”C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials” under Windows XP and ”C:\ProgramData\Bruker AXS\Tutorials” under Windows 7.
To access the folder with the explorer, select “Display hidden files and folders” in the Folders options.

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 —
   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.

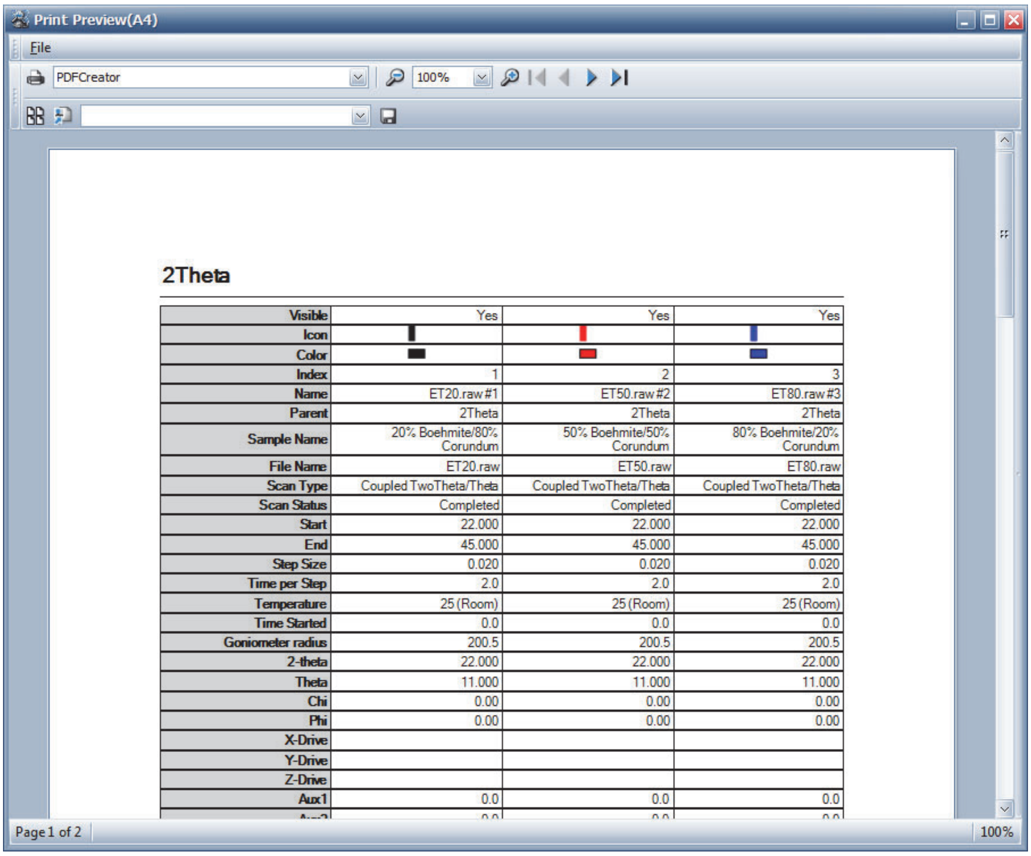
   A Scan Column View will be created.



	Visible	Icon	Color	Index	Name	Parent	Sample Name	File Name	Scan Type	Scan Status	Start
	☑	▮	⬛	1	ET20.raw #1	2Theta	20% Boehmite/80% Corundum	ET20.raw	Coupled TwoTheta/Theta	Completed	22.000
	☑	▮	🟥	2	ET50.raw #2	2Theta	50% Boehmite/50% Corundum	ET50.raw	Coupled TwoTheta/Theta	Completed	22.000
	☑	▮	🟦	3	ET80.raw #3	2Theta	80% Boehmite/20% Corundum	ET80.raw	Coupled TwoTheta/Theta	Completed	22.000

7. 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.
8. 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.
9. Check the view is printable.
10. 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.



2Theta

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

Fig. 184: Vertical table visible in the print preview

Repeat Columns

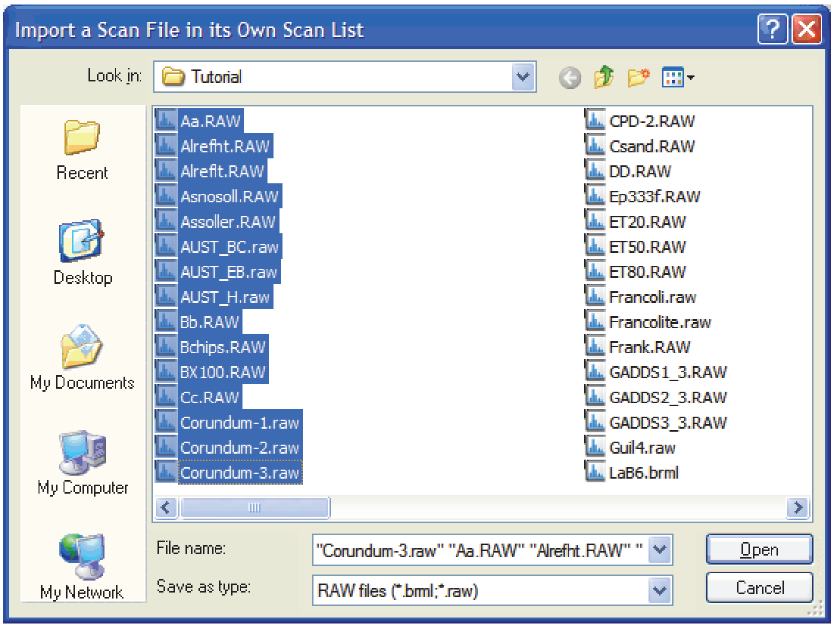
“Repeat Columns” is an option which allows repeating the N first columns of a column view on each “row”. It proves useful when printing a column view with numerous objects and properties.

The “Repeat Columns” feature is available up to version 3.1

New button

Import from file button

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 file** data command or the **Import from file** button. The Import from files dialog box will be displayed.
3. Search the Tutorials/EVA[1] 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.



Look in: Tutorial

Aa.RAW
Alrefht.RAW
Alrefit.RAW
Asnosoll.RAW
Assoller.RAW
AUST_BC.raw
AUST_EB.raw
AUST_H.raw
Bb.RAW
Bchips.RAW
BX100.RAW
Cc.RAW
Corundum-1.raw
Corundum-2.raw
Corundum-3.raw
CPD-2.RAW
Csand.RAW
DD.RAW
Ep333f.RAW
ET20.RAW
ET50.RAW
ET80.RAW
Francoli.raw
Francolite.raw
Frank.RAW
GADDS1_3.RAW
GADDS2_3.RAW
GADDS3_3.RAW
Guil4.raw
LaB6.brml

File name: "Corundum-3.raw" "Aa.RAW" "Alrefht.RAW" "

Save as type: RAW files (*.brml;*.raw)

Fig. 185: Import a Scan File dialog box

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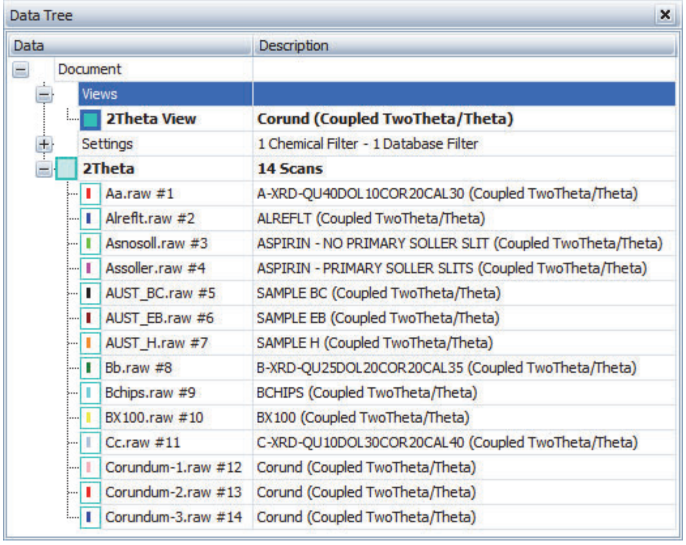
[1] The directory path to the EVA tutorial files is ″C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials″ under Windows XP and ″C:\ProgramData\Bruker AXS\Tutorials″ under Windows 7.
To access the folder with the explorer, select “Display hidden files and folders” in the Folders options.

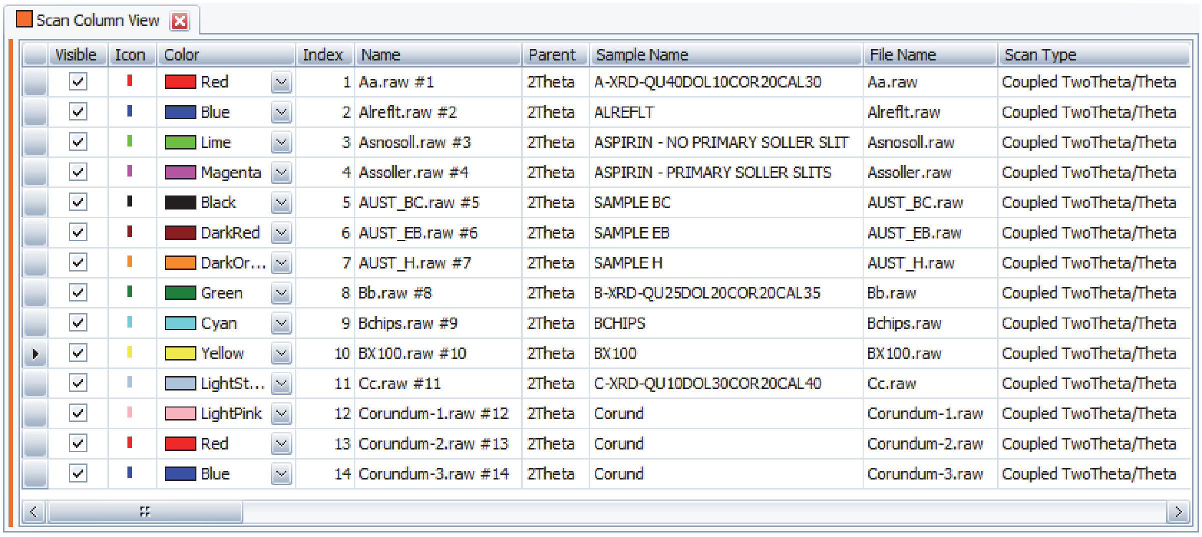


Data	Description
Document	
Views	
2Theta View	**Corund (Coupled TwoTheta/Theta)**
Settings	1 Chemical Filter - 1 Database Filter
2Theta	**14 Scans**
Aa.raw #1	A-XRD-QU40DOL10COR20CAL30 (Coupled TwoTheta/Theta)
Alreflt.raw #2	ALREFLT (Coupled TwoTheta/Theta)
Asnosoll.raw #3	ASPIRIN - NO PRIMARY SOLLER SLIT (Coupled TwoTheta/Theta)
Assoller.raw #4	ASPIRIN - PRIMARY SOLLER SLITS (Coupled TwoTheta/Theta)
AUST_BC.raw #5	SAMPLE BC (Coupled TwoTheta/Theta)
AUST_EB.raw #6	SAMPLE EB (Coupled TwoTheta/Theta)
AUST_H.raw #7	SAMPLE H (Coupled TwoTheta/Theta)
Bb.raw #8	B-XRD-QU25DOL20COR20CAL35 (Coupled TwoTheta/Theta)
Bchips.raw #9	BCHIPS (Coupled TwoTheta/Theta)
BX100.raw #10	BX100 (Coupled TwoTheta/Theta)
Cc.raw #11	C-XRD-QU10DOL30COR20CAL40 (Coupled TwoTheta/Theta)
Corundum-1.raw #12	Corund (Coupled TwoTheta/Theta)
Corundum-2.raw #13	Corund (Coupled TwoTheta/Theta)
Corundum-3.raw #14	Corund (Coupled TwoTheta/Theta)

Fig. 186: 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 —
   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.

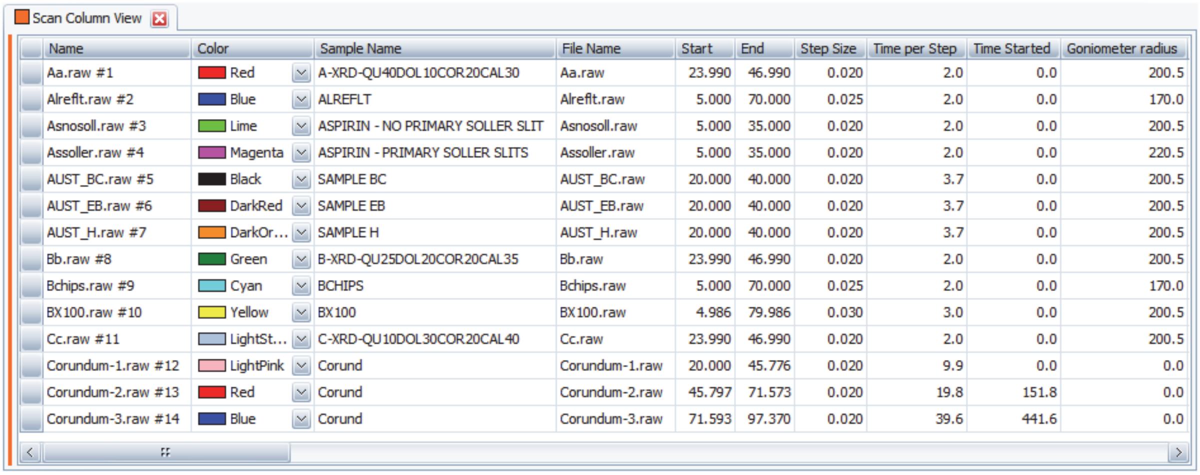
   A Scan Column View will be created.



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

Fig. 187: 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.

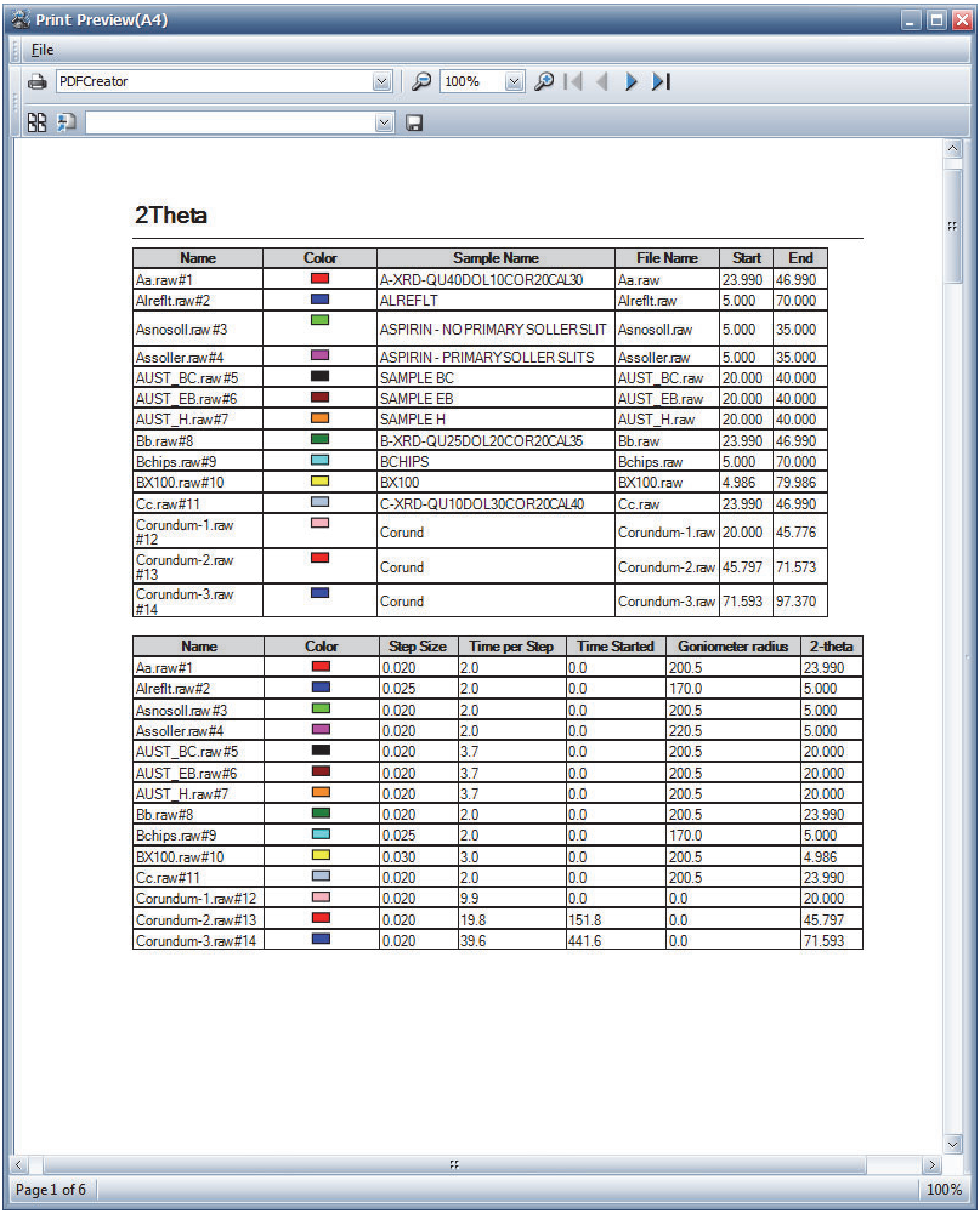


Name	Color	Sample Name	File Name	Start	End	Step Size	Time per Step	Time Started	Goniometer radius
Aa.raw #1	Red	A-XRD-QU40DOL10COR20CAL30	Aa.raw	23.990	46.990	0.020	2.0	0.0	200.5
Alrefit.raw #2	Blue	ALREFLT	Alrefit.raw	5.000	70.000	0.025	2.0	0.0	170.0
Asnosoll.raw #3	Lime	ASPIRIN - NO PRIMARY SOLLER 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

Fig. 188: Scan column view with a new column configuration: file name and color in first

8. 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.
9. 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.
10. Check the view is printable.
11. 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

Fig. 189: The two first columns “Name” and “Color” are repeated in the print preview