

DIFFRAC.SUITE

Tutorial

DIFFRAC.EVALUATION PACKAGE DIFFRAC.EVA

Original Instructions

Innovation with Integrity

XRD

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

All configurations and specifications are subject to change without notice.

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1 Performing a Search/Match Operation

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

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

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

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

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

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

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

Steps

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

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

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

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* 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.

🔏 Import from Files				
Solution Struker AXS	• Tut	orials 🕨 EVA 🕨	✓ ✓ Search : EVA	Q
Organize 🔻 New folder			8	* 🔳 📀
 My Favorites Desktop Downloads Recent Places EVA My Documents Libraries Documents Music Pictures 		D Frame Data A.raw A.raw A.raw A.refht.raw Anrefht.raw Asnosoll.raw Assoller.raw AUST_BC.raw AUST_EB.raw AUST_EB.raw AUST_H.raw B.raw B.raw B.raw B.Raw AUST_A.raw A.SUD.raw A.	Cc.raw Corundum-1.raw Corundum-2.raw Corundum-3.raw CPD-2.raw CSand.raw DD.raw Description.txt Ep333f.raw ET20.raw ET20.raw ES200.raw	Francolite.raw Frank.raw Guil4.raw KCP.raw La86.brml m1.raw m2.raw m3.raw Mineral_Mixtur Nh4no3.raw Niore.raw
🚼 Videos	-	BX100.txt	ET80.raw	E Pchips.raw
File	∢ name	Bchips.raw	 ✓ Measurement fil Open 	► les (*.brml;*.rav Cancel

Figure 1.1: Importing the Bchips.Raw file

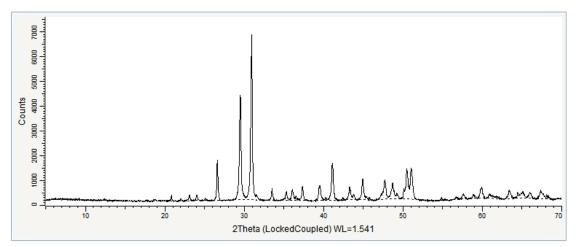


Figure 1.2: Bchips.RAW file imported in the graphical view

1.2 Step 2: Setting the Search Parameters

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



1. Click Search / Match in the Data Command panel

— or — click the **Search/Match** button on the Search/Match toolbar

— or —

right-click the scan, click **Tool** on the context menu and then **Search / Match** on the related submenu.

■ The Search / Match dialog box will be displayed.

Search / Match Bchips.raw #1	×
Databases Match Lists Names Options	
PDF-4+ 2016 RDB	to 📃
DB Filter	Q
Chemical	Aatch

Figure 1.3: Search/match dialog box

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

Search / Match Bchips.raw #1	×
Databases Match Lists Names Options	
Criterion:	
2: Neutral	
Whole Range 💿	
Subrange 🔵	

Figure 1.4: Options tab



- 6. In the **Databases** tab, click the **Match** button.
- ⇒ The candidates are listed in the **Search list** tab of the Data Tree Panel.

1.3 Step 3: Matching Procedure

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

\odot	*	E	FOM	Match	%	Name	ID	Quality	Status	I/ICor	Inc
	Ð		33,18 %		79	Dolomite	PDF 04-008-0789	®	👩 Primary	2,53	^
		2	24,81 %		61	Calcium Magnesium	PDF 04-012-6929	🛞	Primary	2,99	::
	Ð	3	22,42 %		60	Calcite, magnesian,	PDF 01-089-1304	🛞	Primary	3,12	
		4	19,58 %		81	Minrecordite	PDF 00-035-0667	🛞	Primary		
		7	16,90 %		42	Calcium Magnesium	PDF 04-012-6930	🛞	Primary	2,84	
	Ð	12	14,23 %		37	Calcite	PDF 04-012-0489	1	Primary	3,45	
		13	14,09 %		41	Calcite, magnesian,	PDF 01-089-1305	🛞	Primary	3,07	
	Ð	14	1 <mark>4,04 %</mark>		72	Dolomite, ferroan	PDF 04-011-9834	1	Primary	2,77	
		18	12,33 %		79	Dolomite	PDF 00-001-0942	📵	🚂 Deleted		
		21	10,90 %		23	quartz-alpha, syn	PDF 04-018-2594	1	Primary	3,25	
	Ð	22	10,62 %		25	quartz-alpha Fe-dop	PDF 04-007-0522	📵	Primary	1,04	
		25	9,99 %		21	Quartz-alpha, syn	PDF 04-018-2595	1	Primary	3,33	
		27	9,86 %		28	Dolomite	PDF 04-011-9829	1	Primary	2,56	
	Ð	30	9,33 %		36	Ankerite, magnesian	PDF 04-017-1391	🛞	Primary	3	
		31	9,28 %		20	Quartz-alpha, syn	PDF 04-018-2596	1	Primary	3,43	
		32	8,73 %		53	Calcium Carbonate	PDF 04-012-8783	1	Primary	2,09	
		33	8,46 %		20	Calcium Cadmium Ca	PDF 04-012-5238	📵	Primary	4,56	~
			#							>	ĵ.

 \triangleright It is recommended to select the Group Duplicates check box.

Figure 1.5: Candidate List with the first pattern selected

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

Scans Search List DB View												
	0	*	E	FOM	Match	%	Name	ID				
Þ	~	Ð	1	33,18 %		79	Dolomite	PDF 04-008-0789				
			2	24,81 %		61	Calcium Magnesium	PDF 04-012-6929				
		A	2	<u>22 4</u> 2 %		60	Calcite magnesian	DDE 01-080-1304				

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

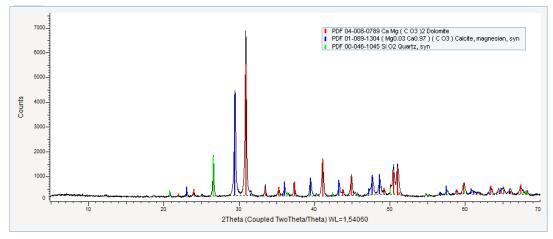


Figure 1.6: Bchips scan displayed in the graphical view with the three identified patterns

Results

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

1.4 Step 4: Preparing the Residual Scan

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

- 1. Multi-select the three identified patterns in the Data tree.
- 2. Click Auto Residue in the Tool list of the Data Command panel

— or — click the **Auto Residue** button on the Pattern toolbar

 or right-click the multi-selection and then click **Tool** on the context menu. Click **Auto Residue** on the Tool submenu.

The already explained areas are automatically removed. They are displayed with the ghost color in the Graphical view.



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

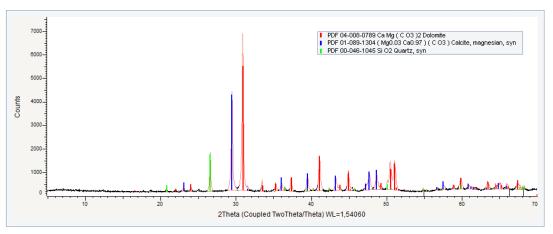


Figure 1.7: Scan with the removed zones in red (ghost color)

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

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

1.6 Step 6: Matching Procedure

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

Scans Search List DB View											
	\odot	品	i E	FOM	Match	%		Name	ID		
			1	116,13 %		-	8	Nickel Tin	PDF 00-004-0851		
			2	102,21 %			4	Erbium Titanium Oxide	PDF 04-001-9755		
			3	101,63 %			4	Hafnium Silicate	PDF 04-002-0611		
			4	100,85 %			4	Gadolinium Lutetium Titanium	PDF 04-001-9758		
I	<		5	98,49 %		_	2	Clinochlore-2MIIb	PDF 00-029-0854		
		Ð	6	93,55 %			1	Clinochlore, ferroan, oriented	PDF 00-060-0325		

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

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

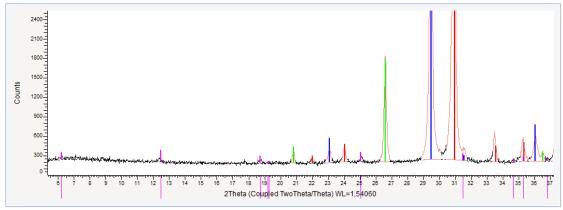


Figure 1.8: Zoom on the first half of the diagram with the Clinochlore phase identified

1.7 Step 7: Saving

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

🔏 Save EVA File As		×
🔾 🗢 📕 « Bruker	AXS → Tutorials → EVA →	م
Organize 🔻 New f	lder III -	• • • •
Wy Favorites Desktop Desktop Donioads Sected Places EVA Control Places Documents Music Pictures Videos	Document.eva	
File name: Bo	ips	-
Type : EV	files (*.eva)	-
Hide Folders	Save 🔊 Can	cel

Figure 1.9: Bchips.EVA document

2

Performing an Automatic Search/ Match Operation

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

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

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

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

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

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

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

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

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

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

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

Steps

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

2.1 Case #1: m1.RAW

M1 is a mixture of Calcite, Aragonite and Brucite.

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

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



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

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

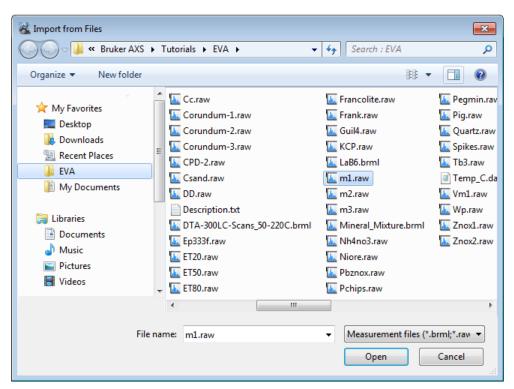


Figure 2.1: Importing the m1.RAW file

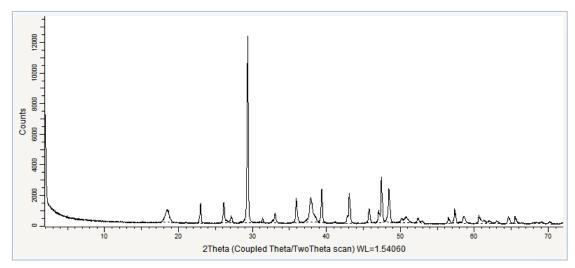


Figure 2.2: m1.RAW file imported in the Graphical view

2.1.2 Step 2: Setting the Search Parameters

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



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click the Search/Match button on the Search/Match toolbar

— or — right-click the scan, click **Tool** on the context menuand then **Search / Match** on the related submenu.

• The Search / Match dialog box will be displayed.

Search / Matc	hm1.raw #2	×
Databases	Match Lists Names Options	
PDF-4+ 201	6 RDB	Auto 📃
✓ DB Filter✓ Chemical	✓✓	Match

Figure 2.3: Search/Match dialog box

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

Database F	ilter m1.raw #2			×
PDF-4+ 20	16 RDB			\sim
Auto Re	build Click to filter Ca	ndidates		Clear
*				✓ Share
Filter		Value	Candidates	
+ 🗸 Co	lors			^
🕂 🗸 So	urces			
🖃 💷 Sul	ofiles			
	Organic		42229	
	Pharmaceutical a		8164	
· 🗖	Common phase		21539	**
	Inorganic		351612	
🗖	Forensic		13783	
	Pigment dye		1382	
	Educational pattern		1071	
🗸	Mineral		44341	
	Metal & Alloy		139072	
	Ceramic (all)		15199	
	Cement and Hyd		1568	
	Explosive		1330	~
				Ľ

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



- 7. In the **Databases** tab, click the **Match** button.
- \Rightarrow The candidates are listed in the **Search list** tab of the Data tree panel.

2.1.3 Step 3: Automatic Matching Procedure

Sca	ans Sear	ch List	DB Vie	w							
	0	*	E	FOM	Match	%		Name		ID	Quality
F	~			2,84 %			71	Calcite		PDF 01-083-1762	🔒 Blank
	~		2	0,56 %		-	11	Brucite, syn		PDF 00-044-1482	🚱 Star (*)
	~		3	0,45 %		_	10	Aragonite		PDF 00-001-0628	📵 Blank
_											
<			::								2
~	Group Du	plicate	s				Ŧ	é è	2 × 4		ß

Figure 2.4: Candidate List with the identified patterns marked



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

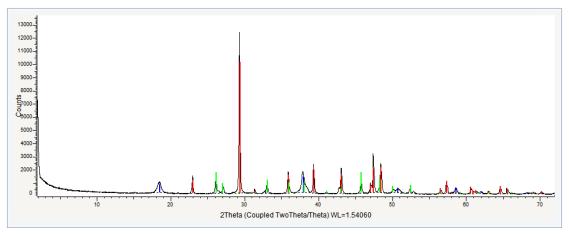


Figure 2.5: m1 scan displayed in the Graphical view with the three identified patterns (Calcite, Brucite and Aragonite)

Results

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

"Normal" matching procedure

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

Scans	Sear	rch List	DB Vie	w							
	\oslash	*	Ξ	FOM	Match	%		Name	ID	Quality	Sta
I		Ð	1	49,62 %			71	Calcite	PDF 01-083-1762	📵 Blank	^
		Ð	8	6,46 %		-	15	Calcite, magnesian, syn	PDF 01-089-1304	🚱 Star (*)	[#
			9	5,09 %			10	Aragonite	PDF 00-001-0628	📵 Blank	
			10	4,89 %			77	Calcite	PDF 00-001-0837	📵 Blank	
		Ð	11	4,61 %			11	Aragonite	PDF 00-041-1475	🚱 Star (*)	[
		Ð	12	4,50 %			11	Brucite, syn	PDF 00-044-1482	🚱 Star (*)	
			14	4,00 %			10	Manganocalcite	PDF 00-002-0604	🙆 Low p	
			16	3,60 %		-	19	Calcite	PDF 00-003-0596	🙆 Low p	
			20	3,00 %		3	34	Carlinite, syn	PDF 00-029-1344	 Indexed 	l
			21	2,88 %			8	Brucite, syn	PDF 00-007-0239	 Indexed 	[
		Ð	22	2,35 %			11	Briartite, syn	PDF 00-042-0565	🕝 Calcul	[
		Ð	24	1,83 %		_ 3	27	Calcite	PDF 00-004-0637	📵 Blank	
			26	1,74 %			4	Ruthenium-Hollandite Lithiu	PDF 04-013-0659	📵 Blank	l
			27	1,73 %			16	Calcite	PDF 00-002-0623	 Indexed 	-
<			#							· · ·	>
✓ Gro	oup Du	plicates	5			Ŀ	ł		<u>*</u>	ľ	

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

- The first pattern 01-083-1762 matches a part of the peaks of the scan.
- 5. Mark this pattern by selecting the corresponding check box.
 - The pattern is associated to a color. The image of its stick patterns remains when it is no longer selected (highlighted) in the Candidate List.
- 6. Go down in the list. Compare the stick patterns to the scan peaks.
 - The Aragonite and Brucite patterns (00-001-0628 and 00-044-1482) appear to match the scan.
- 7. Select the corresponding check boxes:
 - The images of their stick patterns remain when they are no longer selected.
- 8. Leave the non-matching stick patterns unchecked.

	\odot	品	Ξ	FOM	Match	%	Name	ID	Quality	Stat
۶.	~	Ð		49,62 %		7	1 Calcite	PDF 01-083-1762	🕑 Blank	^
		Ð	8	6,46 %		1	5 Calcite, magnesian, syn	PDF 01-089-1304	🚱 Star (*)	[===
	~		9	5,09 %		10) Aragonite	PDF 00-001-0628	📵 Blank	
			10	4,89 %		7	7 Calcite	PDF 00-001-0837	📵 Blank	1
		Ð	11	4,61 %		_ 1	1 Aragonite	PDF 00-041-1475	🚱 Star (*)	[
	~	Ð	12	4,50 %		1	1 Brucite, syn	PDF 00-044-1482	🚱 Star (*)	
			14	4,00 %		_ 10) Manganocalcite	PDF 00-002-0604	🙆 Low p	
			16	3,60 %		19	9 Calcite	PDF 00-003-0596	🧿 Low p	
			20	3,00 %		34	4 Carlinite, syn	PDF 00-029-1344	 Indexed 	[
			21	2,88 %		_ 8	Brucite, syn	PDF 00-007-0239	 Indexed 	[
		Ð	22	2,35 %		_ 1	1 Briartite, syn	PDF 00-042-0565	Calcul	[
		Ð	24	1,83 %		2	7 Calcite	PDF 00-004-0637	📵 Blank	
			26	1,74 %		- 1	4 Ruthenium-Hollandite Lithiu.	. PDF 04-013-0659	📵 Blank	[
			27	1,73 %		16	5 Calcite	PDF 00-002-0623	 Indexed 	
<			#						<u> </u>	>

Figure 2.6: Search List with the three patterns identified

Results

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

2.2 Case #2: CPD-2.RAW

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

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

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

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

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* 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.

Import from Files	▶ Tu	torials + EVA +	✓ 4y Search : EVA	× م
Organize 🔻 New folder				# • 🔳 🛛
 ★ My Favorites Desktop Downloads Recent Places EVA My Documents Libraries Documents Music Picturess Videos 		2D Frame Data 2A Arenfh.raw Alrefh.raw Asnosoll.raw Assoller.raw Assoller.raw ASSOLER.raw AUST_H.raw Bb.raw Bb.raw Bb.raw Bchips.raw BK100.raw BK100.raw	Ccraw Ccraw Corundum-1.raw Corundum-2.raw Corundum-3.raw CoPD-2.raw Ccand.raw DD.raw DD.raw DE-creption.tst DTA-300LC-Scans_50-220C.brm EF20.raw EF20.raw EF20.raw EF10.raw EF10.raw	Francolite.raw Frank.raw Guil4.raw KCP.raw Lab6.brml mt.raw m2.raw Mineral_Mistl Nh4no3.raw Nincer.aw Poznov.raw Poznov.raw
Fi	e nam	e: CPD-2.raw	Measurement f Open	files (*.brml;*.rav ▼ Cancel

Figure 2.7: Importing the CPD-2.RAW file

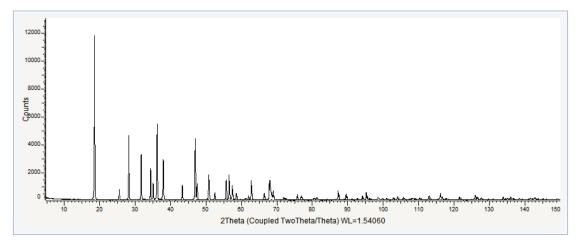


Figure 2.8: CPD-2.RAW file imported in the graphical view

2.2.2 Step 2: Setting the Search Parameters

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

1. Click Search / Match in the Data Command panel

— or —

Q

- click the Search/Match button on the Search/Match toolbar
- or —

right-click the scan, click **Tool** on the context menuand then **Search / Match** on the related submenu.

■ The Search / Match dialog box will be displayed.

Search / Matc	h CPD-2.raw #1	×
Databases	Match Lists Names Options	
PDF-4+ 201	16 RDB 🕥 ,	Auto 📃
DB Filter		Q
Chemical		Match

Figure 2.9: Search/Match dialog box

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

Database F	filter CPD-2.raw #1			×								
PDF-4+ 20	PDF-4+ 2016 RDB											
Auto Rebuild Click to filter Candidates Clear												
Shar												
Filter		Value	Candidates									
	n Ambient		43950	^								
🕂 🗸 Qu	ality Marks											
+ 💷 Sta	atus											
	lors											
+·✓ So	urces			££								
🖃 💷 Su	bfiles											
	Organic		42229									
	Pharmaceutical a		8164									
	Common phase		21539									
	Inorganic		351612									
	Forensic		13783									
	Pigment dye		1382									
	Educational pattern		1071									
🗸	Mineral		44341									
	Metal & Allloy		139072	\sim								

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



- 7. In the **Databases** tab, click the **Match** button.
- \Rightarrow The candidates are listed in the **Search list** tab of the Data tree panel.

o 🔗 🐰	1	FOM	Match	%	Name	ID	Quality	Sta
	1	3,77 %		47	Zincite, syn	PDF 01-089-7102	1 Indexed	-
~	2	2,04 %		38	Fluorite, syn	PDF 04-002-2191	🕕 Indexed	G
~	3	0,71 %		9	Corundum, syn	PDF 00-043-1484	Calculated	
~	4	0,48 %		46	Brucite, syn	PDF 04-011-5938	🚱 Star (*)	œ

2.2.3 Step 3: Automatic Matching Procedure

Figure 2.10: Search List with the identified patterns marked

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

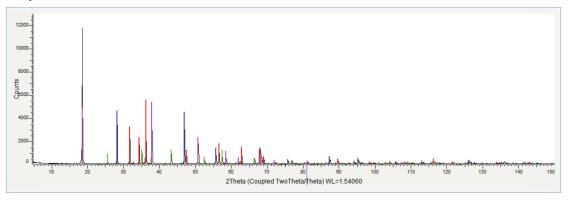


Figure 2.11: CPD-2 scan displayed in the **Graphical view** with the four identified phases: Zincite, Fluorite, Corundum and Brucite

Results

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

3 Using a Match Peak

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

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

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

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

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

Steps

H-

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

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

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



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

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

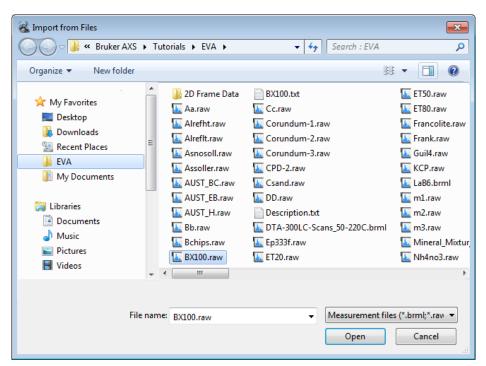


Figure 3.1: Importing BX100.raw

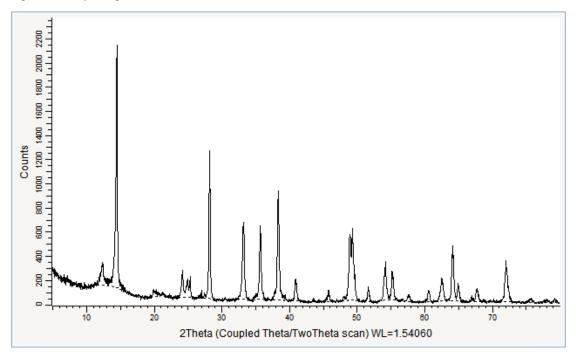


Figure 3.2: BX100.RAW imported in the graphical view

3.2 Step 2: Setting the Search Parameters

- ▷ Make certain the scan is selected; if not, select it either in the Data tree or in the graphical view.
- 2
- 1. Click **Search / Match** in the Data Command panel or —

click the **Search/Match** button on the Search/Match toolbar — or —

right-click the scan, click **Tool** on the context menu and then **Search / Match** on the related submenu.

• The Search / Match dialog box will be displayed.

Search / Match BX100.raw #1										
Databases	Match Lists Names Options									
PDF-4+ 201	.6 RDB	🔺 Auto 🗌								
✓ DB Filter	×	IQ								
Chemical	×	Match								

Figure 3.3: Search/match dialog box

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

Search / Match BX100.raw #1	×
Databases Match Lists Names Options	
2: Neutral	
Whole Range Subrange	



- 6. In the **Databases** tab, click the **Match** button.
- \Rightarrow The candidates are listed in the **Search list** tab of the Data Tree Panel.

3.3 Step 3: Matching Procedure

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

	\odot	*	Ξ	FOM	Match	%	ID	Name	Quality	Status	I/ICor	Org
Þ			1	35,10		91	PDF 00-021-1307	Boehmite, syn	1	👩 Primary		^
			2	26,04		33	PDF 04-002-2984	Vanadium Iron O	P	👩 Primary	2,62	**
		Ð	3	25,52		33	PDF 04-010-7290	Titanium Nickel O	😣	Primary	2,6	
			4	25,33		33	PDF 04-009-6569	Titanium Iron Oxide	1	👩 Primary	2,53	
			5	25,31		33	PDF 04-009-5898	Titanium Iron Oxide	📵	👩 Primary	2,58	
			6	25,15		32	PDF 01-073-8433	a-Fe1.85 H0.45	😣	👩 Primary	2,9	
			7	24,75		31	PDF 04-017-9544	Manganese Iron	🕑	👩 Primary	2,81	
		Ð	8	24,19		34	PDF 04-006-6579	Iron Oxide	1	👩 Primary	3,04	
		Ð	9	23,36		32	PDF 01-077-9924	Hematite, syn	®	👩 Primary	3,17	
			10	23,13		34	PDF 04-006-5322	Iron Aluminum Ox	🕑	👩 Primary	2,6	
			11	22,46		29	PDF 01-088-0434	Iron Tin Oxide	😣	👩 Primary	2,43	
			14	22,21		33	PDF 04-011-9587	Manganese Iron	1	👩 Primary	3,27	
			15	21,97		30	PDF 04-018-8870	Iron Neodymium	🔁	👩 Primary	3,37	
			16	21,90		32	PDF 04-018-8871	Iron Neodymium	😣	👩 Primary	3,95	
			18	21,52		31	PDF 04-020-1978	a-Fe1.95 Rh0.05	1	👩 Primary	3,18	
			19	21,48		30	PDF 04-017-4585	a-Fe1.981 Ge0.0	🕑	👩 Primary	2,82	
			20	21,14		29	PDF 00-042-0410	Chromium Rhodiu	🔁	👩 Primary	1,4	\sim
<				££								>
v 6	Group Du	plicate	s				₽ ₽ ĕ	2 × 🗞	X	(no 🖻		

 \triangleright It is recommended to select the Group Duplicates check box.

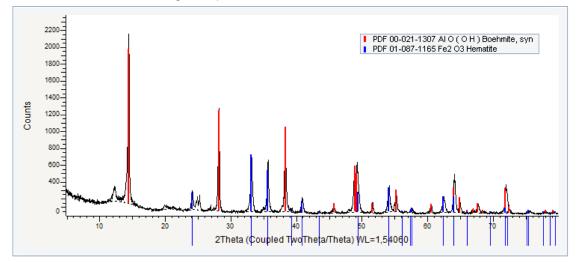
Figure 3.4: Candidate List with the first pattern highlighted

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

Scar	Scans Search List DB View											
	\odot	*	Ξ	FOM	Match	%	Name	ID				
Þ	✓	Ð	1	33,18 %		79	Dolomite	PDF 04-008-0789				
			2	24,81 %		61	Calcium Magnesium	PDF 04-012-6929				
		A	2	22 42 %		60	Calcite magnesian	DDF 01-080-1304				

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

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



6. Leave the non-matching stick patterns unchecked.

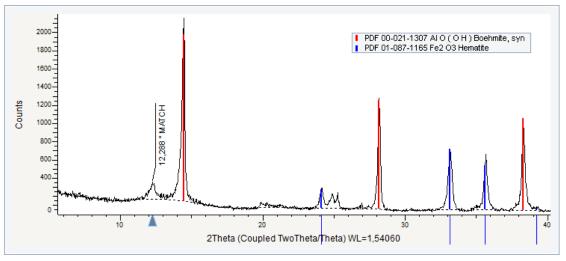
Figure 3.5: BX100 scan displayed in the graphical view with the two identified patterns

3.4 Step 4: Defining a Match Peak

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

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

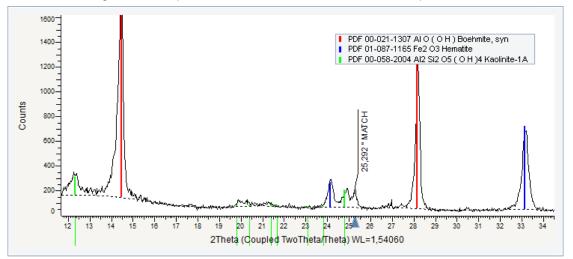
- \triangleright The Search/Match dialog box must be opened.
- 1. Point and right-click the peak at about 12.29°, one of the strongest residual peaks.
- 2. On the contextual menu that appears, click the **Create Match Peak at 2Th=... Cnt=...** command to make it a Match peak.
 - The Match peak is highlighted by a large blue triangle pointing to it in the bottom ruler and the string MATCH which is added to its caption.



- 3. Run another search.
 - Kaolinite will rank 3rd.
- 4. Select the corresponding check box.

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

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



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

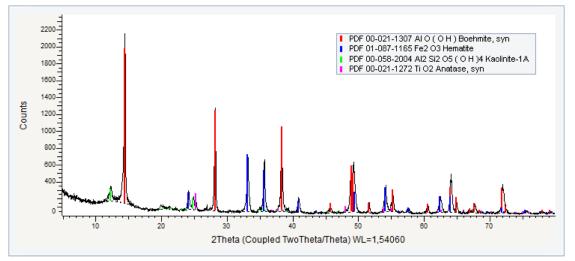


Figure 3.6: BX100 scan with the 4 phases identified

3.5 Step 5: Saving

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

🔏 Save EVA File As		×
😋 🗢 🖉 « Br	uker AXS → Tutorials → EVA →	م
Organize 🔻 N	ew folder	······································
 ▲ My Favorites ■ Desktop ֎ Downloads Secent Places ■ EVA ▲ EVA ▲ Documents ▲ Music ■ Pictures ■ Videos 	Documenteva	
File name:	BX100_Match_peak.eva	•
Type:	EVA files (*.eva)	•
Hide Folders	Save 🔊	Cancel

Figure 3.7: Saving BX100_Match_peak.EVA document

4 Creating and Using Filter Lists

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

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

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

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

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

Steps:

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

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

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

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



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

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

🐮 Import from Files											
Sruker AXS	► T	utorials 🕨 EVA 🕨	→ 4	Search : EVA	Q						
Organize 👻 New folder				••• •							
My Favorites Desktop Constant Desktop Constant Desktop Constan		Cc.raw Corundum-1.raw Corundum-2.raw Corundum-3.raw CPD-2.raw Csand.raw DD.raw		Francolite.raw Frank.raw Guil4.raw KCP.raw LaB6.brml m1.raw m2.raw	Pegmin.rav Pig.raw Quartz.raw Spikes.raw Tb3.raw Temp_C.da Vm1.raw						
 ➢ Libraries ➢ Documents ➢ Music ➢ Pictures ☑ Videos 		Description.bt Description.bt DTA-300LC-Scans_50-; Ep333f.raw ET20.raw ET20.raw ET50.raw ET50.raw	220C.brml [m3.raw Mineral_Mixture.brml Nh4no3.raw Niore.raw Pbznox.raw Pchips.raw	Wp.raw Wp.raw Cox1.raw Cnox1.raw						
Fil	e nan	< m1.raw		Measurement files (*.	brml;*.rav Cancel						

Figure 4.1: Importing the m1.RAW file

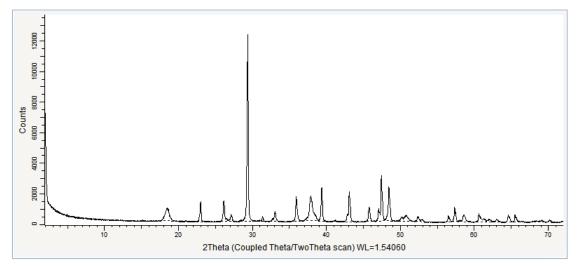


Figure 4.2: m1.RAW file imported in the Graphical view

4.2 Step 2: Creating a Filter List

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

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

Scar	ns Sear	ch List	DB View									
	\odot	品	1	FOM	Match	%	Source	ID	Name	Quality	Status	I/I
Þ	~			2,84 %		71	PLU	PDF 01-083-1762	Calcite	📵 Blank	😼 Deleted	Ì
	~		2	0,56 %		11	PLU	PDF 00-044-1482	Brucite, syn	🚱 Star	🚂 Deleted	
	~		3	0,45 %		10	PLU	PDF 00-001-0628	Aragonite	📵 Blank	🚂 Deleted	
<				**								>
✓ G	iroup Du	olicate	s			F		* 2 ×	<u>×</u>	1		

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- 2. Below the Search list, click the **New list** button to create a new filter list.
 - A new tab containing an empty list will be added.
- 3. In the **Search list** tab, select the three identified patterns and click the **Copy Section to Clipboard** button.
- 4. Go back to the new List tab and click the Paste Selection to Clipboard.
- The patterns will be added to the list.
- 5. Perform a Search by Name:

Course Course List DD Mary List 4

6. In the **Names** tab of the Search/Match dialog box, type *Magnesian Calcite* and click the **Search by Name** button.

	9
Databases Match Lists Names Options	
Magnesian calcite Use Filters	
Use ? and * for partial names e.g. BO*HMIT: parenthesis for authors e.g. (BOGUE), curly brackets for formulas e.g. {CaCO3}, dash to negate the result e.g. QUARTZ -BETA Or Or Name	

Candidates will be listed in the Search list.

Sca	ns S	earc	th List	DB View	Lis	t1 🔣							
	0		*	E		Match	%		Source	ID	Name	Quality	Status
Þ			Ð	1				2	PLU	PDF 00-043-0697	Calcite, magnesian	🋞 Star	👩 Primar
			Ð	3			-	15	PLU	PDF 01-089-1304	Calcite, magnesian, syn	🚱 Star	🙆 Primar
				4				5	PLU	PDF 01-089-1305	Calcite, magnesian, syn	🛞 Star	🙆 Primar
<													
Group Duplicates													

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

Sc	ans Search List	List 1 * 🔀										
	Source	ID	Quality	Status	I/ICor	Org	Inor	Mineral	Name û	For	Crys	а
	PLU2016	PDF 00-001-0628	📵	L			I	м	Aragonite	Ca	Orth	4,9
	PLU2016	PDF 00-044-1482	🛞		2,8		I	м	Brucite, syn	Mg (Hex	3,144
	PLU2016	PDF 01-083-1762	📵		3,25		I	м	Calcite	Ca (Rho	4,989
Þ	PLU2016	PDF 01-089-1304	®	<u>@</u>	3,12		I	М	Calcite, magnesi	(Mg	Rho	4,97
<			#									>



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

Write a Filter List	
Ores	
My Match list	
	Replace
New filter:	<u> </u>
Tutorial list	
	Write

10. Close the document.

4.3 Step 3: Using a Filter List

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

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

Se	arch / Match Csand.raw #1	×
	Databases Match Lists Names Options	
	Tutorial list 🛛	Auto 📃
	Ores	
	My Match list	And I
	 Tutorial list 	Match
	OK Cancel	

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

5 Creating a User Database

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

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

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

It is possible to create and maintain a separate database containing the user own patterns. This database is called a user database.

This chapter describes the basic procedure to create a user database and to use it when performing a search.

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

Steps:

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

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

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



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* 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.

🔏 Import from Files										
Search : EVA >										
Organize New folder										
My Favorites Desktop Downloads Eva Eva My Documents		Cc.raw Corundum-1.raw Corundum-2.raw Corundum-3.raw CPD-2.raw CSand.raw	 Francolite.raw Frank.raw Guil4.raw KCP.raw LaB6.brml m1.raw m2.raw 	Pegmin.rav Pig.raw Quartz.raw Spikes.raw Tb3.raw Tcmp_C.da						
 ➢ Libraries ➢ Documents ➢ Music ➢ Pictures ➢ Videos 		Description.bt Description.bt DTA-300LC-Scans_50-220C.brml Ep333f.raw ET20.raw ET20.raw ET50.raw	I m3.raw Mineral_Mixture.brml Mineral_Mixture.brml Minoral_mixture.brml Niore.raw Discrete Pbznox.raw Compos.raw	Wp.raw Znox1.raw Cnox2.raw						
F	ile na	< III me: m1.raw	Measurement files (*. Open	brml;*.rav ▼ Cancel						

Figure 5.1: Importing the m1.RAW file

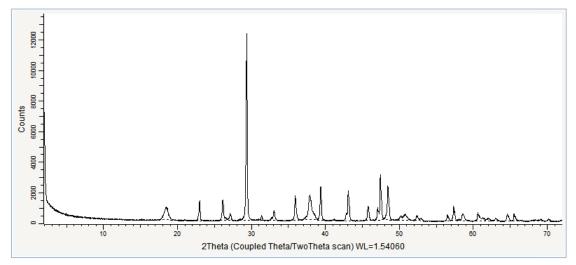


Figure 5.2: m1.RAW file imported in the Graphical view

5.2 Step 2: Performing the Search by Name

- ▷ Make certain the scan is selected; if not, select it either in the **Data tree** or in the **Graphical view**.
- 1. Click Search by Name in the Data Command panel

— or —

click the $\ensuremath{\textbf{Search}}$ by $\ensuremath{\textbf{Name}}$ button on the Search/Match toolbar

— or —

right-click the scan, click **Tool** on the context menu and then **Search by Name** on the related submenu.

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

Abo

Search / Match m1.raw #1	×
Databases Match Lists Names	Options
	Use Filters
Use ? and * for partial names	And And And And And And And And

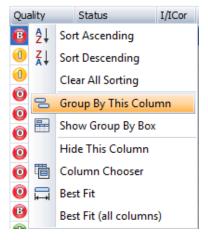
Figure 5.3: Names tab of the Search / Match dialog

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

	\odot	晶	Ξû	%		Name	ID	Quality	Status	I/ICor	Inor
Þ			1		77	Calcite	PDF 00-001-0837	📵 Blank	🚽 Deleted		I ^
			2		16	Calcite	PDF 00-002-0623	 Indexed 	🕞 Deleted		I
			3		5	Calcite	PDF 00-002-0629	 Indexed 	🕞 Deleted		I **
			4		0	Calcite, manganoan	PDF 00-002-0714	🧿 Low p	👩 Primary		I
			5		4	Calcite	PDF 00-003-0569	🧿 Low p	🕞 Deleted		I
			6		26	Calcite	PDF 00-003-0593	🧿 Low p	🕞 Deleted		I
			7		19	Calcite	PDF 00-003-0596	🧿 Low p	🕞 Deleted		I
			8		4	Calcite	PDF 00-003-0612	🧿 Low p	🕞 Deleted		I
			9		0	Calcite	PDF 00-003-0670	🧿 Low p	🚂 Deleted		Ι
		Ð	10		27	Calcite	PDF 00-004-0636	📵 Blank	🚂 Deleted		I ~
Group Duplicates											

Here, we will group patterns by quality.

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



Sci	ans	Sear	ch List								
		0	i E	%	Name	I	-	Status	 Inor		
Þ	E Quality: 🔞 Blank										
	+	Qua	lity: 🙆	Calcula	ted						
	+	Qua	lity: 🕲	Hypoth	netical						
	+	Qua	lity: 创	Indexe	ed						
	+	Qua	lity: 🧿	Low pr	ecision						
	+	Qua	lity: 🕑	Prototy	yping						
	+	Qua	lity: 🔞	Rietve	ld						
	+	Qua	lity: 🛞	Star (*)						
<					#						>
	Grou	up Du	plicates			(+	s è	2 × -	x n	P	

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

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

Scans	Seard	h List	DB View								
Qual	Quality û										
	0	Ξû	%	Name		ID	Status	I/ICor	Inor	Mineral	Crysta
▶ Œ	Quali	ty: 📵	Blank								
E H	Quali	ty: 🕝	Calcula	ited							
	Quali	ty: 🕄	Hypoth	netical							
E E	Quali	ty: 创	Indexe	ed							
t.	Quali	ty: 🧿	Low pro	ecision							
E E	Quali	ty: 🕑	Prototy	yping							
t.	🔄 🕀 Quality: 🔞 Rietveld										
E E	📃 🗄 Quality: 🚱 Star (*)										
<				::							>

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

Scan	s Searc	th List [OB View								
Qu	Quality 0										
	\odot	Ξû	%	Name	ID	Status	I/ICor	Inor	Mineral	Cryst	tal
Þ	- Quali	ity: 🛞	Star (*)							^
		12	68	Calcite, syn	PDF 00-005-0586	👍 Alternate	2	I	м	Rhor	::
		15	_ 2	Calcite, magnesian	PDF 00-043-0697	🚯 Primary		I	м	Rhor	
		19	<u>7</u> 4	Calcite, syn	PDF 01-071-3699	👍 Alternate	3,23	I	м	Rhor	
		20	90	Calcite	PDF 01-072-1937	👍 Alternate	3,23	I	м	Rhor	
		22	67	Calcite	PDF 01-075-6049	👍 Alternate	3,2	I	м	Rhor	
		24	76	Calcite, syn	PDF 01-078-4614	👍 Alternate	3,13	I	м	Rhor	
		25	76	Calcite, syn	PDF 01-078-4615	👍 Alternate	3,14	I	м	Rhor	
		26	81	Calcite	PDF 01-080-2791	👍 Alternate	3	I	м	Rhor	
		27	71	Calcite	PDF 01-080-2792	👍 Alternate	2,99	I	м	Rhor	×
<			5	:						>	

- 6. Mark the first pattern PDF 00-005-0586 by selecting the corresponding check box.
- \Rightarrow The pattern will be added to the Data tree and displayed in the graphical view.

Data Tree							
Data		Description					
Ξ	Document						
E	Views						
	2Theta	1 Scan					
Ė	✓ I m1.raw #1	(Coupled TwoTheta/Theta)					
	Pattern List #1	1 Pattern					
	🦾 🔽 📘 PDF 00-005-0586	Ca C O3 Calcite, syn					

5.3 Step 3: Performing the Tune Cell Operation

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



- 1. Select the Calcite pattern in the Data tree.
- 2. Click **Tune Cell** in the **Data Command** panel or —

click the Tune Cell button of the **Pattern** toolbar

right-click the pattern, then click Tune Cell on the context menu.

► The **Tune cell** dialog box will be displayed.

Tune Co	ell PDF 00-005	5-0586				×
	a 🚩]	System	Rhombo.H.axe	es	Default
	5.03889	Max	Show	All 🕥]	••
	4.98899	Width	All Stick	s indexed	Filter <	5 % 🄶
<u> </u>	4.93911	Min		Replace		Append

3. Do not modify anything and click the **Replace** button.

The Calcite pattern PDF 00-005-0586 will be replaced by the pattern PDF 00-005-0586 (Tune Cell) in the Graphical view as well as in the Data Tree.

Data		Description
=	Document	
E	Views	
.	2Theta	1 Scan
	▼ ■ m1.raw #1	(Coupled TwoTheta/Theta)
	Pattern List #1	1 Pattern
	🛄 🔽 📘 PDF 00-005-0586 (Tune Cell)	Ca C O3 Calcite, syn

78

5.4 Step 4: Creating the User Database

1. Click User Database in the Data Command panel

— or — click the **User Database** button on the **Pattern** toolbar — or —

right-click the tuned pattern and click User Database on the context menu.

► The User Database dialog box will be displayed.

User Databa	se PDF 00-005-0586 (Tune Cell)	×
Description	Bibliography Experimental Cell Peaks	User Database:
Name:	Calcite, syn	dick + to create a database
Formula:	Ca C O3	Click + to create a database
	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	Update ID Delete ID
		and Document Append ID

Figure 5.4: User Database dialog box

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

User Databa	ase Creation 📃 🗖 🔀
Short Name:	
Prefix:	ex: ABC
Digit groups:	ex: 25 meaning: XX-XXXXX
Example:	A Prefix is required.
Cancel	Create

Figure 5.5: User database creation dialog box

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

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

User Database Creation							
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						
Cancel	Create						

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

User Databas	se PDF 00-005-0586 (Tune Cell)	×
Description	Bibliography Experimental Cell Peaks	User Database:
Name:	Calcite, syn	DATABASE1 Y + X
Formula:	Ca C O3	My first user database
	Open to test the formula's validity	Pattern ID:
Keywords:		USR 000-0001
	2 or more alphabetical characters	This pattern number is a vailable.
Color:		
	Choose one of the colors, or type a new one	Update ID Delete ID
Subset:	Inorganic 🛛 Mineral	Land Degreent
		Append ID

5.5 Step 5: Adding the Calcite pattern to the database

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

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

H-

M,

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

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

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

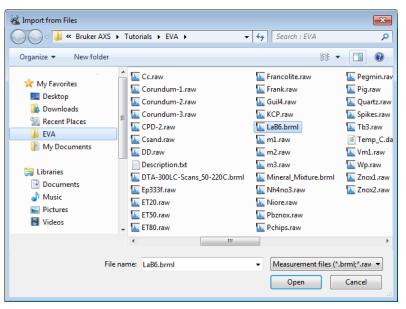


Figure 5.6: Importing LaB6.brml

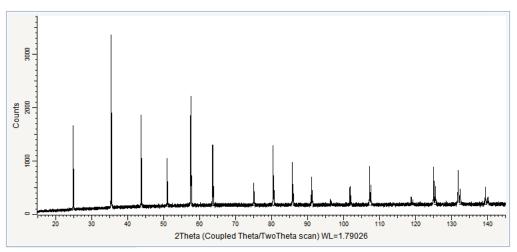


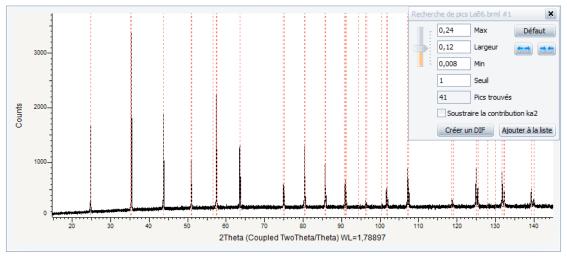
Figure 5.7: LaB6 file imported in the graphical view

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

- 1. Make sure the scan has been selected. If not, select it either in the data tree or in the 1D view.
- 2. Click Peak Search in the Tool list of the Data Command panel

click the Peak Search button on the Peak/Area toolbar

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.

Г

– or —

— or -

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

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

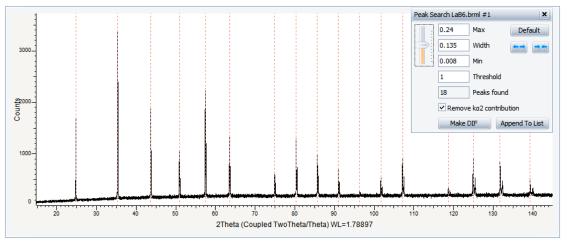
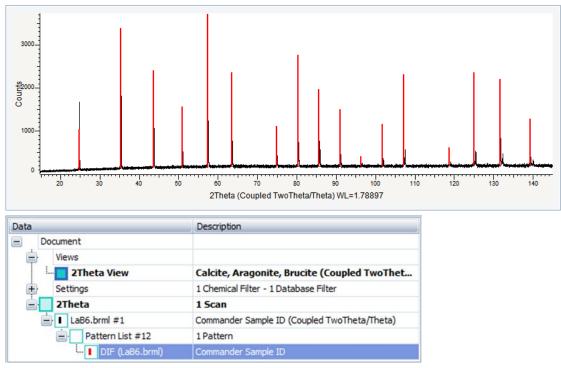


Figure 5.9: Performing a peak search on the LaB6 scan

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



6. Click **User Database** in the Data Command panel

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).

User Database DIF (LaB6.brml)	×
Description Bibliography Experimental Cell Peaks	User Database:
Name: Commander Sample ID	DATABASE1
Formula:	My first user database
Open to test the formula's validity	Pattern ID:
Keywords:	USR 000-0002
2 or more alphabetical characters	This pattern number is available.
Color:	
Choose one of the colors, or type a new one	Update ID Delete ID
Subset: Inorganic Mineral	and Document Append ID

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

User Databas	e DIF (LaB6.brml)	×
Description	Bibliography Experimental Cell Peaks	User Database:
Name:	Lanthanum hexaboride	DATABASE1 🛛 🖌 💌
Formula:	LaB6	My first user database
	Open to test the formula's validity	Pattern ID:
Keywords:		USR 000-0002
Color:	2 or more alphabetical characters	This pattern number is available.
Subset:	Choose one of the colors, or type a new one Inorganic	Update ID Delete ID
		and Document Append ID

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

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

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

- 1. Select the LaB6.BRML scan.
- 2. Click Search / Match in the Data Command panel

— or click the **Search / Match** button on the Search/Match toolbar — or —

right-click the current scan, click **Tool** on the menu which appears and then **Search** / **Match** on the related submenu.

3. In the **Databases** tab, select *My first user database* in addition to the PDF database (here the PDF-4+ 2016) drop-down list. Let the **DB filter** and **Chemical** fields empty.

Database Filter LaB6.brml #1						
PDF-4+ 2016 RDB, My	first user dat	abase				
Crystallography Op	en Database	(REV8924	4 20 13. 10	. 11)		
Crystallography Op		(REV1734	45 2016.0	1.04		
PDF-2 Release 201						
PDF-2 Release 201	6 RDB					
✓ PDF-4+ 2016 RDB						
 My first user datab 	ase					
	OK Cancel					
+ Colors						
+ 🗸 Sources						
📄 🔲 Subfiles						
🗸 Organic 42229						
··· Pharm		8164				
Comm		21539		\sim		



4. Click the Search/Match button.

Scar	ns Sear	ch List	DB V	/iew								
	\odot	*	Û	FOM	Match	%	Source	ID	I/ICor	Quality	Name	Status
			1	146,72 %	29 0	-	PLU2016	PDF 04-005-3486	9,56	Prototyping	Boron Lanthanum Samarium	🔞 Primary 🖉
			2	125,06 %	30 0	_	PLU2016	PDF 04-005-7139	9,5	😰 Prototyping	Boron Lanthanum Samarium	🔞 Primary ²
		Ð	3	124,95 %	30 0	_	PLU2016	PDF 04-005-9344	9,54	🕑 Prototyping	Boron Lanthanum Samarium	👩 Primary
			4	116,63 %	29 0	_	PLU2016	PDF 00-058-0337		🚱 Star (*)	Boron Lanthanum Samarium	👩 Primary
			5	98,70 %	24 0	_	PLU2016	PDF 00-040-1310	9,31	🕝 Calculated	Boron Europium Carbide	🔞 Primary
			6	90,01%	24 0	-	PLU2016	PDF 04-005-7137	9,45	😰 Prototyping	Boron Cerium Lanthanum	🔞 Primary
			7	89,04 %	30 0		PLU2016	PDF 04-005-9736	10,71	🕑 Prototyping	Boron Lanthanum Tungsten	👩 Primary
			8	77,83 %	21 0	_	PLU2016	PDF 00-057-0823	5,23	🚱 Star (*)	Potassium Bismuth Zirconium	👩 Primary
		Ð	9	72, <mark>83 %</mark>	34 0	_	PLU2016	PDF 00-059-0332		🚱 Star (*)	Lanthanum Boride	🔞 Primary
Þ		Ð	10	72,83 %	34 0		DATABASE1	USR 000-0003			Lanthanum Boride	
			11	71, <mark>87 %</mark>	13 0	-	PLU2016	PDF 00-058-0593		🚱 Star (*)	Barium Indium Lanthanum Yt	🔞 Primary
		Ð	12	62,34 %	28 2	-	PLU2016	PDF 04-010-2753	10,34	🕑 Prototyping	Cesium Lithium Molybdate	👩 Primary
			13	61,61 %	33 0		PLU2016	PDF 01-070-8265	9,26	🚱 Star (*)	lanthanum boride Boron La	🚳 Primary
		Ð	14	59,43 %	24 0		PLU2016	PDF 00-031-0254		🚱 Star (*)	Boron Calcium	👩 Primary 🗸
<				::								>

Figure 5.10: Search Results including the user pattern

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

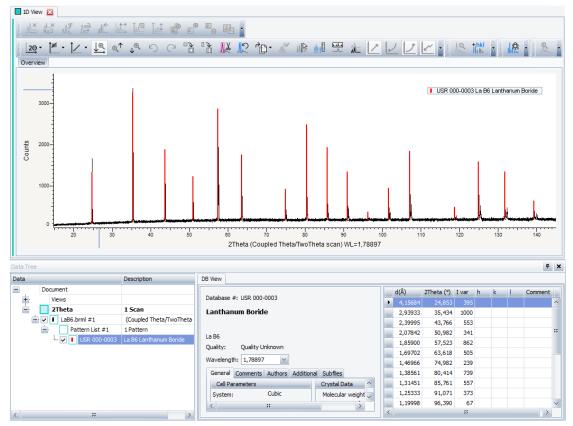


Figure 5.11: User pattern added to the data tree and the graphical view

6 Performing a Peak Search

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

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

Steps

H-

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

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

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



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

🔏 Import from Files				×
Goo Karaker AXS	 Tut 	orials 🕨 EVA 🕨	✓ ✓ Search : EVA	٩
Organize 🔻 New folder			88	•
My Favorites My Favorites Desktop Downloads Recent Places EVA My Documents Libraries Documents Music		CD Frame Data A.raw Alrefht.raw Alrefht.raw Alrefht.raw Asnosoll.raw Assoller.raw AUST_BC.raw AUST_EB.raw AUST_EB.raw AUST_H.raw B.raw	 BX100.txt Cc.raw Corundum-1.raw Corundum-2.raw Corundum-3.raw CPD-2.raw Csand.raw DD.raw Description.txt DTA-300LC-Scans_50-220C.brml 	ET50.raw ET80.raw Francolite.raw Frank.raw Guil4.raw LaB6.brml Mn1.raw Mn2.raw Mn3.raw
PicturesVideos		L Bchips.raw BX100.raw	🚾 Ep333f.raw 🚾 ET20.raw	Mineral_Mixture Nh4no3.raw
Fil	name	Csand.raw	Measurement files Open	; (*.brml;*.raw ▼ Cancel

Figure 6.1: Importing Csand.raw

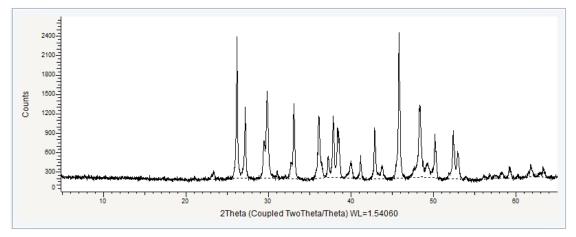


Figure 6.2: Csand scan imported in the graphical view

6.2 Step 2: Setting the Peak Search Parameters

- \triangleright Make certain the scan is selected; if not, select it either in the data tree or in the 1D view.
 - R
- 1. Click **Peak Search** in the Tool list of the Data Command panel

— or — click the **Peak Search** button on the Peak / Area toolbar

— or —

right-click the scan, and then click **Tool** on the context menu. Click **Peak Search** on the Tool submenu.

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

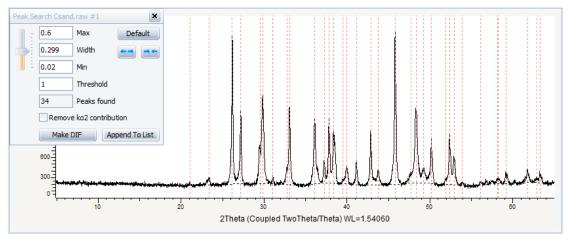
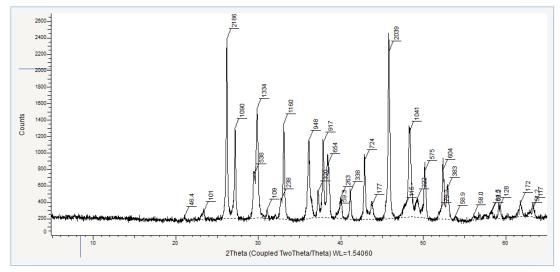


Figure 6.3: Peak Search dialog box and graphical view showing the ghost peaks

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

6.3 Step 3: Appending the Peaks

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



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

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

Data Tree	2		×
Data		Description	
E Do	ocument		
	Views		
		CSAND (Coupled TwoTheta/Theta)	
E	Settings	1 Chemical Filter - 1 Database Filter	F1
	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	
	···· I Peak #4	1090	
	··· I Peak #5	538	
	Peak #6	1334	
	… 📘 Peak #7	109	
	Peak #8	238	
	Peak #9	1160	
	Peak #10	948	~

Figure 6.5: Peak List added in the Data Tree

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



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

6.4 Step 4: Saving

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

🔏 Save EVA File As 🛛 🕰								
🔾 🗢 📕 « Bruke								
Organize 👻 New	folder	• • 🕡						
My Favorites Desktop Downloads Recent Places EVA	2D Frame Data 2D Ocument.eva							
 Eibraries Documents Music Pictures Videos 								
File name: C	sand							
_	/A files (*.eva)	-						
) Hide Folders	Save	Cancel						

Figure 6.6: Saving Csand.EVA document

7 Computing Kα2 Stripping

The following procedure describes the basic procedure for computing K α 2 Stripping. The scan used is held as a tutorial file, Quartz.RAW, found in the Tutorial directory.

Steps

H-

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

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

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

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* 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.

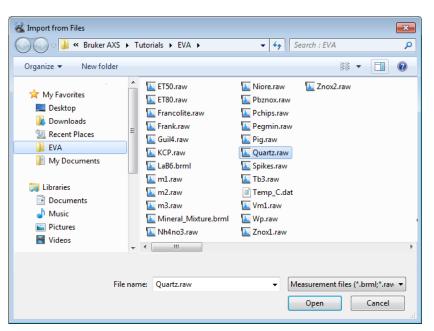


Figure 7.1: Importing Quartz.raw

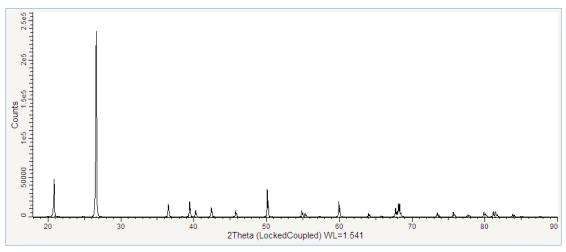
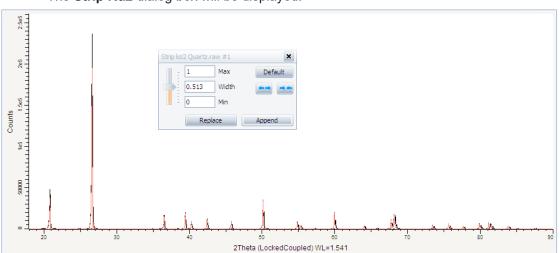


Figure 7.2: Quartz scan imported in the graphical view

7.2 Step 2: Computing the Kα2 Stripping

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

1. Right-click the scan, and then click **Tool** on the context menu. Click **Strip Ka2** on the related submenu.



The Strip Kα2 dialog box will be displayed.

Figure 7.3: Strip K α 2 dialog box and in the graphical view: ghost K α 2-stripped line

- 2. The default parameters are set in the Strip K α 2 dialog box and the ghost line shows the K α 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.

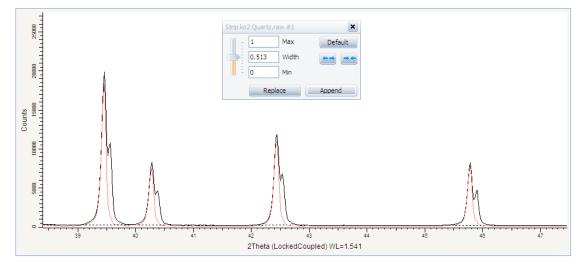
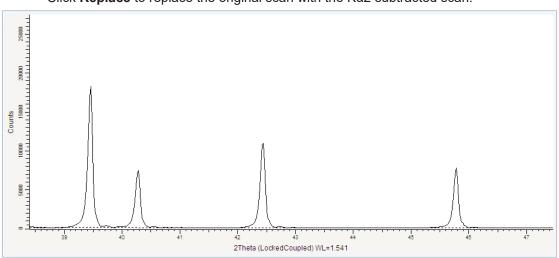


Figure 7.4: Zoom on the peaks (2θ =38° to 48°)

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



- Click **Replace** to replace the original scan with the K α 2 subtracted scan.

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

7.3 Step 3: Saving

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

🔏 Save EVA File As		×
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Figure 7.6: Saving the Quartz.EVA document

8 Smoothing Scans

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

Steps

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

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

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

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* 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.

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Fi	e name: Quartz.raw	Measurement files (*.brml;*.raw Open Cancel	• •

Figure 8.1: Importing Quartz.raw

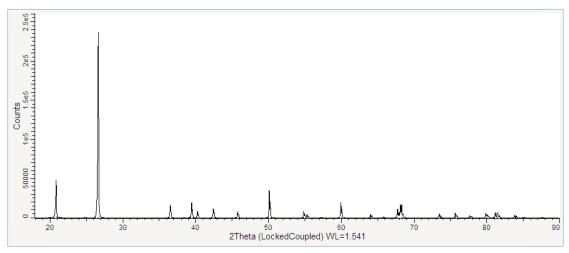
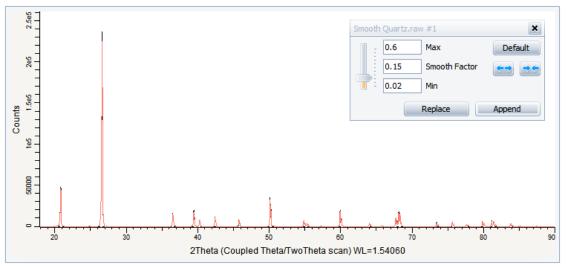


Figure 8.2: Quartz scan imported in the graphical view

8.2 Step 2: Smoothing the Scan

Case #1: Smoothing

- \triangleright Make certain the scan is selected; if not, select it either in the data tree or in the 1D view.
- 1. Right-click the scan, and then click **Tool** on the context menu. Click **Smooth** on the related submenu:



the Smooth dialog box will be displayed.

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

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

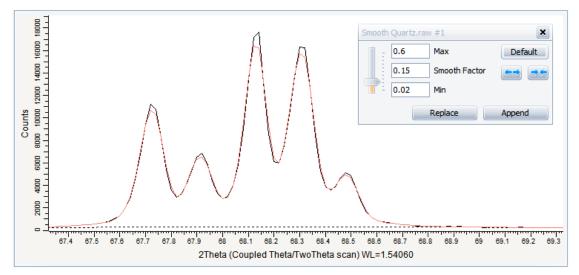


Figure 8.4: Zoom on peaks (20=67° to 69°)

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



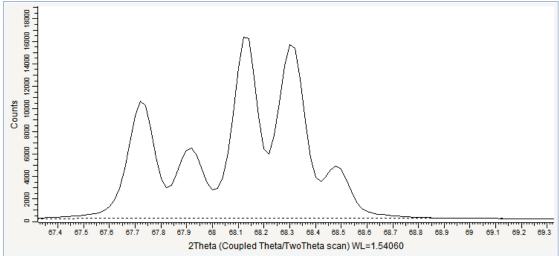


Figure 8.5: Original scan replaced with the smoothed scan - Zoom on peaks ($2\theta=67^{\circ}$ to 69°)

Case #2: Fourier Smoothing

- \triangleright Make certain the scan is selected; if not, select it either in the data tree or in the 1D view.
- 1. Right-click the scan, and then click **Tool** on the context menu. Click **Fourier Smooth** on the related submenu.
 - The Fourier Smooth dialog box will be displayed.

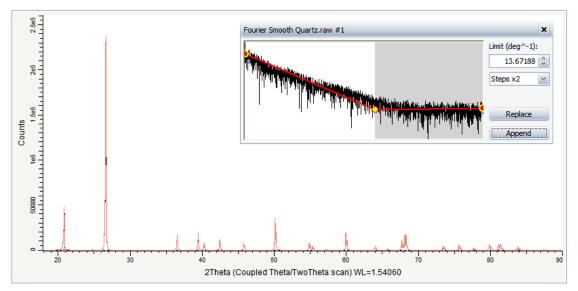
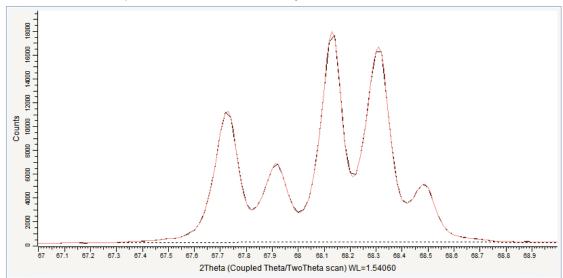


Figure 8.6: Smooth dialog box and in the graphical view: ghost smoothed line

- 2. Automatic adjustments are done. The ghost line shows the smoothed line in the graphical view.
- 3. You can modify the cutoff graphically or by changing the limit value. You can modify the expansion by selecting another **Steps multiplied by** value.



4. Zoom in on the peaks to see the result clearly.

Figure 8.7: Zoom on peaks (20=67° to 69°)

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

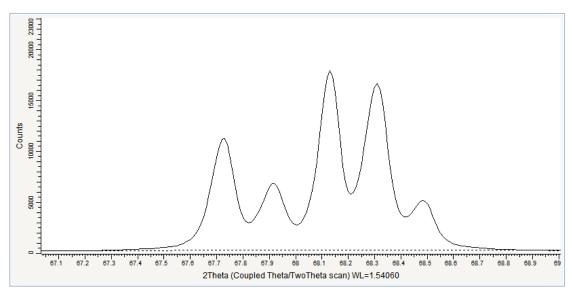


Figure 8.8: Original scan replaced with the smoothed scan - Zoom on peaks (20=67° to 69°)

8.3 Step 3: Saving

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

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Figure 8.9: Saving the Smooth_Quartz.EVA document

9 Removing Aberrant Points

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

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

Steps

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

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

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



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

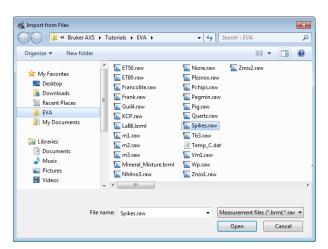


Figure 9.1: Importing Spikes.raw

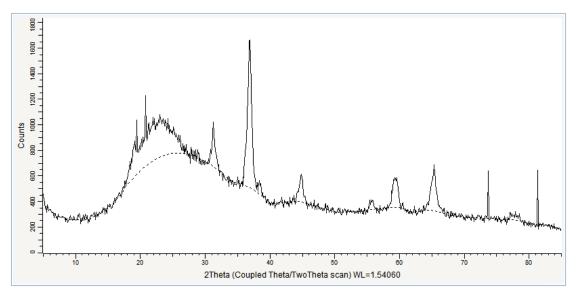


Figure 9.2: Spikes scan imported in the graphical view

9.2 Step 2: Removing Aberrant Points

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

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

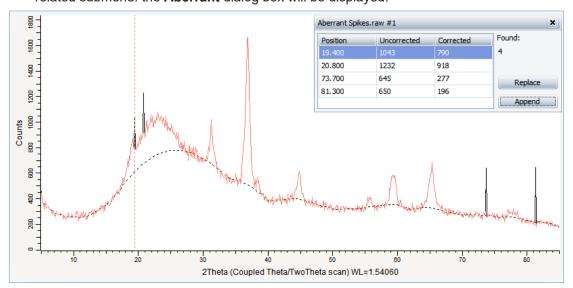


Figure 9.3: Aberrant dialog box and graphical view displaying a ghost line with the aberrant points removed

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

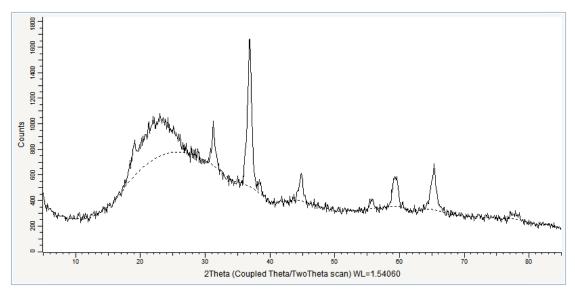


Figure 9.4: Original scan replaced with the corrected scan

9.3 Step 3: Saving

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

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Figure 9.5: Saving the Spikes.EVA document

10 Computing Areas

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

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

Steps

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

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

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

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* 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.

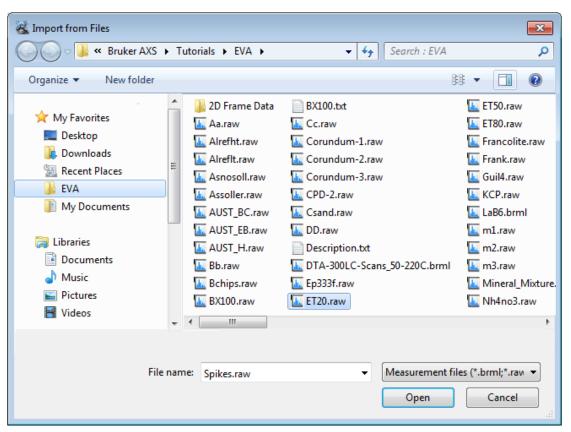


Figure 10.1: Importing ET20.raw

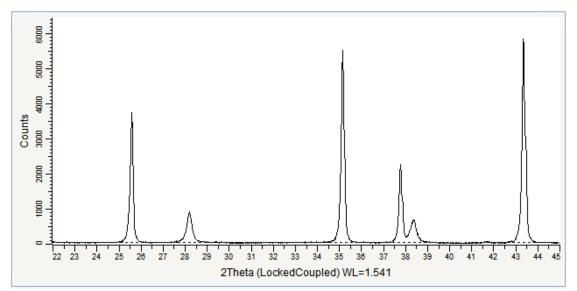


Figure 10.2: ET20.RAW file imported in the graphical view

10.2 Step 2: Selecting and Computing an Area

- \triangleright Make certain the scan is selected; if not, select it either in the data tree or in the 1D view.
- 1. Click Create Area in the Tool list of the Data Command panel,
 - click the Create Area button on the Peak /Area toolbar,
 - or —

– or —

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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.

Create Area ET20.RAW #1	×
Angle (deg.)	Intensity (cps)
Left	Left
Right	Right
Max	Max
FWHM	Net Height
Chord Mid.	Scherrer evaluation
I. Breadth	Crystallite Size
Gravity C.	Use FWHM 🔘
Area (cps x deg.)	Use I. Breadth 🔘
Raw Area	K = 1
Net Area	Instr. Width = 0
Press and select an Area	Append this Area

Figure 10.3: Create Area dialog box

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

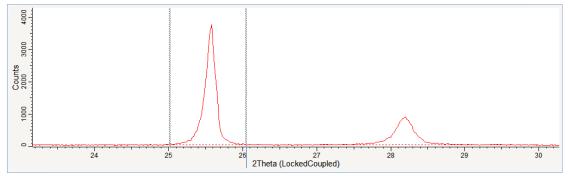


Figure 10.4: Selecting an area

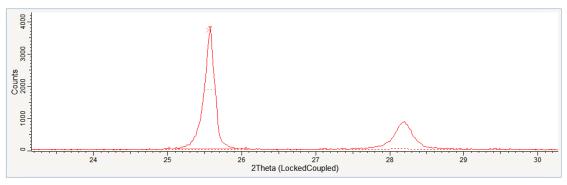


Figure 10.5: Area selected

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

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Create Area ET20.RAW #1				
Angle (deg.)		Intensity (cps)		
Left	24.940	Left	28.3	
Right	26.080	Right	28.6	
Max	25.571	Max	1870.5	
FWHM	0.149	Net Height	1842.0	
Chord Mid.	25.569	Scherrer evaluation		
I. Breadth	0.181	Crystallite Size	605.809	
Gravity C.	25.552	U	lse FWHM 🍥	
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Net Area	333.1	Instr. Width =	0	
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Figure 10.6: Results of the area computation

- 4. Once the selection is satisfactory, click **Append this Area** to add the area to an Area list in the Data tree.
- ⇒ The results will be displayed in the Area Property table.

10.3 Step 3: Saving

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

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Figure 10.7: Saving ET20.EVA document

11 Adding Scans

The following procedure describes the basic procedure for adding scans.

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

Steps

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

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



- 1. Click New on the File menu or use the dedicated button in the toolbar.
 - The EVA document is empty.
- 2. Click the Import from files data command or the Import from files button.
 - The Import From Files dialog box will be displayed.
- 3. Search the Tutorials/EVA* directory and multi-select the ET20.RAW, ET50.RAW and ET80.RAW files.
- 4. Click Open.
- ⇒ The scan ET20, ET50 and ET80 will be added to the Data tree and displayed in the graphical view of the EVA document.

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

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Figure 11.1: Importing the 3 scans

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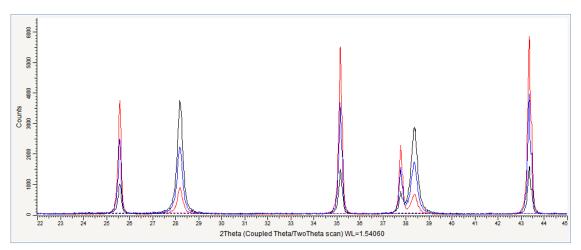


Figure 11.2: ET20.RAW, ET50.RAW and ET80.RAW files imported in the graphical view

11.2 Step 2: Adding the Scans

- 1. Multi-select the scans in the data tree.
- 2. Click Add in the Tool list of the Data Command panel

— or — click the **Add** button on the Scan toolbar

— or —

right-click the multi-selection, and then click **Tool** on the context menu. Click **Add** on the Tool submenu.

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

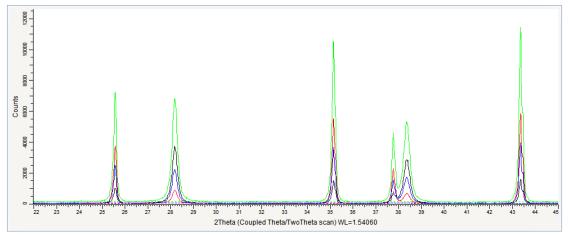


Figure 11.3: Original scans and the scan resulting from the addition

11.3 Step 3: Saving

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

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Figure 11.4: Saving ET_addition.EVA document

12 Subtracting Scans

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

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

Steps

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

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

- 1. Click New on the File menu or use the dedicated button in the toolbar.
 - ► The EVA document is empty.
- 2. Click the Import from files data command or the Import from files button.
- The Import From Files dialog box will be displayed.
- 3. Search the Tutorials/EVA* directory and multi-select the files ET20.RAW and ET50.RAW.
- 4. Click Open.
 - The scans ET20 and ET50 will be added to the Data tree and displayed in the graphical view of the EVA document.

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

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Figure 12.1: Importing ET50.raw and ET20.raw

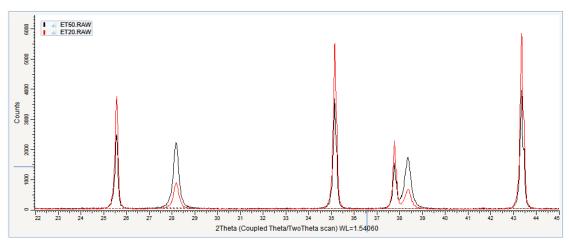


Figure 12.2: ET20.RAW and ET50.RAW files imported in the graphical view

12.2 Step 2: Subtracting the Scans

Case #1: Subtraction result with positive values

- 1. Multi-select the scans in the data tree (select ET50.RAW first).
- 2. Click Subtract in the Tool list of the Data Command panel

— or — click the **Subtract** button on the Scan toolbar

— or —

right-click (the multi-selection), and then click **Tool** on the context menu. Click **Subtract** on the Tool submenu.

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

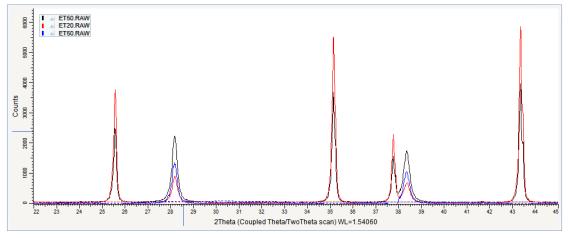


Figure 12.3: Original scans and the scan resulting from the subtraction

Case #2: Subtraction result with negative values

- 1. Multi-select the scans in the data tree (select ET20.RAW first).
- 2. Click Subtract in the Tool list of the Data Command panel



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- or click the **Subtract** button on the Scan toolbar
- or —

right-click (the multi-selection), and then click **Tool** on the context menu. Click **Subtract** on the Tool submenu.

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



Figure 12.4: Difference curve displayed in the extended view

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

12.3 Step 3: Saving

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

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Figure 12.5: Saving ET_subtraction.EVA document

13 Merging Scans

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

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

Steps

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

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

- 1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
 - The EVA document is empty.
- 2. Click the Import from files data command or the Import from files button.
 - The Import From Files dialog box will be displayed.
- 3. Search the Tutorials/EVA1 directory and multi-select the files Corundum-1.RAW, Corundum-2.RAW and Corundum-3.RAW.
- 4. Click Open.
- ⇒ The scans Corundum-1, Corundum-2 and Corundum-3 will be added to the Data tree and displayed in the graphical view of the EVA document.

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

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Figure 13.1: Import the 3 scans

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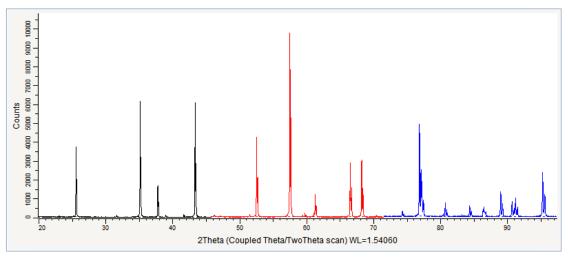


Figure 13.2: Corundum-1.RAW, Corundum-2.RAW and Corundum-3 files imported in the graphical view

13.2 Step 2: Merging the Scans

- 1. Multi-select the scans from Corundum-1 to Corundum-3 in the data tree; the Corundum-1 is taken as the reference.
- 2. Click Merge in the Tool list of the Data Command panel

— or click the **Merge** button on the Scan Toolbar — or —

right-click the multi-selection, and then click **Tool** on the context menu. Click **Merge** on the Tool submenu.

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

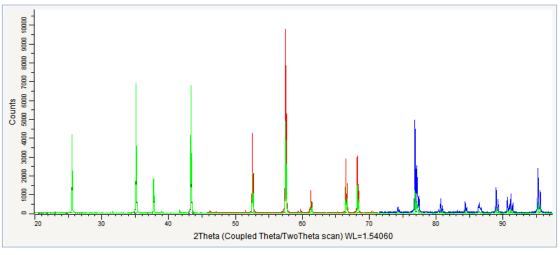


Figure 13.3: Original scans and the scan resulting from the merging

13.3 Step 3: Saving

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

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G v Karakar AXS > Tutorials > EVA > v 4	earch : EVA 🔎
Organize 🔻 New folder	ii • 🔞
▲ ★ My Favorites ▲ ■ Desktop ▲ ▶ Downloads ▲ ▶ EvA ▲ ▲ Eva ▲ ▶ Eva ▲ ▶ Documents ▲ ▶ Videos ▼	
File name: Merge_corundum	-
Type : EVA files (*.eva)	
Hide Folders	Save Cancel

Figure 13.4: Saving Merge_corundum.EVA document

14 Normalizing Scans

The following procedure describes the basic procedure for normalizing scans.

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

Steps

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

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

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

j

* 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.

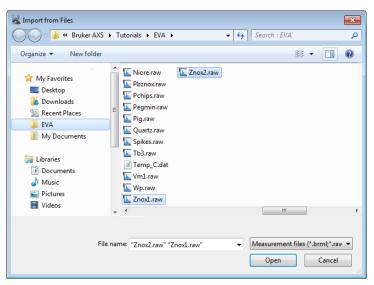


Figure 14.1: Importing the scans

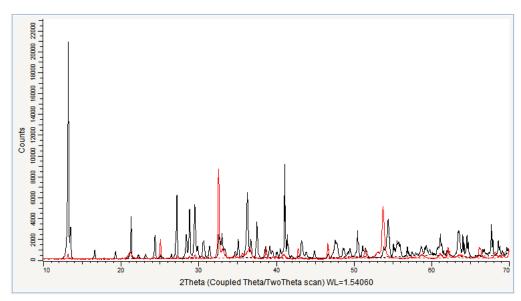


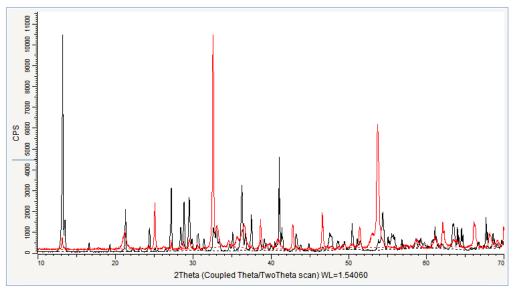
Figure 14.2: Znox1.RAW (in red) and Znox2.RAW (in black) files imported in the graphical view

14.2 Step 2: Normalizing the Scans

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

To normalize on the Znox2 scan:

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



• The scans are normalized on the maximum of the Znox2 scan.

Figure 14.3: Original scans and the scan resulting from normalizing

14.3 Step 3: Saving

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

🔏 Save EVA File As		×
😋 🔍 🗢 📕 « Bru	uker AXS → Tutorials → EVA →	٩
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 ★ My Favorites ■ Desktop Downloads ≅ Recent Places EVA ■ Libraries ■ Documents Music ■ Pictures ■ Videos 	Document.eva	
File name:	Znox	•
Type :	EVA files (*.eva)	
) Hide Folders	Save Save	

Figure 14.4: Saving Znox.EVA document

15 Computing the Crystallinity

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

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

Steps

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

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



- 1. Click New on the File menu or use the dedicated button in the toolbar.
 - The EVA document is empty.
- 2. Click the Import from files data command or the Import from files button.
 - The Import From Files dialog box will be displayed.
- 3. Search the Tutorials/EVA* directory and select the m2.RAW file.
- 4. Click **Open**. The scan m2 will be added to the Data tree and displayed in the graphical view of the EVA document.
- * The directory path to the EVA tutorial files is C:\Documents and Settings\All Users\Application Data\Bruker AXS\Tutorials under Windows XP and C: \ProgramData\Bruker AXS\Tutorials under Windows 7.

Crganize New folder	▶ T	utorials > EVA > -	Search : EVA ₿₿ ▼	<u>ب</u> م ا
 ★ My Favorites ■ Desktop ➡ Downloads ™ Recent Places ➡ EVA ➡ My Documents ➡ Libraries ➡ Documents ➡ Music 	E	BX100.bt Cc.raw Corundum-1.raw Corundum-2.raw Corundum-3.raw CPD-2.raw CPD-2.raw DD.raw Description.bt D=DatableC-Scans_50-220C.brml Ep333f.raw	ET50.raw ET80.raw Francolite.raw Frank.raw Guil4.raw KCP.raw LaB6.brml m1.raw M.raw m3.raw Mineral Mixture.brml	Niore.raw Pbznox.rav Pbznox.rav Pchips.rav Pegmin.ra Pig.raw Quartz.rav Spikes.raw Tb3.raw Temp_C.d Mul.raw Wup.raw
 Pictures Videos 	-	▲ ET20.raw	wh4no3.raw	Znox1.raw
File	e nar	ne: "Znox2.raw" "Znox1.raw"	Measurement files (*.i Open	brml;*.rav 💌 Cancel

Figure 15.1: Importing m2.raw

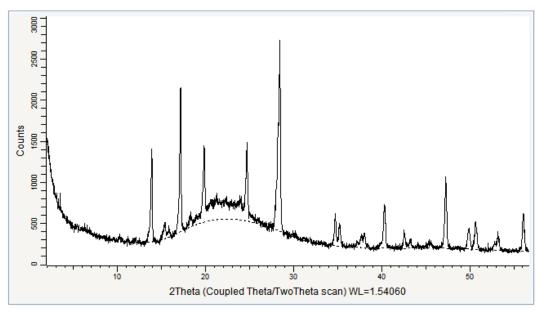


Figure 15.2: m2 file imported in the graphical view

15.2 Step 2: Computing the Crystallinity

 \triangleright Make certain the m2 scan is selected in the data tree.

- 1. Adjust the background. To do so:
- 2. Click **Background** in the Tool list of the Data Command panel

click the **Background** button on the Scan toolbar

right-click the scan in the data tree and then click **Tool** on the context menu. Click **Background** on the Tool submenu.

- The background dialog box will be displayed.
- 3. Adjust the background curvature as shown below.

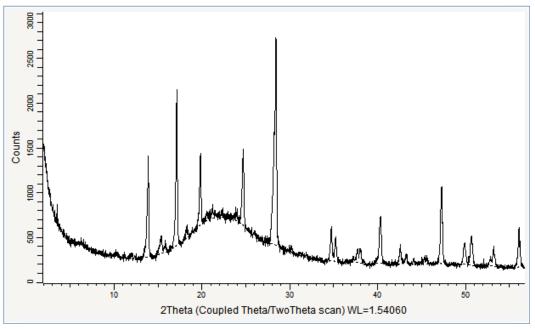


Figure 15.3: Background adjusted

X

- 4. 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 Crystallii	~
Cristallinity - From	2,000
Cristallinity - To	56,700
%-Crystallinity	39,8 %
%-Amorphous	60,2 %
Global Area	2878
Reduced Area	1146

15.3 Step 3: Checking the Results

You can check the results by computing the global area "manually".

 \triangleright Make certain the m2 scan is selected in the data tree.

1. Click **Background** in the Tool list of the Data Command panel

click the Background button on the Scan toolbar

— or —

— or —

right-click the scan in the data tree and then click **Tool** on the context menu. Click **Background** on the Tool submenu.

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

click the Create Area button on the Peak / Area toolbar

— or —

– or -

right-click the multi-selection, and then click **Tool** on the context menu. Click **Create Area** on the Tool submenu.

- The Create Area dialog box will be displayed.
- 7. Enter the left and right angle values (2 and 56.7) of the scan to compute the corresponding area. The value to look at is the raw area.



Create Area m2.RAW #3	×
Angle (deg.)	Intensity (cps)
Left Angle 2.000	Left Int0.67
Right Angle 56.700	Right Int3.15
Obs. Max 28.412	Gross Int. 834
FWHM 6.131	Net Height 836
Chord Mid. 25.449	Scherrer evaluation
I. Breadth 3.566	Crystallite Size 14.9
Gravity C. 27.176	Use FWHM 🔘
Area (cps x deg.)	Use I. Breadth 🔵
Raw Area 2878	K = 1
Net Area 2982	Instr. Width = 0
Press and select an Area	Append this Area

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

%Amorphous= Global area - Reduced area Global area

%Crystallinity=100 - %Amorphous

15.4 Step 4: Saving

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

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File name: m Type : EV	2 (A files (*.eva)	•
Hide Folders		ancel

Figure 15.4: Saving m2.EVA document

16 Simulating a Slit Mode

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

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

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

The following chapter describes the basic procedure for simulating a slit mode. The scan used is held as a tutorial file, LaB6.BRML, found in the Tutorial directory. LaB6 was measured using variable slits.

Steps

Ŧ

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

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

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



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

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My Favorites Desktop Cownloads Recent Places EVA My Documents		Cc.raw Corundum-1.raw Corundum-2.raw Corundum-3.raw CPD-2.raw CSand.raw DD.raw		Francolite.raw Frank.raw Guil4.raw KCP.raw LaB6.brml m1.raw m2.raw	Pegmin.rav Pig.raw Quartz.raw Spikes.raw Tb3.raw Temp_C.da Vm1.raw
 □ Libraries □ Documents □ Music □ Pictures □ Videos 		Docription.txt Description.txt DTA-300LC-Scans_50-220C.brml Ep333f.raw ET20.raw ET20.raw ET50.raw ET50.raw ET80.raw		m3.raw Mineral_Mixture.brml Nh4no3.raw Niore.raw Pbznox.raw Pchips.raw	Wp.raw Wp.raw Znox1.raw
Fil	e nam	< III III	•	Measurement files (* Open	.brml;*.rav 👻 Cancel

Figure 16.1: Importing LaB6.brml

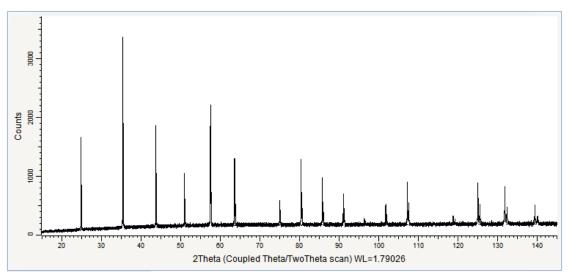


Figure 16.2: LaB6 file imported in the graphical view

16.2 Step 2: Performing the Search/Match Operation

 \triangleright Make certain the LaB6 scan is selected in the data tree.

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

品	ΙΞ	FOM	Match	%	Source	ID	Name	Quality	Status	Formula
	1	146,72 %	29 0	_	PLU2016	PDF 04-005-3486	Boron Lanthanum Samarium	Prototyping	👩 Primary	La0.56 Sm0.44 B5.9
	2	125,06 %	30 0	_	PLU2016	PDF 04-005-7139	Boron Lanthanum Samarium	Prototyping	👩 Primary	La0.59 Sm0.41 B6
Ð	3	124,95 %	30 0	-	PLU2016	PDF 04-005-9344	Boron Lanthanum Samarium	Prototyping	👩 Primary	La0.5 Sm0.5 B6
	4	116,63 %	29 0	-	PLU2016	PDF 00-058-0337	Boron Lanthanum Samarium	🚱 Star (*)	👩 Primary	B6 La0.6 Sm0.4
	5	98,70 %	24 0	_	PLU2016	PDF 00-040-1310	Boron Europium Carbide	Calculated	👩 Primary	B5.80 C0.20 Eu
	6	90,01%	24 0	-	PLU2016	PDF 04-005-7137	Boron Cerium Lanthanum	Prototyping	👩 Primary	La0.59 Ce0.41 B6
	7	89,0 <mark>4 %</mark>	30 0		PLU2016	PDF 04-005-9736	Boron Lanthanum Tungsten	Prototyping	👩 Primary	La0.5 W0.5 B6
	8	77,83 %	21 0	_	PLU2016	PDF 00-057-0823	Potassium Bismuth Zirconium	🚱 Star (*)	👩 Primary	K0.5 Bi0.5 Zr O3
Ð	9	72, <mark>83 %</mark>	34 0		PLU2016	PDF 00-059-0332	Lanthanum Boride	🛞 Star (*)	👩 Primary	La B6
	10	71, <mark>87 %</mark>	13 0	-	PLU2016	PDF 00-058-0593	Barium Indium Lanthanum Yt	🚱 Star (*)	👩 Primary	La0.6 Ba0.4 In0.9 Y
Ð	11	62,34 %	28 2	-	PLU2016	PDF 04-010-2753	Cesium Lithium Molybdate	Prototyping	👩 Primary	Cs Li (Mo O4)
			#				1 A 1 A 1 - A			>

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

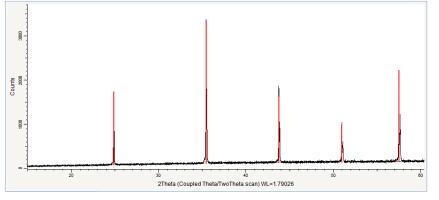


Figure 16.3: Zoom on the scan and the pattern (2θ =20° to 60°)

16.3 Step 3: Simulating a Slit Mode

 \triangleright Make certain the LaB6 scan is selected in the data tree.

- In the Scan Property Table, change the Simul. Slit Mode property from Variable to Fixed.
 - The intensities of the scan will be recalculated. The other scan related data, a pattern in this example, will be projected as well.

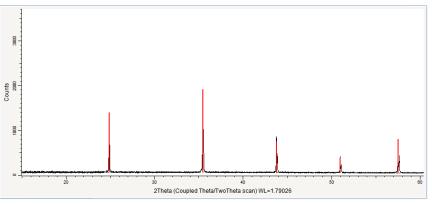


Figure 16.4: Zoom on the scan and the pattern (2θ =20° to 60°)

16.4 Step 4: Saving

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

🔏 Save EVA File As		×
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File name: LaB6		-
Type : EVA files (*.eva)		
Hide Folders	Cancel	

Figure 16.5: Saving LaB6.EVA document

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

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

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

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

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

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

Steps

H-

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

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

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



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

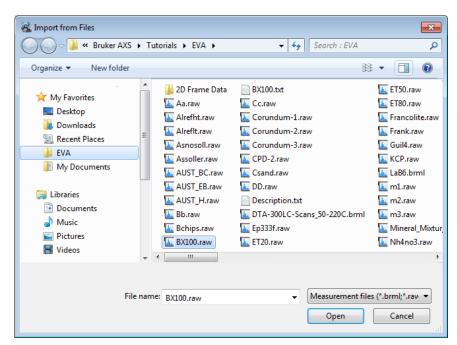


Figure 17.1: Importing BX100.raw

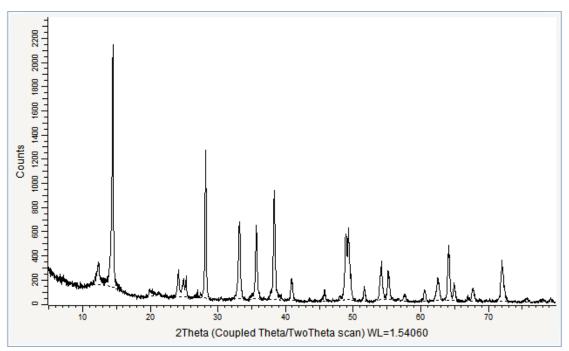


Figure 17.2: BX100.RAW imported in the graphical view

17.2 Step 2: Performing the Search/Match Operation

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

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

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

	\odot	品	Ξ	FOM	Match	%	Source	ID	Name	I/ICor	Quality	Status	Formula	
•		İİ		34,85 %	26	1	PLU2016	PDF 00-021-1307	Boehmite, syn		1 Indexed	🙆 Primary	AlO(OH)	^
			2	26,06 %	26 (0	PLU2016	PDF 04-002-2984	Vanadium Iron Oxide	2,62	Prototyping	👩 Primary	V Fe O3	::
		Ð	3	25,50 %	27	3	PLU2016	PDF 04-010-7290	Titanium Nickel Oxide	2,6	🚱 Star (*)	👩 Primary	Ti Ni O3	
			4	25,32 %	25	2	PLU2016	PDF 04-009-6569	Titanium Iron Oxide	2,53	 Indexed 	👩 Primary	Ti0.228 Fe1.698 O3	
			5	25,26 %	27	2	PLU2016	PDF 04-009-5898	Titanium Iron Oxide	2,58	📵 Blank	👩 Primary	Ti0.22 Fe1.78 O3	
			6	25,09 %	27	2	PLU2016	PDF 01-073-8433	a-Fe1.85 H0.45 O3, Hem	2,9	🚱 Star (*)	👩 Primary	Fe1.85 H0.45 O3	
			7	24,70 %	27	1	PLU2016	PDF 04-017-9544	Manganese Iron Oxide	2,81	Prototyping	👩 Primary	Mn0.2 Fe1.8 O3	
		Ð	8	24,39 %	25	1	PLU2016	PDF 04-006-6579	Iron Oxide	3,04	 Indexed 	👩 Primary	Fe2 O3	
		Ð	9	23,28 %	26	2	PLU2016	PDF 01-077-9924	Hematite, syn	3,17	🚱 Star (*)	👩 Primary	Fe1.92 O3	
			10	23,14 %	26	2	PLU2016	PDF 04-006-5322	Iron Aluminum Oxide	2,6	Prototyping	👩 Primary	Fe1.78 Al0.22 O3	
			11	22,40 %	27	2	PLU2016	PDF 01-088-0434	Iron Tin Oxide	2,43	🚱 Star (*)	👩 Primary	Fe1.727 Sn0.205 O3	
			14	22,16 %	26	3	PLU2016	PDF 04-011-9587	Manganese Iron Oxide	3,27	 Indexed 	👩 Primary	Mn0.176 Fe1.824 O3	
			15	21,90 %	26	4	PLU2016	PDF 04-018-8870	Iron Neodymium Oxide	3,37	🚱 Star (*)	👩 Primary	Nd0.1 Fe1.9 O3	
			16	21,84 %	25	1	PLU2016	PDF 04-018-8871	Iron Neodymium Oxide	3,95	🚱 Star (*)	🙆 Primary	Nd0.3 Fe1.7 O3	\sim
					::								>	

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

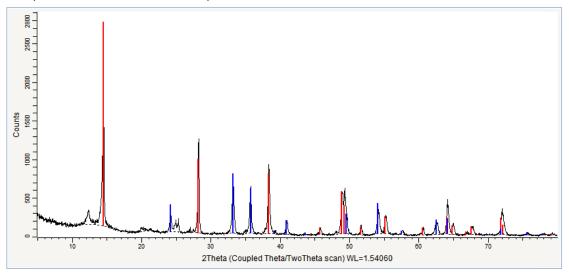


Figure 17.3: Boehmite pattern in red and Iron Oxide pattern in blue

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

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

₽Ļ	Sort Ascending
Z↓	Sort Descending
8	Group By This Column
	Show Group By Box
	Hide This Column
1	Column Chooser
↓	Best Fit
	Best Fit (all columns)

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

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

7. Drag first the **Name** column header and then the **I/ICor** column to the grouping area.

Candidates will be grouped first by Name and then by I/ICor value.

Sc	ans	Search List	DB View									
	Vame	e û I/ICo	r û									
		0	FOM	Match	%	Source	ID	Quality	Status	Formula	Organic	Inorg
	÷	Name: Iro	n Yttrium P	hosphide								^
	÷.	Name: Iro	n(III) trifo	rmate (carb	on di	oxide) hy	drate Iron Carl	bon Oxide Fo	ormate Hydrate	2		
	÷	Name: Jia	nshuiite									
		Name: Kad	linite-1A									
	1	+ I/ICor										
Þ	1	I/ICor	0,98									
			49 18,83	% 30 30		PLU2016	PDF 04-010-4800	 Indexed 	👩 Primar	y Al2 Si2 O5 (O H)4		I
	÷.	Name: Kad	linite-1Ad									
	÷	Name: Kad	linite-mon	itmorillonite								
	۰.	Name: Kor	nelite, syn									
	÷	Name: Lan	thanum Br	romide Hydr	oxide	Hydrate						~
<					::							>

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

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

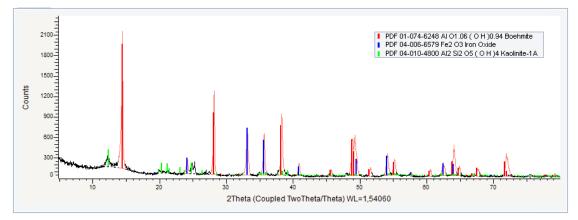


Figure 17.4: Boehmite pattern in red, Iron Oxide pattern in blue and Kaolinite-1A pattern in green.

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

- 1. Select the scan BX100.RAW either in the data tree or in the graphical view.
- 2. Click Import XRF Results in the Data Command panel

— or -

Right-click the scan, then click Import XRF Results on the context menu.

- The Open an XRF results filename dialog box will be displayed.
- 3. Select the BX100.txt file in the Open an XRF results filename dialog box and click Open.
 - The results of the chemical analysis will be displayed in the element list in the data tree next to the SQD results.

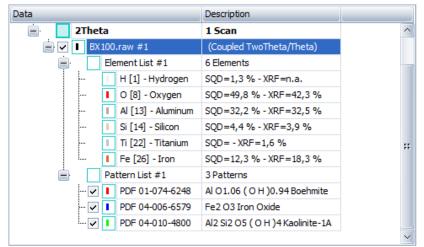


Figure 17.5: The chemical analysis indicates that the sample contains titanium.

Create a chemical filter from Titanium. To do so:

- 1. Select the Titanium in the data tree.
- 2. Click Green Filter data in the Data Command panel.

Right-click the scan, then click Create|Green Filter data on the context menu.

- A new chemical filter is created: BX100.RAW #1 Green Filter.
- 3. Another run using this new chemical filter makes it then possible to identify Anatase (PDF 04-014-0491).

— or –

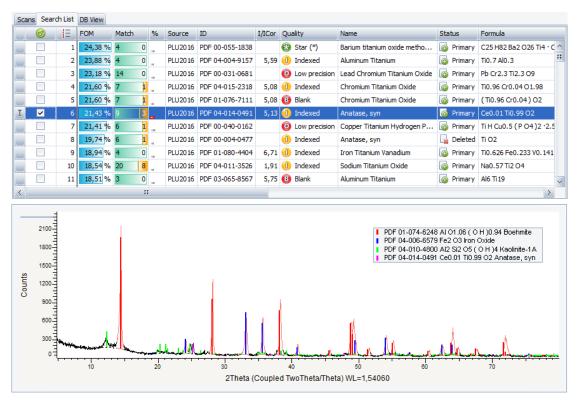


Figure 17.6: Boehmite pattern in red, Iron Oxide pattern in blue, Kaolinite-1A pattern in green and Anatase pattern in pink.

17.3 Step 3: Performing the Semi-Quantitative Phase Analysis

Once all the phases have been identified, the semi-quantitative analysis can be performed The first phase identified in the list is Boehmite.

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

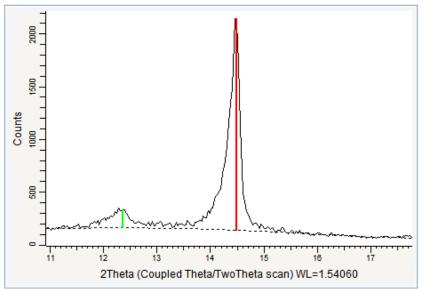


Figure 17.7: Zoom on the peaks (2θ =38° to 48°)

3. Proceed the same way for the other phases.

1.

- 4. Select the BX100 scan either in the data tree or in the 1D view.
- 5. Click **Pattern Column View** in the Create list of the Data Command panel or
 - click the Pattern Column View button on the Create View toolbar. or —

right-click and then click Create. Click Pattern Column View on the submenu.

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

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

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

To display the results as a pie or bar chart:

- 1. Select the pattern list in the data tree.
- 2. Click **Pattern Chart View** in the Create list of the Data Command panel or —

click the Pattern Chart View button on the Create View toolbar.

- or Right-click and then click **Create.** Click **Pattern Chart View** on the submenu.
- 3. Select either **Pie Chart** or **Bar Chart** in the Pattern Chart View table.

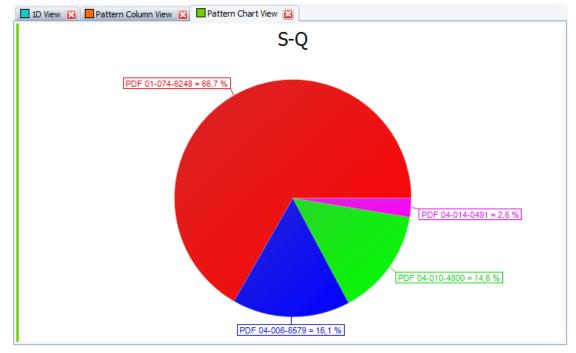


Figure 17.9: Semi-quantitative analysis results as a pie chart

17.4 Step 4: Saving

1. Click Save As on the File menu.

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

🔏 Save EVA File As		×
😋 🗢 🕨 « Bru	iker AXS → Tutorials → EVA →	٩
Organize 👻 Ne	w folder	
 My Favorites Desktop Downloads Recent Places EVA EVA Libraries Documents Music Pictures Videos 	Document.eva	
File name:	BX100	-
Type : [EVA files (*.eva)	•
Alide Folders	Save	Cancel

Figure 17.10: Saving BX100.EVA document

18 Using the d Multiplied By Tool

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

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

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

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

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

Csand is white coral sand from a beach in Hawaii.

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

Steps

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

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

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

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



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

🔏 Import from Files				—
Sruker AXS	• Tute	orials 🕨 EVA 🕨	✓ Search : EVA	٩
Organize 🔻 New folder			8.8	•
My Favorites Desktop Downloads Recent Places EVA My Documents Cibraries Documents		2D Frame Data Aa.raw Alrefht.raw Alrefht.raw Asnosoll.raw Assoller.raw AUST_BC.raw AUST_EB.raw AUST_H.raw Bb.raw	BX100.txt Cc.raw Corundum-1.raw Corundum-2.raw Corundum-3.raw CPD-2.raw CPD-2.raw DD.raw Dc.raw Dc.raw Dr.raw Dr.raw Dr.raw Dr.raw	ET50.raw ET80.raw Francolite.raw Frank.raw Guil4.raw KCP.raw LaB6.brml LaB6.brml m1.raw m2.raw M3.raw
 Music Pictures Videos 	+ (L Bchips.raw BX100.raw	🗽 Ep333f.raw 🗽 ET20.raw	L Mineral_Mixture Nh4no3.raw
File	name:	Csand.raw	Measurement file Open	s (*.brml;*.rav 💌 Cancel

Figure 18.1: Importing Csand.raw

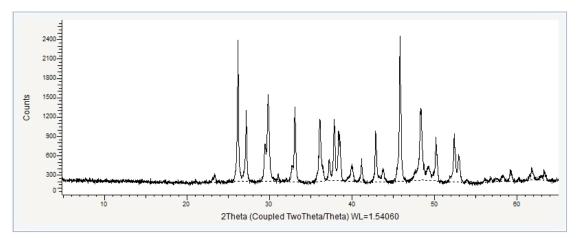


Figure 18.2: Csand scan imported in the graphical view

18.2 Step 2: Performing the Search/Match Operation

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

Scans	Sear	ch List	DB \	/iew										
	0	品	Û	FOM	Match	%	Source	ID	I/ICor	Quality	Name	Sta	itus	
۱.				33,66 %			PLU2016	PDF 00-001-0628		📵 Blank	Aragonite		Delete	^
		Ð	2	27,10 %	35 2		PLU2016	PDF 04-013-9616	0,33	🚱 Star (*)	Aragonite	œ	Primar	11
			7	14,27 %	26 1		PLU2016	PDF 00-036-1149		 Indexed 	Iridium Silicon	œ	Primar	
			8	13,83 %	19 2	-	PLU2016	PDF 01-080-3277	3,15	Hypothetical	Calcite, syn	œ	Primar	
			9	11,71 %	10 0	-	PLU2016	PDF 04-016-4799	30,71	 Indexed 	Thorium Uranium Telluride	œ	Primar	
		Ð	10	11,67 %	19 2	-	PLU2016	PDF 00-043-0697		🚱 Star (*)	Calcite, magnesian	œ	Primar	
		Ð	11	10,99 %	19 2	-	PLU2016	PDF 04-014-6291	5,45	 Indexed 	perovskite group Cobalt Str	¢	Primar	
			12	10,84 %	10 0	-	PLU2016	PDF 04-005-3806	11,16	 Indexed 	Titanium Niobium Carbide	œ	Primar	
			13	10,69 %	10 1	-	PLU2016	PDF 01-075-5492	9,25	🚱 Star (*)	Neodymium Strontium Cobalt	œ	Primar	
			14	10,57 %	10 0		PLU2016	PDF 01-082-8288	6,25	Hypothetical	Iron Nickel	œ	Primar	
			15	10,57 %	8 0	-	PLU2016	PDF 00-019-0745		📵 Blank	Lutetium Telluride	œ	Primar	
			16	10,50 %	10 0	-	PLU2016	PDF 04-019-6237	12,17	 Indexed 	Chromium Niobium Carbide	œ	Primar	
			17	10,47 %	10 0		PLU2016	PDF 04-002-2765	2,3	Prototyping	Europium Aluminum Nitride O	œ	Primar	,
<				::									>	

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

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

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

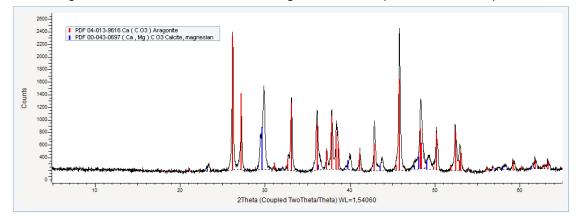


Figure 18.3: Aragonite pattern in red and Magnesian calcite in blue

18.3 Step 3: Using the d Multiplied By Tool

- 1. Insert the pure Calcite pattern (PDF 00-005-0586) by using the Search by name tool.
- 2. Zoom in around the location of the 100% line of pure Calcite.
- 3. Select the Calcite pattern in the data tree.
- 1. Click **d x by** in the Data Command panel — or —

click the d x by command on the Pattern toolbar

— or —

right-click the pattern, then click **d x by** on the context menu.

- The d x by dialog box will be displayed.
- 2. Set the **d Multiplied by value** to 0.990 using the slider. It shows the Magnesian calcite pattern (PDF 00-043-0697) corresponds to the pure Calcite d-spacing multiplied by about 0.990.

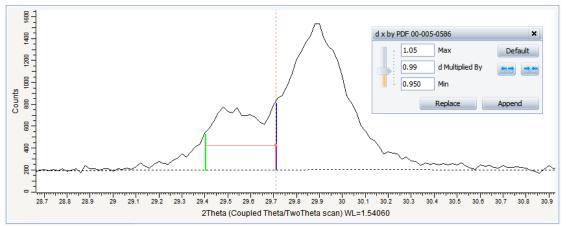
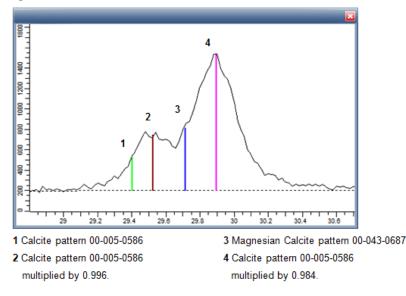


Figure 18.4: Adjusting the d Multiplied by value to 0.990 using the slider

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





18.4 Step 4: Saving

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

🔏 Save EVA File As		×
😋 🔍 🗢 📕 « Bri	uker AXS > Tutorials > EVA > - 47 Search : EVA	Q
Organize 🔻 No	ew folder 👫	• 🕡
 My Favorites Desktop Downloads Recent Places EVA EVA Libraries Documents Music Pictures Videos 	Document.eva	
File name:	Csand_dxBy	•
Type :	EVA files (*.eva)	
) Hide Folders	Save Save	ancel

Figure 18.5: Saving Csand_dxBy.EVA document

19 Using the Tune Cell Tool

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

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

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

The following procedure describes how use the Tune Cell tool.

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

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

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

Steps

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

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

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



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

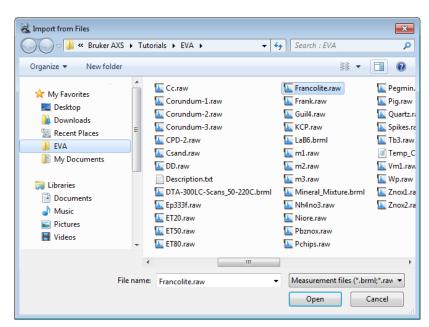


Figure 19.1: Importing Francolite.raw

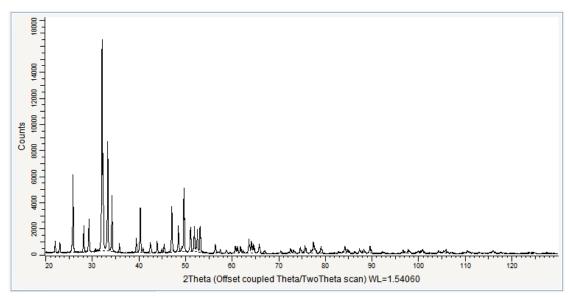


Figure 19.2: Francolite.RAW imported in the graphical view

19.2 Step 2: Performing the Search/Match Operation

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

Scan	is Sea	rch List	DB \	/iew									
	\bigcirc	*	Û	FOM	Match	%	Source	ID	I/ICor	Quality	Name	Sta	tus
		Ð	1	56,37 %	90 0		PLU2016	PDF 01-073-9695	0,96	 Indexed 	Carbonate-fluorapatite (NR)	~	
			4	19,53 %	81 18		PLU2016	PDF 04-006-8991	1,16	Prototyping	Sodium Calcium Yttrium Fluori	œ	Prii ^{FF}
			5	19,44 %	80 1 <mark>4</mark>		PLU2016	PDF 04-002-2456	1,08	Prototyping	Calcium Carbonate Phosphate	œ	Prii
			6	19,09 %	83 1 <mark>9</mark>		PLU2016	PDF 01-073-9462	1,1	 Indexed 	Fluorapatite, manganous, syn	œ	Prii
			7	18,85 %	81 18		PLU2016	PDF 04-009-8338	1,11	📵 Blank	Fluorapatite, syn	œ	Prii
			13	1 6,88 %	80 1 <mark>5</mark>	-	PLU2016	PDF 04-015-6661	1,35	 Indexed 	Fluorapatite, strontian, hydr	œ	Prii
I	~		15	15,74 %	82 <mark>29</mark>	_	PLU2016	PDF 01-080-8486	1,11	🛞 Star (*)	Fluorapatite, syn	Ð	Pri
			16	15,43 %	82 <mark>2</mark> 1		PLU2016	PDF 04-017-1403	1,09	 Indexed 	Fluorapatite, manganoan	œ	Pri
			19	15,25 %	81 28		PLU2016	PDF 01-076-0560	1,06	 Indexed 	Fluorapatite, neodymian, syn	œ	Pri
			23	14,88 %	80 30		PLU2016	PDF 01-076-0559	1,05	 Indexed 	Fluorapatite, neodymian, syn	œ	Pri
			37	12,98 %	76 24	_	PLU2016	PDF 04-015-2186	1,02	🚱 Star (*)	Fluorapatite, syn	æ	Prii 🗠
<				££									>

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

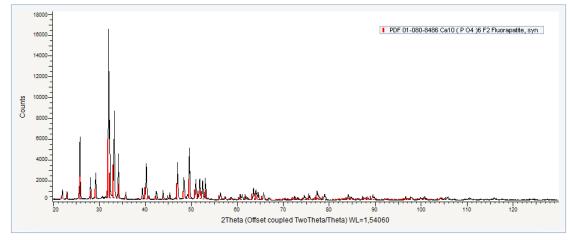


Figure 19.3: Fluorapatite pattern in blue

19.3 Step 3: Performing the Tune Cell Operation

- 1. Select the Fluorapatite pattern in the data tree.
- 2. Click Tune Cell in the Data Command panel

— or — click the **Tune Cell** button on the Pattern toolbar

— or —

- right-click the pattern, then click Tune Cell on the context menu.
- The Tune cell dialog box will be displayed.
- 3. In the list of parameters, click **a**, and then click **hk0** in the **Show** drop-down list to see lines which position depend only on *a*.

Tune Cell PDF 01-080-8486	×
a 🖂	System Hexagonal Default
9,460902 Max	Show h k 0 💌 😁 🛤
9,36723 Width	All Sticks indexed Filter < 1 % 💌
9,273559 Min	Replace Append

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

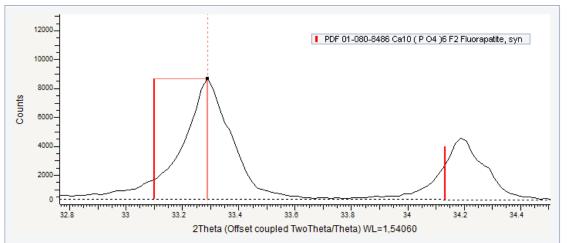


Figure 19.4: (300) stick (located at 2theta=33.129°) of the pattern PDF 00-015-0876 shifted to fit the corresponding peak.

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

19.4 Step 4: Saving

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

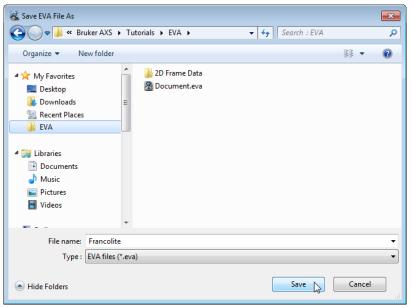


Figure 19.5: Saving Francolite.EVA document

20 Displaying a Pattern with Another Wavelength

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

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

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

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

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

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

Steps

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

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

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WÌ,

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

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



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

🔏 Import from Files										
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	∢ File name:	Francolite.raw	Measurement files (*.brr Open C	► ml;*.raw ▼ Cancel						

Figure 20.1: Importing Francolite.raw

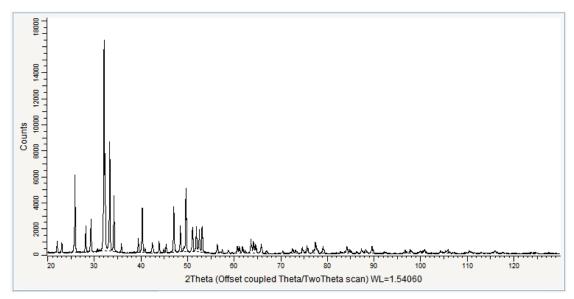


Figure 20.2: Francolite.RAW imported in the graphical view

20.2 Step 2: Performing the Search/Match Operation

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

	\odot	*	E	FOM	Match	%	Source	ID	I/ICor	Quality	Name	5
	~	0	1	56,37 %	90 0		PLU2016	PDF 01-073-9695	0,96	 Indexed 	Carbonate-fluorapatite (NR)	^
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			38	12,95 %	76 22	-	PLU2016	PDF 01-073-7334	0,86	🚱 Star (*)	Carbonate-hydroxylapatite,	
			57	9,91 %	33 2	-	PLU2016	PDF 00-019-0272		📵 Blank	Carbonatehydroxylapatite, s	
			4	19,53 %	81 1 <mark>8</mark>	-	PLU2016	PDF 04-006-8991	1,16	Prototyping	Sodium Calcium Yttrium Fluori	
			5	19,44 %	80 1 <mark>4</mark>	-	PLU2016	PDF 04-002-2456	1,08	Prototyping	Calcium Carbonate Phosphate	
		Ð	6	19,09 %	83 1 <mark>9</mark>	-	PLU2016	PDF 01-073-9462	1,1	 Indexed 	Fluorapatite, manganous, syn	
			8	18,74 %	76 1 <mark>2</mark>	-	PLU2016	PDF 04-013-7494	1,05	 Indexed 	Hydroxylapatite, sulfatian	
		A	٥	18 57 %	81 14		PU12016	DDE 01-073-0607	1.01	Indexed	Carbonate-fluoranatite (NP)	\sim

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

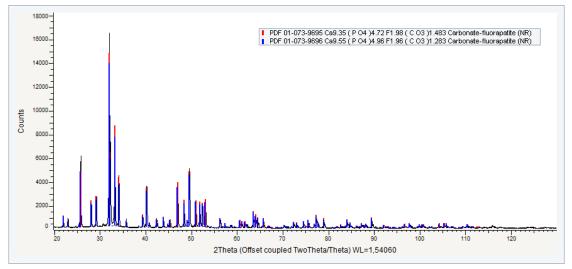


Figure 20.3: The two patterns of Carbonate-fluorapatite are superposed.

20.3 Step 3: Changing the Wavelength

We want to check if there is a pollution of the X-ray tube. The WL α 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 WL α 1 radiation.

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

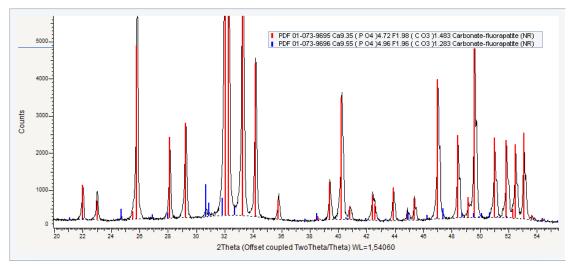


Figure 20.4: Carbonate-fluorapatite pattern displayed with the WLa1 wavelength in blue and original pattern in red.

- 5. Zoom on the 20-55° 2Theta range. The modified pattern looks to match some parts of the scan.
- ⇒ It makes it possible to conclude there is likely a pollution of the X-ray tube.

20.4 Step 4: Saving

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

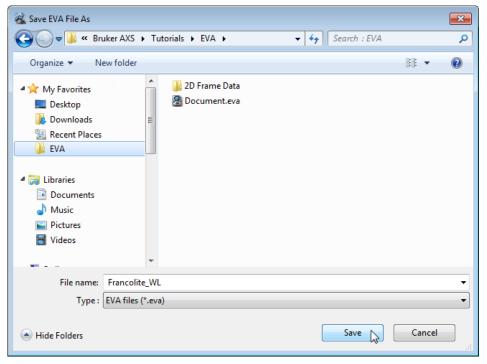


Figure 20.5: Saving Francolite_WL.EVA document

21 Working with the Waterfall View

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

Steps

H-

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

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

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



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File name: Ep333f.raw Measurement files (*.brml;*.raw Den Cancel							

Figure 21.1: Import a Scan File dialog box

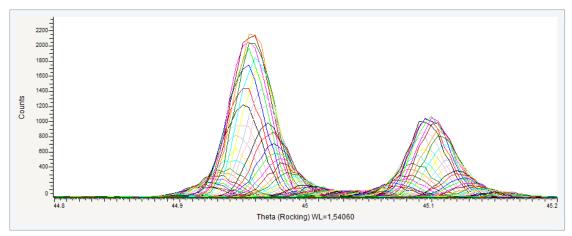


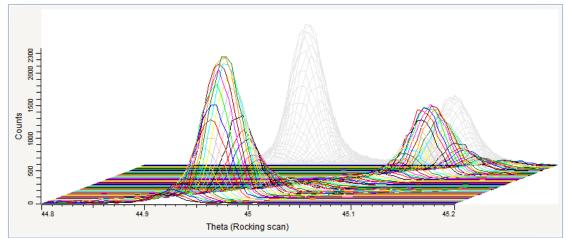
Figure 21.2: Ep333f.RAW file imported in the graphical view

21.2 Step 2: Creating and Working with the Waterfall View



1. Click the **Waterfall Display** button on the 1D View toolbar — or —

select the Waterfall display check box in the View property panel.



• The scans will be displayed as a waterfall.

Figure 21.3: Waterfall display

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

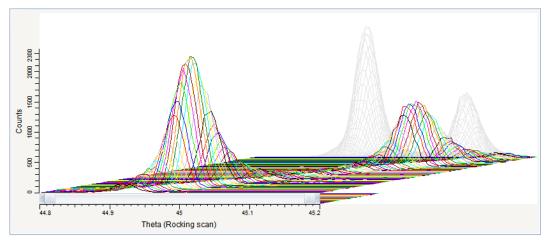


Figure 21.4: Perspective horizontally modified

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

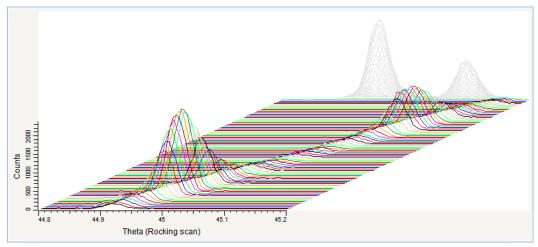


Figure 21.5: Perspective horizontally and vertically modified

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

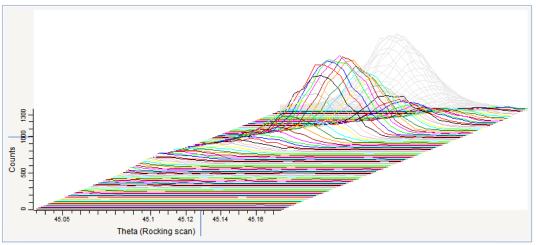


Figure 21.6: Zoom on the right peak

21.3 Step 3: Saving

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

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Figure 21.7: Saving Ep333f.EVA document

22 Working with the 2D View

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

Steps

H-

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

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

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



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

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Figure 22.1: Import a Scan File dialog box

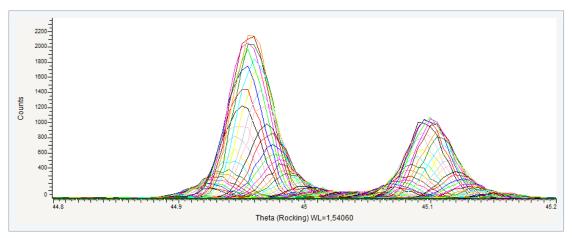


Figure 22.2: Ep333f.RAW file imported in the graphical view

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

Case #1: 2D view with intensity map

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

1. Click 2D View in the Create list of the Data Command panel

— or —

click the **2D View** button on the Create View toolbar — or —

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

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

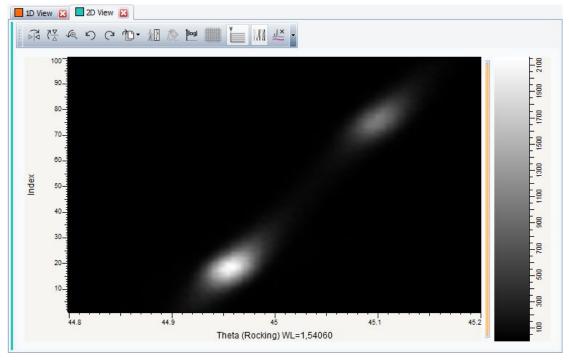


Figure 22.3: 2D view with intensity map

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

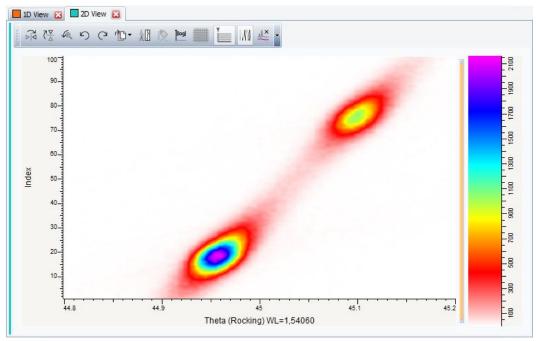


Figure 22.4: 2D view with colored intensity map

Case #2: 2D view with levels

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

1. Click **Create Level** in the Tool list of the Data Command panel — or —

right-click the scan list in the data tree to display the context menu. Click **Tool** and then **Create Level** on the related submenu.

The Create Level Theta dialog box will be displayed. By default 5 automatic levels will be created. They are displayed as ghost levels on the graphical view.

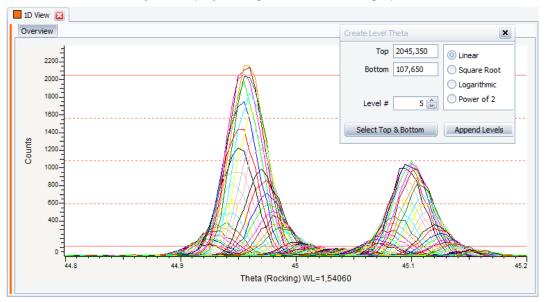
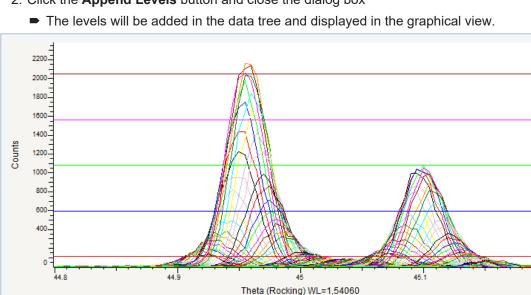


Figure 22.5: Creating levels: Create Level dialog box and ghost levels in the graphical view

80



2. Click the Append Levels button and close the dialog box

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

3. Click 2D View in the Create list of the Data Command panel — or —

click the 2D View button on the Create View toolbar

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

The 2D View will be displayed in a new tab. The Intensity map and the Levels are displayed by default. Leave the Intensity map and the Levels check boxes selected.

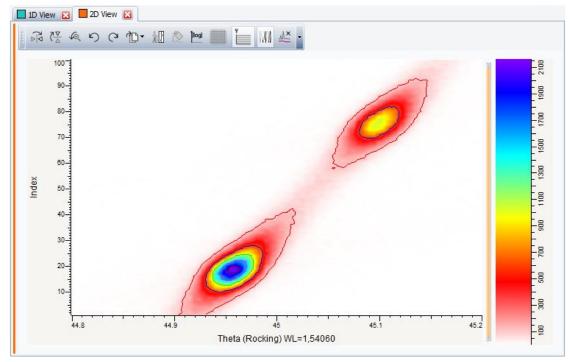


Figure 22.7: 2D view with intensity map and levels

45.2

22.3 Step 3: Saving

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

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Figure 22.8: Saving Ep333f-2D.EVA document

23 Working with the Side View

The following procedure describes how to work with waterfall view.

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

Steps

+

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

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

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

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

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Figure 23.1: Importing the scan

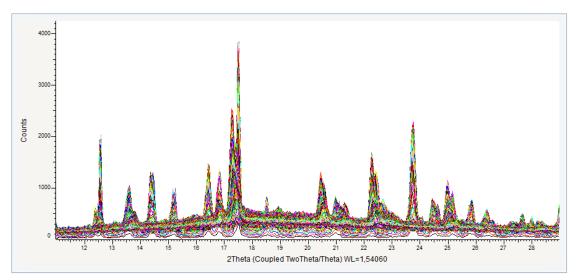
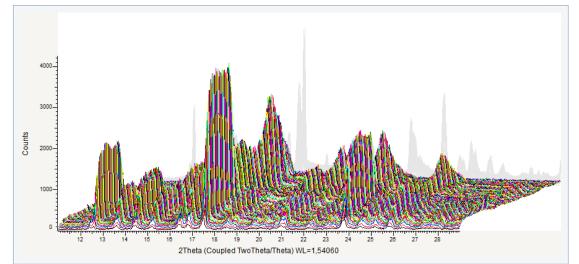


Figure 23.2: DTA-300LC-Scans_50-220C.BRML file imported in the graphical view

23.2 Step 2: Creating and Working with the Side View

1. Click the Waterfall Display button on the 1D View toolbar

— or — select the **Waterfall display** check box in the View property panel.



The scans will be displayed as a waterfall.

Figure 23.3: Waterfall display



AL_

2. Click the **Side View Display** button on the 1D View toolbar — or —

select the Side View Display check box in the View property panel.

• The side view will be displayed at the right of the waterfall view.

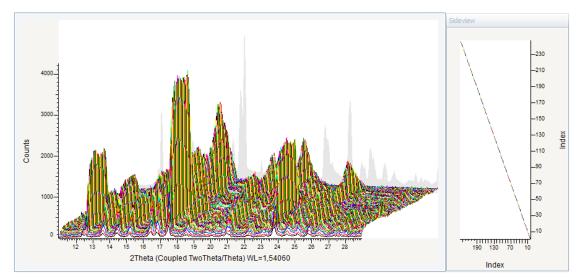


Figure 23.4: Side view added to the waterfall display

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

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

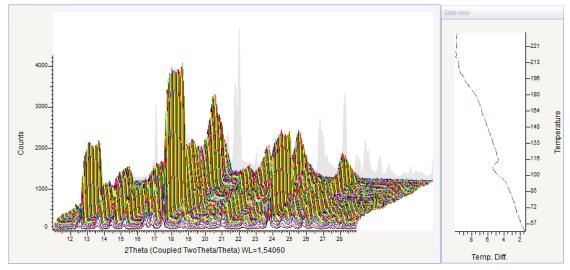


Figure 23.5: Side view with modified axes

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

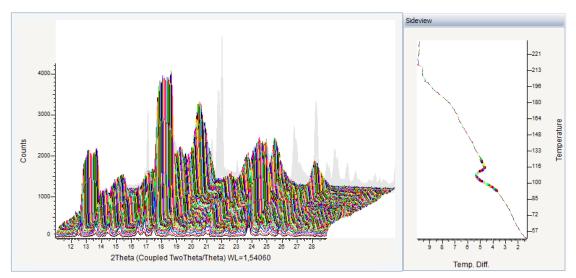


Figure 23.6: Selected scans highlighted in the Side view

23.3 Step 3: Saving

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

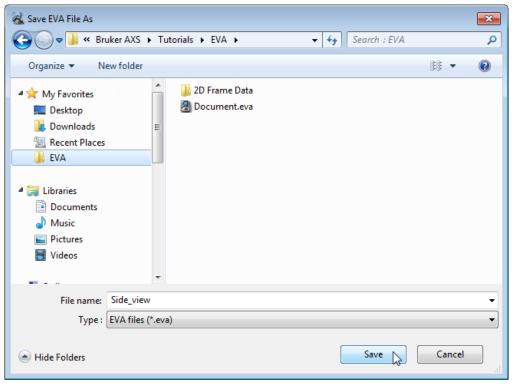


Figure 23.7: Saving Side_view.EVA document

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

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

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

Steps

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

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

- Ŧ
- 1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
 - The EVA document is empty.
- Ø.
- 2. Click the Import from files data command or the Import from files button.
- The Import From Files dialog box will be displayed.
- 3. Search the Tutorials/EVA* directory and select the Guil4.RAW file.
- 4. Click Open.
 - The scan Guil4 will be added to the Data tree and displayed in the graphical view of the EVA document.



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

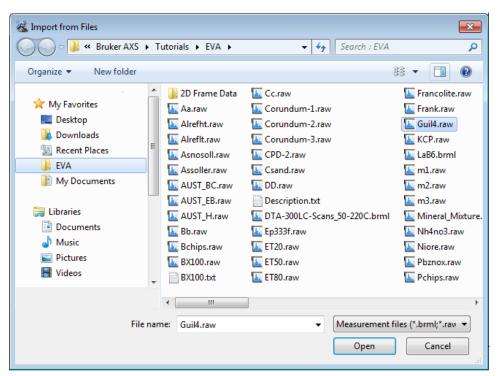


Figure 24.1: Importing Guil4.raw

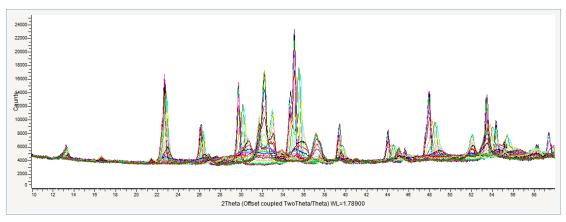


Figure 24.2: Guil4.RAW file imported in the graphical view

24.2 Step 2: Creating the 2D View with Levels

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

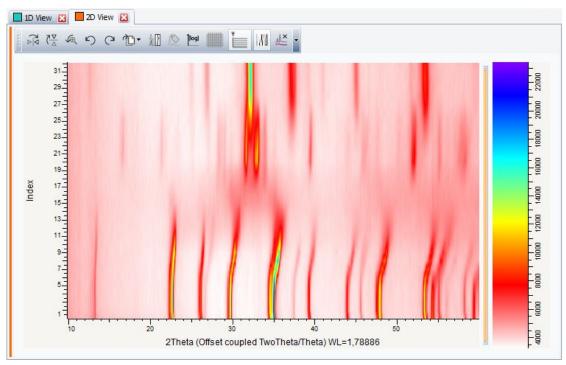
2. Click 2D View in the Create list of the Data Command panel

— or click the **2D View** button on the Create View toolbar

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

The 2D View will be displayed in a new tab.

20



3. Click Create Level in the Tool list of the Data Command panel

— or — right-click the scan list in the data tree to display the context menu. Click **Tool** and then **Create Level** on the related submenu.

 The Create Level Theta dialog box will be displayed. By default 5 automatic levels will be created.

Create Level 2Theta	×
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Bottom 4261,250	O Square Root
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Level # 5 💭	O Power of 2
Select Top & Bottom	Append Levels

Figure 24.3: Creating levels: Create Level dialog box

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

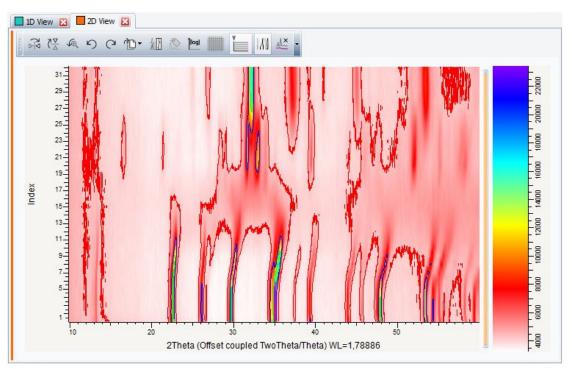


Figure 24.4: 2D view with intensity map and levels, scans sorted by index on the Y-axis

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

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

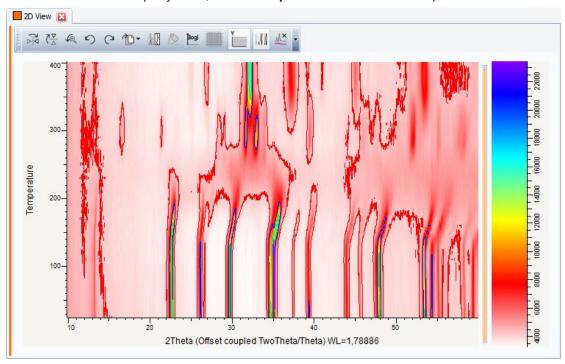


Figure 24.5: 2D view with intensity map and levels - scans sorted by temperature on the Y-axis

24.4 Step 4: Saving

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

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Figure 24.6: Saving Guil4.EVA document

25 Working with the PIP and VIP Views

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

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

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

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

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• The scan m1 will be displayed in the graphical view of the EVA document.

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

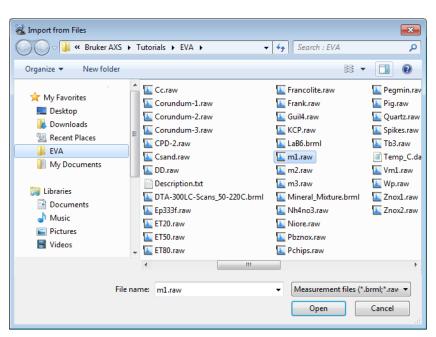


Figure 25.1: Importing the m1.RAW file

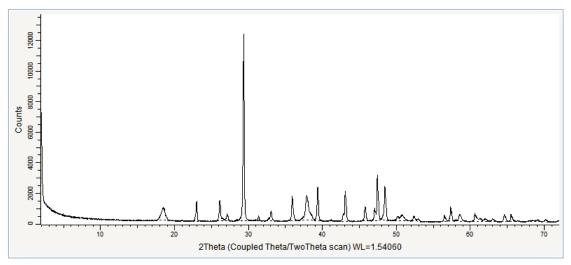


Figure 25.2: m1.RAW file imported in the Graphical view

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

Case #1: Creating a PIP view

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1. Click the PIP mode button on the view toolbar

— or —

right-click anywhere in the graphical view to display the context menu. In the context menu, click the **PIP Mode** command.

- A **PIP** text box will be added below the pointer.
- 2. Select the zone around the peak between the 2θ angles 22° and 24° .
 - A window corresponding to the selected zone is created.

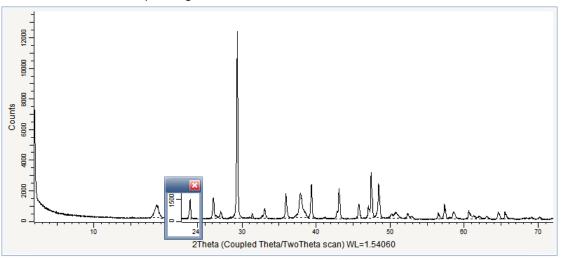


Figure 25.3: Creating a PIP view

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

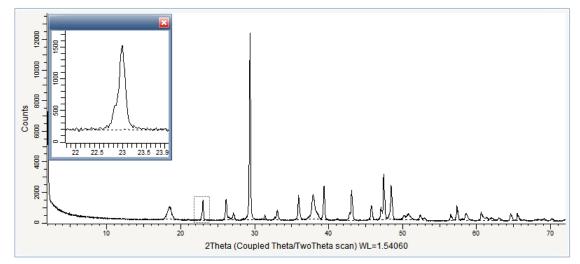


Figure 25.4: Moving and resizing the PIP view

4. Once you are satisfied with the PIP view, click anywhere in the graphical view.



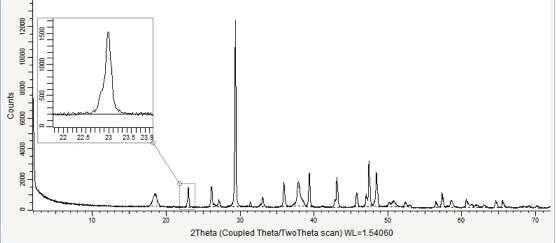


Figure 25.5: PIP view inserted and linked to the original zone

Case #2: Creating a VIP view

- 1. Zoom in on the zone between the 2θ angles 37° and 47° .
- 2. Click the VIP mode button on the view toolbar

— or — right-click anywhere in the graphical view to display the context menu. In the context menu, click the **VIP Mode** command.

- A VIP text box will be added below the pointer.
- 3. Select the zone between the 20 angles 40.5° and 41.5.°
 - The VIP view editor is displayed.



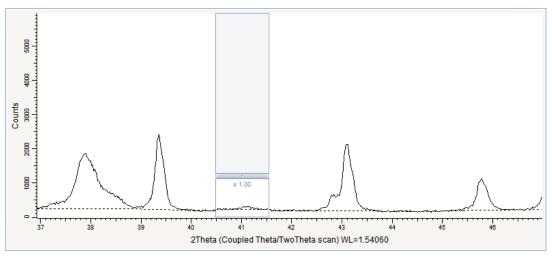


Figure 25.6: Creating a VIP view



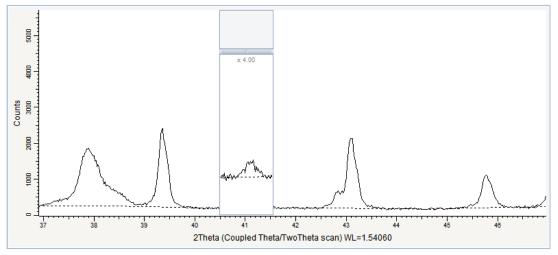


Figure 25.7: Changing the scale

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

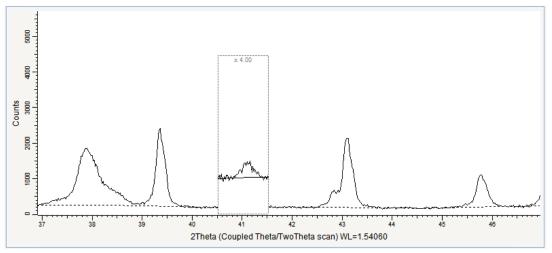


Figure 25.8: VIP view inserted in the graphical view

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

26 Creating a Label from a Peak

Peaks can be used to create labels.

To do so:

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

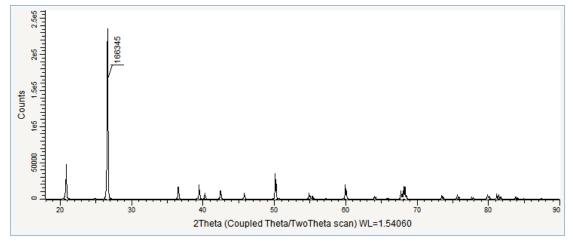
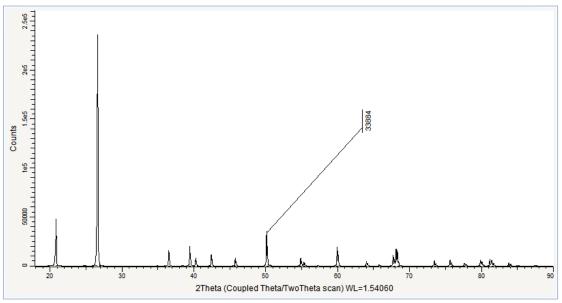
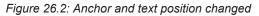


Figure 26.1: Peak inserted manually in the graphical view

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





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

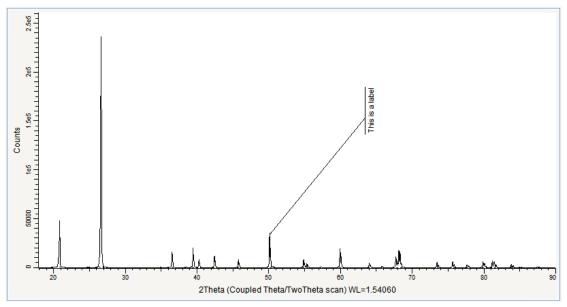


Figure 26.3: Anchor and text position changed

Customize the resulting "label" if necessary:

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

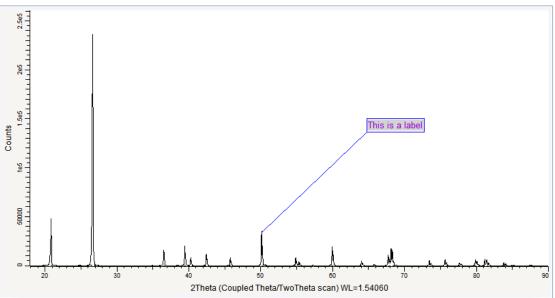


Figure 26.4: Label customized according to the procedure previously described

27 Loading and Integrating Mergeable 2D Frames

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

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

Steps

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

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

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



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

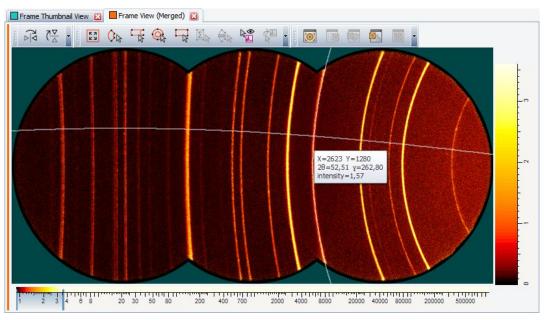


Figure 27.1: 2D Frame View after loading a measurement with three mergeable frames

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

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

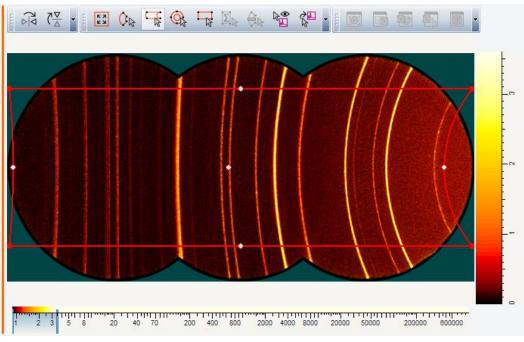


Figure 27.2: Slice Cursor prepared for the subsequent integration

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27.3 Step 3: Displaying the Cursors Preview Tool and Integration

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1. Click the **Cursors Preview** button on the Frame Integration toolbar

— or — click the **Cursors Preview** command in the command bar or the context menu of the slice cursor.

- 2. 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.

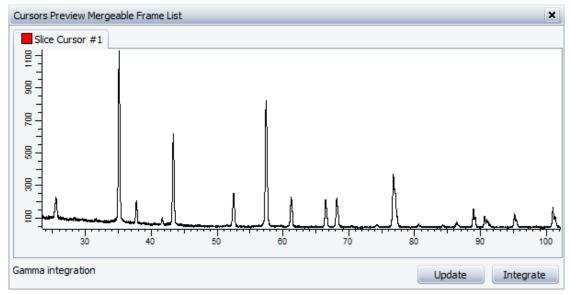


Figure 27.3: The Cursors Preview Tool with the preview of the integration result

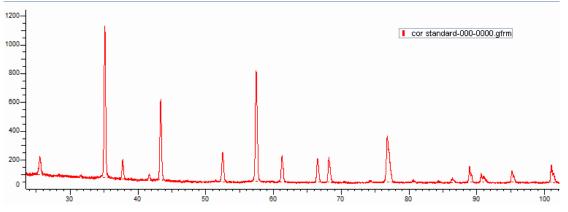


Figure 27.4: The resulting integrated scan

Integrate

28 Loading and Integrating Stackable 2D Frames

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

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

Steps

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

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

- 1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
 - The EVA document is empty.
 - 2. Click the **Import from files** data command or the **Import from files** button.
 - The Import From Files dialog box will be displayed.
 - 3. Search the Tutorials\EVA\2D Frame Data directory* and select all of the "HTSR258*.gfrm" files in the "HTSR258" sub-directory.
 - 4. Click **Open**. The frames will be displayed in the frame view of the EVA document. A **Stackable Frame List** will appear in the tree.

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* 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.

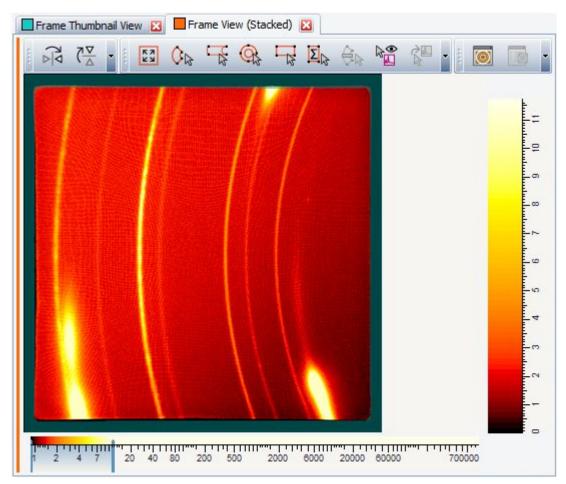


Figure 28.1: 2D Frame View after loading a measurement with stackable frames

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

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

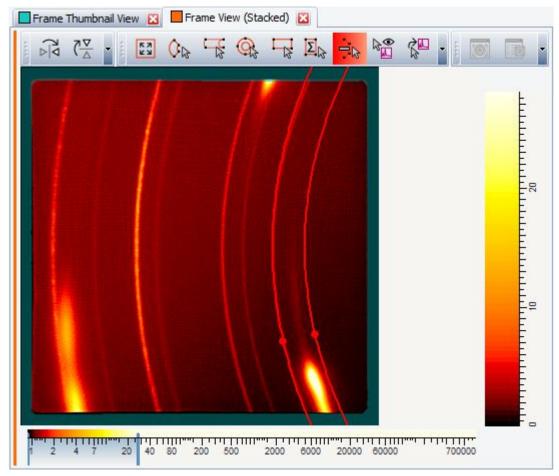


Figure 28.2: Ring Cursor prepared for the subsequent integration

28.3 Step 3: Displaying the Cursors Preview Tool and Integrate

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

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 Click the Cursors Preview button on the Frame Integration toolbar — or —

click on the **Cursors Preview** command in the command bar or the context menu of the cursor.

Integrate

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

Integration Parameters		
Direction	2-Theta integration	\sim
Merge as Single Scan	 Image: A start of the start of	
Integrate in a Separate List		
Step size	0.005 °	\sim

Figure 28.3: The integration parameters of the ring cursor

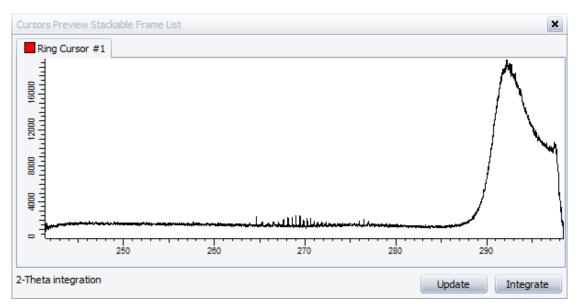


Figure 28.4: The Cursors Preview Tool with the preview of the integration result

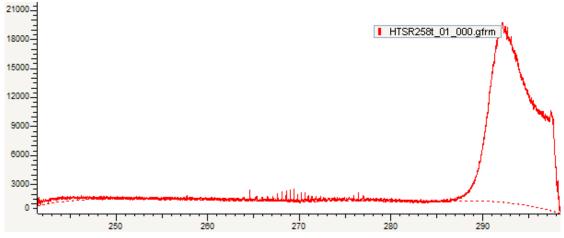


Figure 28.5: The resulting integrated scan

29 Rocking Curve Integration on Stackable 2D Frames

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

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

Steps

H-

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

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

- 1. Click **New** on the **File menu** or use the dedicated button in the toolbar.
 - The EVA document is empty.
- 2. Click the **Import from files** data command or the **Import from files** button.
 - The Import From Files dialog box will be displayed.
- 3. Search the Tutorials\EVA\2D Frame Data directory* and select all of the "GM_XRR*.gfrm" files in the "GM_XRR" sub-directory.
- 4. Click Open.
- ⇒ The frames will be displayed in the frame view of the EVA document. A Stackable Frame List will appear in the tree.



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

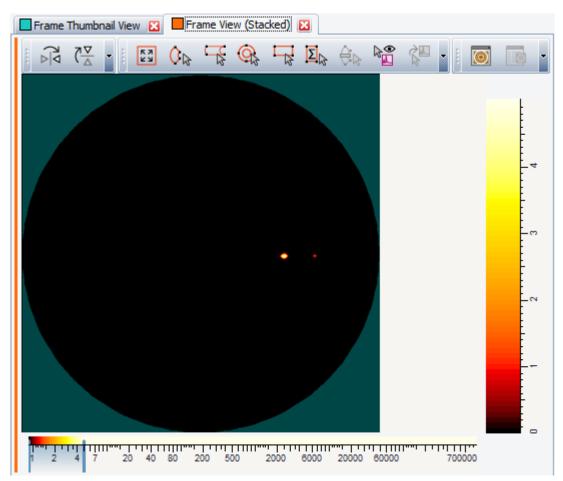


Figure 29.1: 2D Frame View after loading a measurement with stackable frames

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

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

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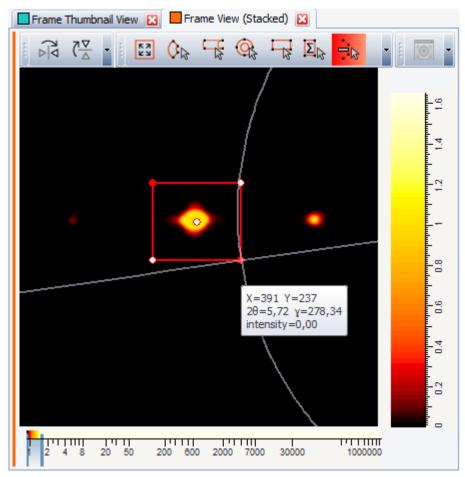


Figure 29.2: Area Cursor prepared for the subsequent integration

29.3 Step 3: Displaying the Cursors Preview Tool and Integrate

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

2. Click the **Cursors Preview** button on the Frame Integration toolbar — or —

click the **Cursors Preview** command in the command bar or the context menu of the cursor.

Integrate

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

Integration Paramete	:rs	
X-axis	Theta	$\mathbf{\mathbf{\nabla}}$
Reverse order		
Area Type	Mean	\checkmark

Figure 29.3: The integration parameters of the ring cursor

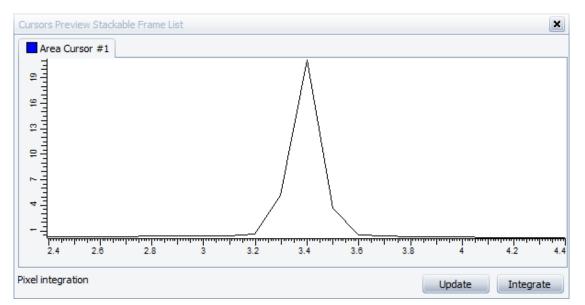


Figure 29.4: The Cursors Preview Tool with the preview of the integration result

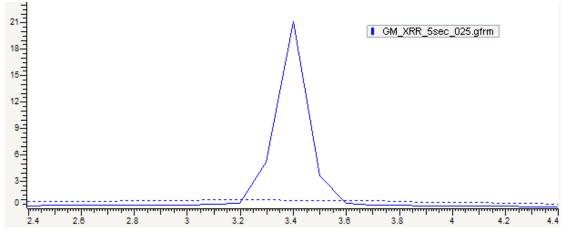


Figure 29.5: The resulting integrated scan

30 Adjusting the Default Mask of a 2D Frame

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

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

Steps

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

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

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



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

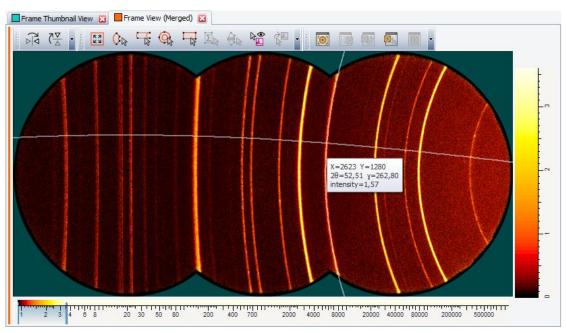


Figure 30.1: 2D Frame View exhibiting non-exposed areas around the frames

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

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

click the **Integrate Cursor** command in the command bar or the context menu of the cursor.

The scan will be created in a separate scan list. A problem is clearly visible at the beginning of the scan where the intensity drops.

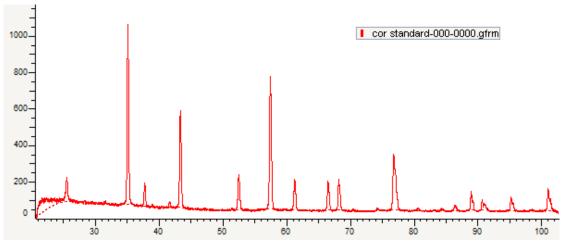


Figure 30.2: Integrated scan with intensity drop at low angles due to mask misalignment

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

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

Multiple properties		+ ×
▲ X ⊻		
Edit multiple properties	\bigcirc	

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

Attributes		
Color		\sim
Use Default Mask	~	
Use Custom Mask		

3. Change the Radius to 980 pixel.

Attributes	
Color	
Use Default Mask	 Image: A start of the start of
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.

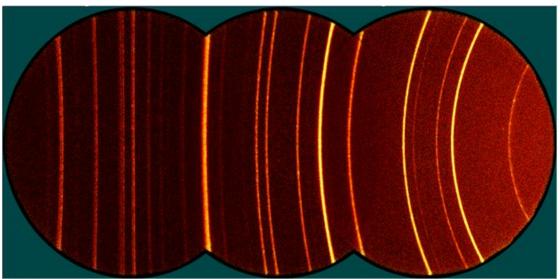


Figure 30.3: 2D Frame View with an adjusted default mask

30.4 Step 4: Selecting the Integration Cursor and Integration



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

— or — click the **Integrate Cursor** command in the command bar or the context menu of the cursor.

The scan is created in a separate scan list.

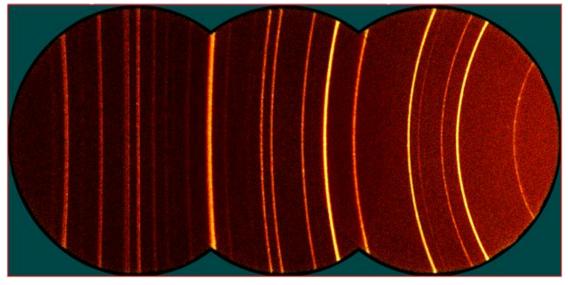


Figure 30.4: 2D Frame View with the full frame cursor drawn along its edges

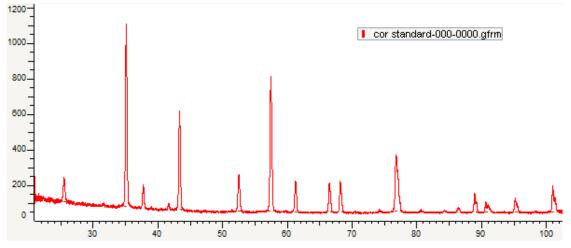


Figure 30.5: The resulting integrated scan

31 Using Printing Options

This chapter will describe how to use some printing options.

31.1 Vertical Table

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

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

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

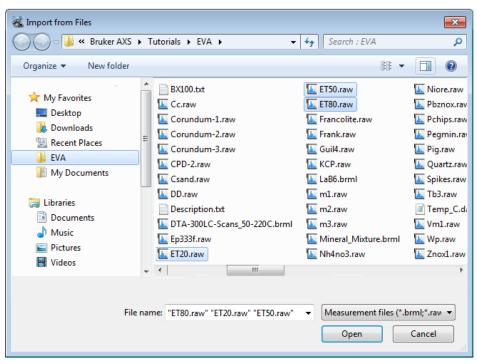


Figure 31.1: Importing the 3 scans

Data Tree	×				
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)				

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

- 1. Select the scan list (2Theta list in the example).
- 2. Click Scan Column View in the Create list of the Data Command panel

— or —

click the Scan Column View button on the Create View toolbar — or —

right-click the scan list in the data tree to display the context menu. Click **Create** and then **Scan Column View** on the related submenu.

A Scan Column View will be created.

Scan	Colum	nn View									
Visi	ible	Icon	Color	Index	Name	Parent	Sample Name	File Name	Scan Type	Scan Status	Start
	~	I	. 🗠	1	ET20.raw #1	2Theta	20% Boehmite/80% Corundum	ET20.raw	Coupled TwoTheta/Theta	Completed	22.000
	~	1	. 🖂	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
<		#									>

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

— or — Right-click the scan column view in the data tree to display the context menu. Click **Print preview**.

• The print preview with the vertical table will be displayed.

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PDFCreator		🖂 🔎 100% 🖂 🖉	0 4 6 6		
3 🔁					
	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%	50% Boehmite/50%	80% Boehmite/20%	
		Corundum	Corundum	Corundum	
	File Name	ET20.raw	ET50.raw	ET80.raw	
	Scan Type	Coupled TwoTheta/Theta	Coupled TwoTheta/Theta	Coupled TwoTheta/Theta	
	Scan Status	Completed	Completed	Completed	
	Start	22.000	22.000	22.000	
	End	45.000	45.000	45.000	
	Step Size	0.020	0.020	0.020	
	Time per Step	2.0	2.0	2.0	
	Temperature	25 (Room)	25 (Room)	25 (Room)	
	Time Started	0.0	0.0	0.0	
	Goniometer radius	200.5	200.5	200.5	
	2-theta	22.000	22.000	22.000	
	Theta	11.000	11.000	11.000	
	Chi	0.00	0.00	0.00	
	Phi	0.00	0.00	0.00	
	X-Drive				
	Y-Drive				
	Z-Drive Aux1	0.0	0.0	0.0	

Figure 31.3: Vertical table visible in the print preview

31.2 Repeat Columns

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



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

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

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

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

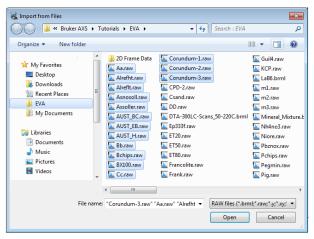


Figure 31.4: Importing Scans

Data Tree			
Data			Description
=	Doc	ument	
		Views	
		2Theta	14 Scans
	~	Aa.raw #1	A-XRD-QU40DOL10COR20CAL30
	~	Alrefit.raw #2	ALREFLT
	~	Asnosoll.raw #3	ASPIRIN - NO PRIMARY SOLLER SLIT
	~	Assoller.raw #4	ASPIRIN - PRIMARY SOLLER SLITS
	~	AUST_BC.raw #5	SAMPLE BC
	~	AUST_EB.raw #6	SAMPLE EB
	~	AUST_H.raw #7	SAMPLE H
	~	Bb.raw #8	B-XRD-QU25DOL20COR20CAL35
	~	Bchips.raw #9	BCHIPS
	✓	BX100.raw #10	BX100
	✓	Cc.raw #11	C-XRD-QU10DOL30COR20CAL40
	~	Corundum-1.raw #12	Corund
	~	Corundum-2.raw #13	Corund
L	~	Corundum-3.raw #14	Corund
<		**	>

Figure 31.5: Scans added to the data tree

— or —

- 5. Select the scan list (2Theta list in the example).
- 6. Click **Scan Column View** in the Create list of the Data Command panel or —

click the Scan Column View button on the Create View toolbar.

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
~	1.1	Red	$\mathbf{\mathbf{v}}$	1	Aa.raw #1	2Theta	A-XRD-QU40DOL10COR20CAL30	Aa.raw	Coupled TwoTheta/Th
~	1.1	Blue	$\mathbf{\sim}$	2	Alrefit.raw #2	2Theta	ALREFLT	Alrefit.raw	Coupled TwoTheta/Th
~	1	Lime	\mathbf{r}	3	Asnosoll.raw #3	2Theta	ASPIRIN - NO PRIMARY SOLLER SLIT	Asnosoll.raw	Coupled TwoTheta/Th
~	1.1	Magenta	\mathbf{r}	4	Assoller.raw #4	2Theta	ASPIRIN - PRIMARY SOLLER SLITS	Assoller.raw	Coupled TwoTheta/Th
~	1	Black	\mathbf{r}	5	AUST_BC.raw #5	2Theta	SAMPLE BC	AUST_BC.raw	Coupled TwoTheta/Th
~	1	DarkRed	\checkmark	6	AUST_EB.raw #6	2Theta	SAMPLE EB	AUST_EB.raw	Coupled TwoTheta/Th
~	1	DarkOr	\checkmark	7	AUST_H.raw #7	2Theta	SAMPLE H	AUST_H.raw	Coupled TwoTheta/Th
~	1	Green	\checkmark	8	Bb.raw #8	2Theta	B-XRD-QU25DOL20COR20CAL35	Bb.raw	Coupled TwoTheta/Th
~	1	Cyan	$\mathbf{\vee}$	9	Bchips.raw #9	2Theta	BCHIPS	Bchips.raw	Coupled TwoTheta/Th
~	-	Yellow	$\mathbf{\mathbf{v}}$	10	BX100.raw #10	2Theta	BX 100	BX100.raw	Coupled TwoTheta/Th
~	1	LightSt	$\mathbf{\mathbf{v}}$	11	Cc.raw #11	2Theta	C-XRD-QU10DOL30COR20CAL40	Cc.raw	Coupled TwoTheta/Th
~	1	LightPink	¥	12	Corundum-1.raw #12	2Theta	Corund	Corundum-1.raw	Coupled TwoTheta/Th
~	1	Red	$\mathbf{\mathbf{v}}$	13	Corundum-2.raw #13	2Theta	Corund	Corundum-2.raw	Coupled TwoTheta/Th
~	1	Blue	\sim	14	Corundum-3.raw #14	2Theta	Corund	Corundum-3.raw	Coupled TwoTheta/Th

Figure 31.6: Scan column view

7. In this example, it is interesting to configure the table columns differently. To do so, rightclick 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	\sim	A-XRD-QU40DOL10COR20CAL30	Aa.raw	23.990	46.990	0.020	2.0	0.0	200.
Alrefit.raw #2	Blue	~	ALREFLT	Alrefit.raw	5.000	70.000	0.025	2.0	0.0	170
Asnosoll.raw #3	Lime	$\mathbf{\mathbf{v}}$	ASPIRIN - NO PRIMARY SOLLER SLIT	Asnosoll.raw	5.000	35.000	0.020	2.0	0.0	200
Assoller.raw #4	Magenta	~	ASPIRIN - PRIMARY SOLLER SLITS	Assoller.raw	5.000	35.000	0.020	2.0	0.0	220
AUST_BC.raw #5	Black	~	SAMPLE BC	AUST_BC.raw	20.000	40.000	0.020	3.7	0.0	200
AUST_EB.raw #6	DarkRed	~	SAMPLE EB	AUST_EB.raw	20.000	40.000	0.020	3.7	0.0	200
AUST_H.raw #7	DarkOr	~	SAMPLE H	AUST_H.raw	20.000	40.000	0.020	3.7	0.0	200
Bb.raw #8	Green	~	B-XRD-QU25DOL20COR20CAL35	Bb.raw	23.990	46.990	0.020	2.0	0.0	200
Bchips.raw #9	Cyan	~	BCHIPS	Bchips.raw	5.000	70.000	0.025	2.0	0.0	170
BX100.raw #10	Yellow	$\mathbf{\mathbf{v}}$	BX100	BX100.raw	4.986	79.986	0.030	3.0	0.0	200
Cc.raw #11	LightSt	~	C-XRD-QU10DOL30COR20CAL40	Cc.raw	23.990	46.990	0.020	2.0	0.0	200
Corundum-1.raw #12	LightPink	~	Corund	Corundum-1.raw	20.000	45.776	0.020	9.9	0.0	C
Corundum-2.raw #13	Red	$\mathbf{\mathbf{v}}$	Corund	Corundum-2.raw	45.797	71.573	0.020	19.8	151.8	C
Corundum-3.raw #14	Blue	$\mathbf{\vee}$	Corund	Corundum-3.raw	71.593	97.370	0.020	39.6	441.6	(

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

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

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

Right-click the scan column view in the data tree to display the context menu. Click **Print preview**.

The print preview will be displayed.

A	2Theta								
A									
A									
-	Name								
		Color		Sample Name			Start	Start End	
Δ	Aa.raw#1			40DOL10COR20C/	AL30	Aa.raw	23.990	46.990)
	Alreflt.raw#2					Alreflt.raw	5.000	70.000)
Δ	Asnosoll.raw #3					Asnosoll.raw	5.000	35.000)
Δ	Assoller.raw#4		ASPIRIN - PRIMARYSOLLER SLITS Assoller.raw 5.000		5.000	35.000			
	AUST_BC.raw #5	ST_BC.raw #5 SAMPLE BC AUST_BC. ST_EB.raw #6 SAMPLE EB AUST_EB. ST_H.raw #7 SAMPLE H AUST_H.raw #7 raw #8 B-XRD-QU25DOL20COR20CAL35 Bb.raw nips.raw #9 BCHIPS Bchips.raw					_		_
	AUST_EB.raw#6			AUST_EB.ray					
Α	AUST_H.raw#7			SAMPLE H			20.000	40.000)
_	3b.raw#8				23.990				
-	3chips.raw#9			Bchips.raw	5.000	70.000			
	3X100.raw#10		BX100			BX100.raw	4.986	79.986	
	Cc.raw#11		C-XRD-QU	C-XRD-QU10DOL30COR20CAL40 Cc.raw				46.990)
	Corundum-1.raw #12 Corundum-2.raw #13 Corundum-3.raw #14 Name		Corund	Corund Corundum-1.raw 20.000 45.7				45.776	5
			Corund			Corundum-2.	aw 45.797	w 45.797 71.573	
			Corund			Corundum-3.	aw 71.593	97.370)
П		Color	Step Size	Time per Step	Time	Started Go	niometer ra	dius 2	2-theta
Δ	Aa.raw#1		0.020	2.0	0.0	200.			3.990
	Alrefit.raw#2		0.025	2.0	_		-		
-					0.0	170.0			000
A	Asnosoll.raw#3		0.020	2.0	0.0	200.		5.	000
-	Asnosoll.raw #3 Assoller.raw #4		0.020	_	_			5. 5.	
Δ				2.0	0.0	200.		5. 5. 5.	000
А А	Assoller.raw#4		0.020	2.0 2.0	0.0 0.0	200.9 220.9		5. 5. 20	000 000
А А А	Assoller.raw#4 AUST_BC.raw#5 AUST_EB.raw#6 AUST_H.raw#7		0.020 0.020 0.020 0.020	2.0 2.0 3.7 3.7 3.7	0.0 0.0 0.0 0.0 0.0	200.9 220.9 200.9 200.9 200.9		5. 5. 20 20 20	000 000 0.000 0.000 0.000
A A B	Assoller.raw#4 AUST_BC.raw#5 AUST_EB.raw#6 AUST_H.raw#7 3b.raw#8		0.020 0.020 0.020 0.020 0.020 0.020	2.0 2.0 3.7 3.7 3.7 2.0	0.0 0.0 0.0 0.0 0.0 0.0 0.0	200.3 220.3 200.3 200.3 200.3 200.3		5. 5. 20 20 20 20 20 20	000 000 0.000 0.000 0.000 0.000 3.990
A A B B	Assoller.raw#4 AUST_BC.raw#5 AUST_EB.raw#6 AUST_H.raw#7 Bb.raw#8 Bchips.raw#9		0.020 0.020 0.020 0.020 0.020 0.020 0.025	2.0 2.0 3.7 3.7 3.7 2.0 2.0	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0	200.3 220.3 200.3 200.3 200.3 200.3 170.0		5. 5. 20 20 20 20 20 20 5.	000 000 0.000 0.000 0.000 0.000 3.990 000
	Assoller raw#4 AUST_BC.raw#5 AUST_EB.raw#6 AUST_H.raw#7 Bb.raw#8 Bchips.raw#9 BX100.raw#10		0.020 0.020 0.020 0.020 0.020 0.020 0.025 0.030	2.0 2.0 3.7 3.7 2.0 2.0 3.0	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0	200.9 220.9 200.9 200.9 200.9 200.9 170.0 200.9		5. 5. 20 20 20 20 20 20 20 20 20 20 20 20 20	000 000 0.000 0.000 0.000 3.990 000 986
	Assoller raw#4 AUST_BC.raw#5 AUST_EB.raw#6 AUST_H.raw#7 Bb.raw#8 Bchips.raw#9 BX100.raw#10 Cc.raw#11		0.020 0.020 0.020 0.020 0.020 0.025 0.030 0.020	2.0 2.0 3.7 3.7 2.0 2.0 2.0 3.0 2.0	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0	200. 220. 200. 200. 200. 200. 200. 200.		5. 5. 20 20 20 23 5. 4. 23	000 000 0.000 0.000 0.000 3.990 000 986 3.990
	Assoller raw#4 AUST_BC.raw#5 AUST_EB.raw#6 AUST_H.raw#7 Bb.raw#8 Bchips.raw#9 BX100.raw#10		0.020 0.020 0.020 0.020 0.020 0.020 0.025 0.030	2.0 2.0 3.7 3.7 2.0 2.0 3.0	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0	200.9 220.9 200.9 200.9 200.9 200.9 170.0 200.9		5. 5. 20 20 20 20 20 20 20 20 20 20 20 20 20	000 000 0.000 0.000 0.000 3.990 000 986

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

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