Lesson 6 BGMN & Profex

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Rietveld Refinement Software BGMN

BGMN:

- Fundamental Parameters Approach
- Free for academic use
- Device independent
- Very robust automatic refinement strategy
- Slightly less steep learning curve
- Powerful scripting language
- Multi-Platform
- Multi-threaded

Visit: http://www.bgmn.de for tutorials and documentation



BGMN Website



Site map

	Up	Program Description	BGMN FAQ	Download Page
Instrumental Function	The following pa (plaster) makes y	ages serve as a short introduction your test runs easier.	on into the BGMN R	ietveld software. A description of an example
Tube Tails and size/strain estimation	First, the generat	tion of the instrumental functio	n is described.	
Structure Description	Second, the cons in detail.	truction of structure files is exp	plained. In an extra to	opic the handling of preferred orientation is mentioned
Preferred Orientation	Third, the calcula	ation control during a problem	specific control file	is shown.
Calculation Control	Last, we have a l	ook at the different result files.	The Carlo	
Result Output	A somewhat exte	ended explanation of the used v	variables is also avail	lable.
BGMN Variables				
Download Structures Preferred Orientation Calculation Control Result Output BGMN Variables	Third, the calcula Last, we have a l A somewhat exte	ation control during a problem ook at the different result files. ended explanation of the used v	specific control file i variables is also avail	is shown. lable.

http://www.bgmn.de/program.html



BGMN Control File (*.sav)





Profex



History

- 2003: Start of development as an alternative GUI for Fullprof.2kFor personal use only (my PhD)Linux only
- 2006: Major rewrite

Support for Windows

- 2012: Support for BGMN Rietveld backend added
- 2014: Support for Mac OS X





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First Use







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	gibix-ads-10mm.geg		Cubiy_ade_10mm a
	Structures		Cubix-aus-romin.g
	File Name	Phase	Comr ^
Projects Plot Options efinement Protocol	 Ardealite.str benzoic-acid.str beta_Ft.str betaCMP.str betaCPP.str betaCPP-tetrahydrate.str betaTCP.str betaTCP-Mg.str Brushite.str C2S-Calcio-Olivine.str C2S-Larnite.STR C3S-Hatrurite.str C3S-rJm.str CaCl2.str CaCl2.str CaCl2.str 	Ardealite Benzoic-Acid beta_Ft betaCaMetaphosphate betaCaPyrophosphate betaCPP-tetrahydrate betaTCP betaTCP-Mg Dicalciumphosphate_Dihydrat C2S_orthorhombic C2SH-Hillebrandite C2S-monoclinic C3S_monoclinic C3S_triclinic C3S_triclinic C3S_rhombohedral CaCl2	04-011 CSD B 01-075 04-005 04-011 Select: betaTCP.str Hydroxylapatite.str
	Expand/Collapse	Ca hudragan sulfata	







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BGMN Control File (*.sav)

What Profex does in the background:

- Generate a control file
- Adjust file names in control file
- Copy all selected **structure files** from local DB to location of scan file
- Copy **instrument configuration files** from local DB to location of the scan file

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4_0012 XRD Bern 2015 Lessons	▶ Examples-Test ▶ Lesson 6 ▶ Änderungsdatu	Example 1 m Typ	 ↓ ↓ Example 1 B = ↓ Größe
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Profex

With Profex:

- 1. Load scan file
- 2. Use «Add phase» dialog to select phases, instrument, and generate control file
- 3. Run refinement

No need to:

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- Copy structure / device files
- Change any file names
- Convert scan files



September - 3.3.1	The second se			
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Name Status lesson6-ex1 idle	<pre>% Theoretical instrumental function VERZERR=cubix-ads-10mm.geq % Wavelength LAMBDA=CU % Polarization (CuKa with Graphite mon POL=sqr(cos(26.6*pi/180))</pre>	ochromator)		
	<pre>pi=2*acos(0) % Phases STRUC[1]=betaTCP.str STRUC[2]=Hydroxylapatite.str % Measured data</pre>		Context Help:	
	VAL[1]=lesson6-ex1-file1.xy % Minimum Angle (2theta) % WMIN=10 % Maximum Angle (2theta) % WMAX=60	Place (Cursor on a key v	vord
Projects Plot Options	% Result list output LIST=lesson6-ex1-file1.lst % Peak list output		Press «F1»	
Context Help B × EPS2 is the specimen out of axis shift of the pattern (sample displacement error). May be refined within BGMN as a global parameter. • EPS2*sin (Theta) for transmission geometry • EPS2*cos (Theta) otherwise, e.g. for BRAGG- BRENTANO geometry	Sofror-Tessono-extrinetion % Diagram output DIAGRAMM=lesson6-extrile1.dia % Global parameters for zero point and EPS1=0 PARAM[1]=EP\$2=00.01^0.01 alpha3ratio=0.02 Sofratio 0 NTHREADS=8 PROTOKOLL=Y Sum=betaTCP+HAp	sample displacement		
gives the pattern shift in one Theta in radians. Attention: Usually, the x axis of the pattern is two Theta.	GOAL[1]=betaTCP/sum GOAL[2]=HAp/sum			
Refinement Protocol	5 ×	Global Parameters and GOALs	₽×	
	Wavelength: 1.5418	Global Parameters and GOALs Chemistry 3 Å Angle: 0.000° Intensity: 0.000 cts	d-Spacing: 0.000 Å Line 24, Column 11	

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Name Status lesson6-ex1 idle	<pre>% Theoretical instrumental function VERZERR=cubix-ads-10mm.geq % Wavelength LAMBDA=CU % Polarization (CuKa with Graphite monochromator) POL=sqr(cos(26.6*pi/180)) pi=2*acos(0) % Phases STRUC[1]=betaTCP.str STRUC[1]=betaTCP.str STRUC[2]=Hydroxylapatite.str % Measured data VAL[1]=lesson6-ex1-file1.xy % Minimum Angle (2theta) % MAXIMUM Angle (2theta) % Transformer (2theta) % Maximum Angle (2theta) % Transformer (2theta) % Maximum Angle (2theta) % Transformer (2theta) % Result list output UITOFTAMM=lesson6-ex1-file1.par % Diagram output DIAGRAMM=lesson6-ex1-file1.dia % Global parameters for zero point and sample displacement EPS1=0 PARAM[1]=EPS2=00.01^0.01 alpha3ratio=0.02 betaratio=0 NTHREADS=8 PROTOKOLL=Y Sum=betaTCP+HAp GOAL [1]=betaTCP/sum GOAL [2]=HAp/sum</pre>	
Refinement Protocol	♂ × Global Parameters and GOALs	₽×
	Global Parameters and GOALs Chemistry	

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- 1. Open Graph File: «Examples\Lesson 6\Example 2\lesson6-ex2.file1.xrdml»
- 2. Click «Add a phase» (+)
 - a) Select instrument: «pw1800-fds»
 - b) Select Phases:
 «AL2O3-Corundum»
 «Fluorite»
- 3. Run the refinement

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	<u>I</u>
Projects Plot Options	20.00 30.00 40.00 50.00 60.00 Angle [°2θ]
Refinement Protocol	Global Parameters and GOALs G
	$R_{\mu\rho}=37.97\%$, $R_{e\nu\rho}=14.40\%$, $X^2=2.6368$
	Corundum/sum 0.5958 0.0093
	fluorite/sum 0.4042 0.0093
	A m
	Global Parameters and GOALs Chemistry Wavelength: 1.54179 Å Angle: 34.019° Intensity: -177.731 cts d-Spacing: 2.635 Å Line 0. Column 0.
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C:/xrd/test/Examples/Lesson 5/Example 2/lesson5-ex2-file1.dia

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BGMN Structure Files (*.str)

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Name Status	<pre>PHASE=Fluorite // 04-002-2191 SpacegroupNo=225 HermannMauguin=F4/m-3 PARAM=A=0.5463_0.54A0.55 // RP=4 k1=0 k2=0 PARAM=B1=0_0A0.003 PARA d=10 // GOAL=GrainSize(1,1,1) // GOAL=d // GOAL:fluorite=GEWICHT*ifthenelse(ifdef E=CA+2 Wyckoff=a TDS=0.0041 E=F-1 Wyckoff=c TDS=0.0062</pre>	2/m // M=GEWICHT=0.1_0 // (d),exp(my*d*3/4),1)
Refinement Protocol	5 ×	Global Parameters and GOALs
		R _{wp} =37.97%, R _{exp} =14.40%, X ² =2.6368
		Parameter / Goal Value ESD
		Corundum/sum 0.5958 0.0093
		fluorite/sum 0.4042 0.0093
		 ₩
		Global Parameters and GOALs Chemistry
1	Wavelength: 1.541/	9 A Angle: 0.000 Intensity: 0.000 cts d-Spacing: 0.000 A Line 0, Column 0

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BGMN Structure Files (*.str)

```
PHASE=Fluorite // 04-002-2191
SpacegroupNo=225 HermannMauguin=F4/m-32/m //
PARAM=A=0.5463_0.54^0.55 //
RP=4 k1=0 k2=0 PARAM=B1=0_0^0.003 PARAM=GEWICHT=0.1_0 //
d=10 //
GOAL=GrainSize(1,1,1) //
GOAL=GrainSize(1,1,1) //
GOAL=my //
GOAL=d //
GOAL=d //
GOAL:fluorite=GEWICHT*ifthenelse(ifdef(d),exp(my*d*3/4),1)
E=CA+2 Wyckoff=a TDS=0.0041
E=F-1 Wyckoff=c TDS=0.0062
```

Phase name // Database reference Space group number & H-M symbol Unit Cell: *a* axis (nm) Peak profile parameters Mean particle size (µm), optional

Goals (optional, these values are reported in the results file)

List of atomic positions

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BGMN Structure Files (*.str)

PHASE=Fluorite // 04-002-2191
SpacegroupNo=225 HermannMauguin=F4/m-32/m //
PARAM=A=0.5463_0.54^0.55 //
RP=4 k1=0 k2=0 PARAM=B1=0_0^0.003 PARAM=GEWICHT=0.1_0 //
d=10 //
GOAL=GrainSize(1,1,1) //
GOAL=my //
GOAL=d //
GOAL:fluorite=GEWICHT*ifthenelse(ifdef(d),exp(my*d*3/4),1)
E=CA+2 Wyckoff=a TDS=0.0041
E=F-1 Wyckoff=c TDS=0.0062

Right mouse button on a parameter:

Refine isotropically Refine anisotropically	Ctrl+A
Colored All	Chilli A
Delete	
Paste	Ctrl+V
Сору	
Cut	Ctrl+X
Redo	Ctrl+Y
Undo	

Fix parameter:	Refined parameter:	Refined parameter with limits:		
A =0.5463	PARAM= <mark>A=</mark> 0.5463	PARAM=A=0.5463_0.54^0.55		
Name Value	Release for Name Starting value refinement	Release for Name Starting Lower Upper refinement value limit limit		

See <u>http://www.bgmn.de/variables.html#real</u> for RP=4 and k1=0

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```
PHASE=Fluorite // 04-002-2191
SpacegroupNo=225 HermannMauguin=F4/m-32/m //
PARAM=A=0.5463_0.54^0.55 //
RP=4 k1=0 k2=0 PARAM=B1=0_0^0.003 PARAM=GEWICHT=0.1_0 //
d=10 //
GOAL=GrainSize(1,1,1) //
GOAL=GrainSize(1,1,1) //
GOAL=my //
GOAL=d //
GOAL:fluorite=GEWICHT*ifthenelse(ifdef(d),exp(my*d*3/4),1)
E=CA+2 Wyckoff=a TDS=0.0041
E=F-1 Wyckoff=c TDS=0.0062
```

B1: refined, but limited to the range 0.000 – 0.003 (upper limit may be too strict)

k2: micro strain effect, not refined (necessary?)

Change:

RP=4 k1=0 k2=0 PARAM=B1=0_0^0.003 PARAM=GEWICHT=0.1_0 //

To:

RP=4 k1=0 k2=0 PARAM=B1=0_0^0.03 PARAM=GEWICHT=0.1_0 //

Repeat Refinement

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Change:

RP=4 k1=0 k2=0 PARAM=B1=0_0^0.03 PARAM=GEWICHT=0.1_0 //

To:

RP=4 k1=0 PARAM=k2=0_0 PARAM=B1=0_0^0.03 PARAM=GEWICHT=0.1_0 //

Repeat Refinement

Preferred Orientation / Texture:

- Refine «GEWICHT» anisotropically:
 - Right mouse button on GEWICHT
 - «Refine anisotropically»

Changes:

RP=4 k1=0 PARAM=k2=0_0 PARAM=B1=0_0^0.03 PARAM=GEWICHT=0.1_0 //

To:

RP=4 k1=0 PARAM=k2=0_0 PARAM=B1=0_0^0.03 GEWICHT=SPHAR4 //

Repeat Refinement

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Summary: Structure Files (*.str)

- Structure file database (*.str) is stored in
 ...\Profex-BGMN-Bundle-3.3.1\Profex\Structures
- Copied by Profex to the location of the scan file
- They contain:
 - Space group information
 - Unit cell dimensions
 - Profile parameters
 - Scaling (weight fraction)
 - List of atoms (element, SOF, Wyckoff sequence, fract. coordinates, TDS)
 - Optional «Goals»: Results / values printed to the results file (*.lst)
- Release parameters for refinement:
 - «PARAM=»
 - Optionally (recommended!): «_lowerLimit» and «^upperLimit»

Summary: Structure Files (*.str)

Refinements are «fine tuned» by editing Structure Files:

Commonly:

- Set reasonable upper and lower limits
- Control peak broadening
- Control texture / preferred orientation

Rarely:

-

- Control structural parameters:
 - atomic coordinates
 - site occupancies
 - thermal displacement parameters

Structure Databases

STR files included in Profex bundle (created manually by Nicola Doebelin)

http://www.bgmn.de/download-structures.html

More on Structure Files: Lesson 8: Creating Structure Files

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Projects B Name Status lesson6-ex3-file01 idle lesson6-ex3-file03 idle lesson6-ex3-file04 idle lesson6-ex3-file05 idle lesson6-ex3-file06 idle lesson6-ex3-file07 idle lesson6-ex3-file09 idle lesson6-ex3-file09 idle lesson6-ex3-file09 idle lesson6-ex3-file10 idle lesson6-ex3-file10 idle lesson6-ex3-file10 idle lesson6-ex3-file10 idle lesson6-ex3-file10 idle lesson6-ex3-file10 idle Refinement Protocol Image: Status	Image: Street and Street
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lesson6-ex3-file01 lesson6-ex3-file02 lesson6-ex3-file03 lesson6-ex3-file04	idle idle idle	<pre>% Theoretical instrumental function VERZERR=cubix-ads-10mm.geq % Wavelength LAMBDA=CU % Polarization (CuKa with Graphite monochromator) POL=sqr(cos(26.6*pi/180))</pre>
lesson5-ex3-file05 lesson5-ex3-file06 lesson6-ex3-file07 lesson6-ex3-file08 lesson6-ex3-file09 lesson6-ex3-file10 < III Context Help	idle idle idle idle idle idle	 pi=2*acos(0) % Phases STRUC[2]=Hydroxylapatite.str % Measured data VAL[1]=lesson6-ex3-file01.xy, % Minimum Angle (2theta) % WMIN=10 % Maximum Angle (2theta) % Maxi
		DIAGRAMM=lessonb-ex3-file01.dla % Global parameters for zero point and sample displacement EPS1=0 PARAM[1]=EPS2=00.01^0.01 alpha3ratio=0.02 betaratio=0 NTHREADS=8 PROTOKOLL=Y sum=betaTCP+HAp GOAL[1]=betaTCP/sum
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		Global Parameters and GOALs Chemistry Local Parameters

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3 G:/Auftr Proi/S-Auftraege/2014/S14 0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file01.lst	lesson6-ex3-file01	HAp/sum	0,706	0.0025		
4 G:/Auftr Proi/S-Auftraege/2014/S14 0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file02.lst	lesson6-ex3-file02	betaTCP/sum	0.2887	0.0024		
5 G:/Auftr Proi/S-Auftraege/2014/S14 0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file02.lst	lesson6-ex3-file02	HAp/sum	0.7113	0.0024		
6 G:/Auftr Proi/S-Auftraege/2014/S14 0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file03.lst	lesson6-ex3-file03	betaTCP/sum	0.2929	0.0024		
7 G:/Auftr Proi/S-Auftraege/2014/S14 0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file03.lst	lesson6-ex3-file03	HAp/sum	0.7071	0.0024		
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9 G:/Auftr Proj/S-Auftraege/2014/S14 0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file04.lst	lesson6-ex3-file04	HAp/sum	0.7059	0.0024		
10 G:/Auftr Proj/S-Auftraege/2014/S14 0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file05.lst	lesson6-ex3-file05	betaTCP/sum	0.2934	0.0024		
11 G:/Auftr Proj/S-Auftraege/2014/S14 0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file05.lst	lesson6-ex3-file05	HAp/sum	0.7066	0.0024		
12 G:/Auftr Proj/S-Auftraege/2014/S14 0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file06.lst	lesson6-ex3-file06	betaTCP/sum	0.2918	0.0023		
13 G:/Auftr Proj/S-Auftraege/2014/S14 0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file06.lst	lesson6-ex3-file06	HAp/sum	0.7082	0.0023		
14 G:/Auftr_Proj/S-Auftraege/2014/S14_0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file07.lst	lesson6-ex3-file07	betaTCP/sum	0.2899	0.0024		
15 G:/Auftr_Proj/S-Auftraege/2014/S14_0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file07.lst	lesson6-ex3-file07	HAp/sum	0.7101	0.0024		
16 G:/Auftr_Proj/S-Auftraege/2014/S14_0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file08.lst	lesson6-ex3-file08	betaTCP/sum	0.2908	0.0024		
17 G:/Auftr_Proj/S-Auftraege/2014/S14_0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file08.lst	lesson6-ex3-file08	HAp/sum	0.7092	0.0024		
18 G:/Auftr_Proj/S-Auftraege/2014/S14_0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file09.lst	lesson6-ex3-file09	betaTCP/sum	0.2896	0.0024		
19 G:/Auftr_Proj/S-Auftraege/2014/S14_0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file09.lst	lesson6-ex3-file09	HAp/sum	0.7104	0.0024		
20 G:/Auftr_Proj/S-Auftraege/2014/S14_0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file10.lst	lesson6-ex3-file10	betaTCP/sum	0.2933	0.0024		
21 G:/Auftr_Proj/S-Auftraege/2014/S14_0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file10.lst	lesson6-ex3-file10	HAp/sum	0.7067	0.0024		
22						
23		-		×		
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