



• • • • • Testing • Research • Consulting

Workshop „Rietveld Refinement with Profex“

Lesson 5: Introduction to Profex - Rietveld Refinement

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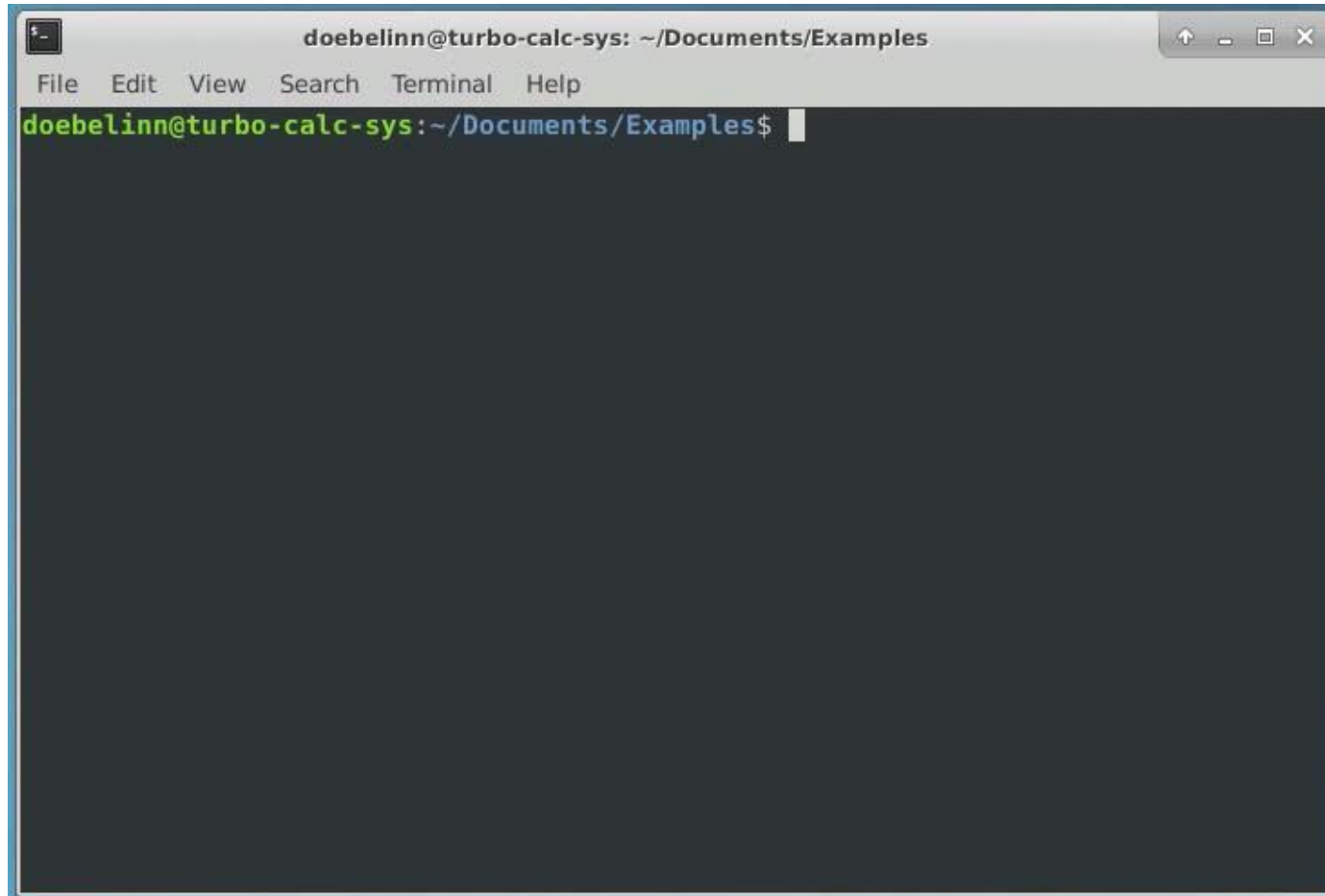
RMS Foundation, Switzerland

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Forschungszentrum Jülich, Germany



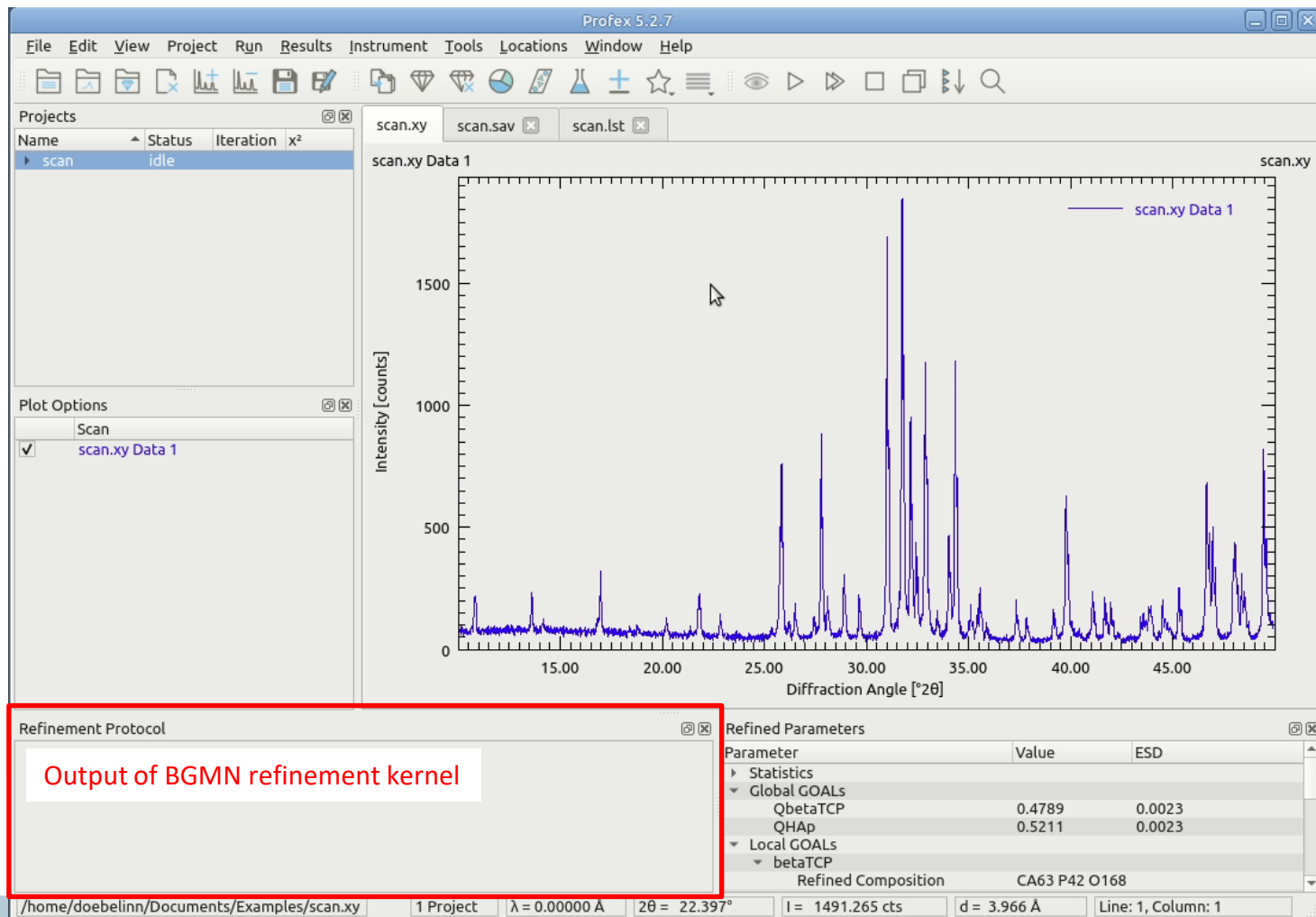
BGMN: Rietveld Refinement Kernel



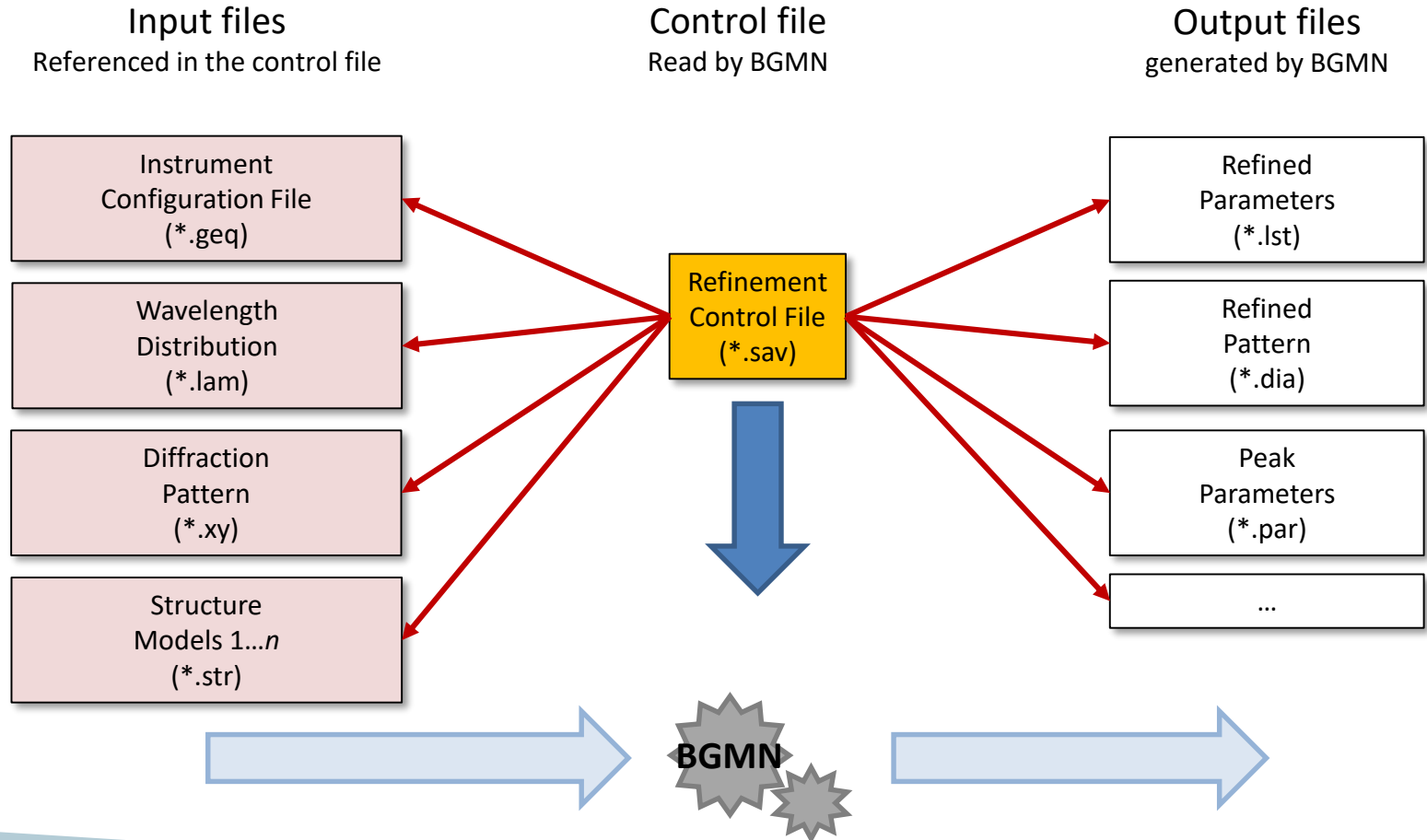
A terminal window titled "doebelinn@turbo-calc-sys: ~/Documents/Examples". The window has a menu bar with "File", "Edit", "View", "Search", "Terminal", and "Help". The terminal content shows the prompt "doebelinn@turbo-calc-sys:~/Documents/Examples\$" with a cursor at the end.

```
doebelinn@turbo-calc-sys: ~/Documents/Examples
File Edit View Search Terminal Help
doebelinn@turbo-calc-sys:~/Documents/Examples$
```

Profex: Graphical User Interface for BGMN



BGMN Rietveld Refinement Kernel



BGMN Input and Output Files

Input files

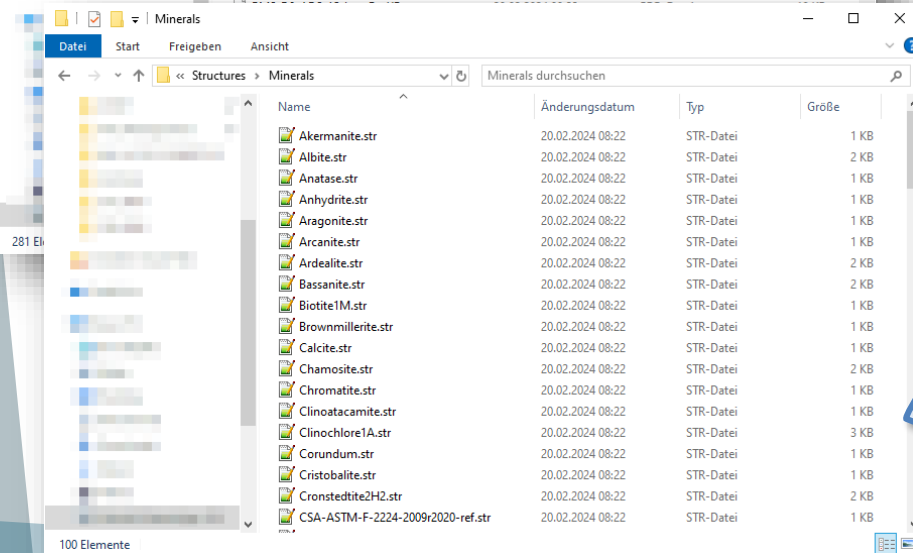
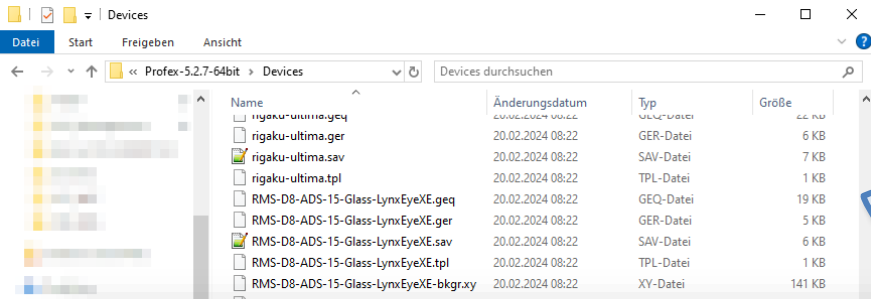
File	Extension	Content
Refinement control file	*.sav	Project configuration
Instrument configuration file	*.geq	Peak profile: Instrument contribution
Wavelength distribution	*.lam	Peak profile: Wavelength contribution
Diffraction pattern	*.xy	Measured diffraction data
Structure models	*.str	Unit cell, atomic positions etc.

Output files

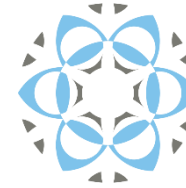
File	Extension	Content
Refined parameters	*.lst	Refinement results
Refined pattern	*.dia	lobs, lcalc, background etc. for graphical representation
Peak parameters	*.par	Position, intensity, width of refined peaks

Profex repositories

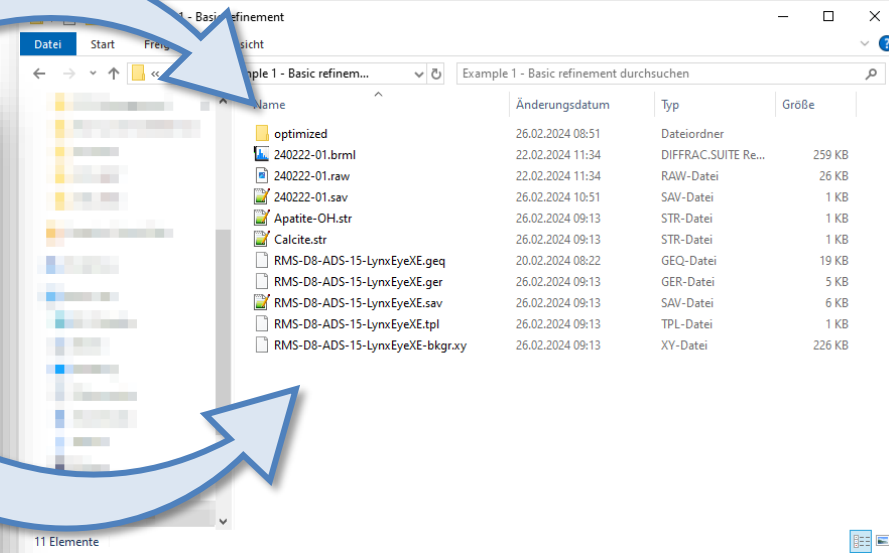
Collections of device and structure files



Profex manages file templates



Working folder



First Rietveld Refinement: Loading the Scan File

The screenshot shows the Profex 5.2.7 interface with the 'Open Raw Data File' dialog box open. The dialog box displays the current directory 'Example 1 - Basic refinement' and a list of files. The file '240222-01.brm1' is selected. The file type filter is set to 'All files (*.*)'. The file name '240222-01.brm1' is entered in the 'Dateiname:' field. The 'Öffnen' button is highlighted.

Name	Änderungsdatum	Typ
optimized	26.02.2024 08:51	Dateiordner
240222-01.brm1	22.02.2024 11:34	DIFFRAC.SUITE Re...
240222-01.raw	22.02.2024 11:34	RAW-Datei

First Rietveld Refinement: Identifying Phases

Profex 5.2.7

File Edit View Project Run Results Instrument Tools Locations Window Help

3. Add/Remove Phase

Projects

Name	Status	Iteration	χ^2
240222-01			

240222-01.brml

S24_0007: S240007_02

240222-01.brml

Intensity [counts]

1. Double click = Apatite-OH

2. Double click = Calcite

S24_0007: S240007_02

Diffraction Angle [2θ]

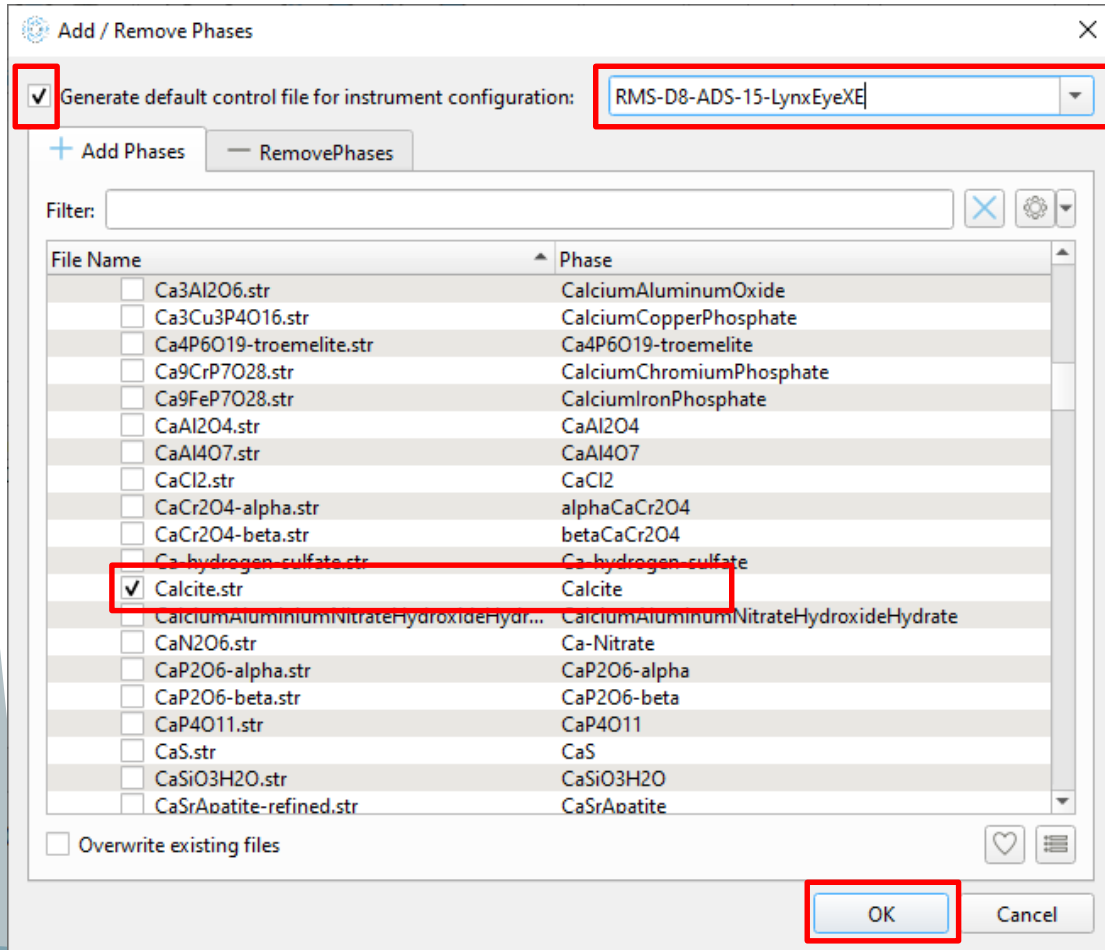
Refinement Protocol

Refined Parameters

Parameter	Value	ESD
Statistics		
Rwp		
Rexp		
χ^2		
GoF		
Background Coefficients		
Global GOALS		
Local GOALS		

G:\Auftr_Proj\S-Auftraege\2024\S24_0007 XRD-Workshop FZ Jülich\E 1 Project $\lambda = 1.54060 \text{ \AA}$ $2\theta = 38.975^\circ$ $I = 8943.797 \text{ cts}$ $d = 2.309 \text{ \AA}$

First Rietveld Refinement: Creating Refinement Project



1. Generate refinement control file for the instrument used to measure the dataset.

Here: „RMS-D8-ADS-15-LynxEyeXE“

2. Select the phases „Calcite.str“ and „Apatite-OH.str“.

(Use filters to find the phases.)

3. Click OK

First Rietveld Refinement: Refinement Control File (*.sav)

The screenshot displays the Profex 5.2.7 software interface. The main window shows a list of projects on the left and a text editor on the right. The text editor contains the refinement control file for '240222-01.sav', which is highlighted with a red box. The file content includes sample information, instrument parameters, phase names, and refinement settings. The status bar at the bottom shows the current project path, wavelength, 2θ, intensity, d-spacing, and line/column coordinates.

Projects

Name	Status	Iteration	χ^2
240222-01			

Plot Options

Scan	Vertical Offset
<input checked="" type="checkbox"/> S24_0007: S240007_02	0.00

```
240222-01.brml 240222-01.sav*
1 % SampleID: S24_0007: S240007_02
2 % Theoretical instrumental function
3 VERZERR=RMS-D8-ADS-15-LynxEyeXE.geq
4 % Wavelength
5 LAMBDA=CU
6 % Phases
7 STRUC[1]=Apatite-OH.str
8 STRUC[2]=Calcite.str
9 % Measured background
10 UNT=RMS-D8-ADS-15-LynxEyeXE-bkgr.xy
11 RU=10
12 % Measured data
13 VAL[1]=240222-01.xy
14 % Minimum Angle (2theta)
15 WMIN=10
16 % Maximum Angle (2theta)
17 % WMAX=60
18 % Result list output
19 LIST=240222-01.lst
20 % Peak list output
21 OUTPUT=240222-01.par
22 % Diagram output
23 DIAGRAMM=240222-01.dia
24 % Global parameters for zero point and sample displacement
25 EPS1=0
26 PARAM[1]=EPS2=0_-0.01^0.01
27 EPS3=0
28 alpha3ratio=0.020
29 betaratio=0.005
30 NTHREADS=8
31 PROTOKOLL=Y
32 SAVE=N
33
34 sum=Hydroxyapatite+ Calcite
35 QHydroxyapatite=Hydroxyapatite/sum
36 QCalcite= Calcite/sum
```

G:\Auftr_Proj\S-Auftraege\2024\S24_0007 XRD-Workshop FZ Jülich\E 1 Project $\lambda = 1.54060 \text{ \AA}$ $2\theta = 0.000^\circ$ $I = 0.000 \text{ cts}$ $d = 0.000 \text{ \AA}$ Line: 1, Column: 1

First Rietveld Refinement: Run Refinement

The screenshot displays the Profex 5.2.7 software interface. The main window shows a Rietveld refinement plot for sample S24_0007: S240007_02. The plot displays Intensity [counts] on the y-axis (0 to 14000) versus Diffraction Angle [°2 θ] on the x-axis (15.00 to 80.00). The plot includes several data series: I observed (black), I calculated (red), I difference (grey), Background (blue), Hydroxyapatite (green), and Calcite (light blue). A red box highlights the play button in the toolbar, with an arrow pointing to it and the text "Run the refinement".

Projects

Name	Status	Iteration	χ^2
240222-01	Running...	8	3.44

Plot Options

Scan	Vertical Offset
<input checked="" type="checkbox"/> I observed	0.00
<input checked="" type="checkbox"/> I calculated	0.00
<input checked="" type="checkbox"/> I difference	-2715.23
<input checked="" type="checkbox"/> Background	0.00
<input checked="" type="checkbox"/> Hydroxyapatite	0.00
<input checked="" type="checkbox"/> Calcite	0.00

Refinement Protocol

0	2.340331E+06			
1	4.856880E+05	3.396E+06	1.000E-01	1.000
2	1.585322E+05	5.482E+05	2.000E-02	1.000
3	5.899777E+04	1.736E+05	3.762E-02	1.000
4	3.760179E+04	3.286E+04	2.725E-02	1.000
5	3.218936E+04	6.891E+03	2.357E-02	1.000
6	2.468206E+04	9.362E+03	4.884E-03	1.000
7	2.042521E+04	6.670E+03	9.768E-04	1.000
8	1.959870E+04	1.405E+03	1.954E-04	1.000

Refined Parameters

Parameter	Value	ESD
Statistics		
Rwp	9.15	
Rexp	4.93	
χ^2	3.44	
GoF	1.85	
Background Coefficients		
Global GOALS		
Local GOALS		

Status Bar

C:\Users\doebelin\AppData\Local\Temp\240222-01.dia | 1 Project | $\lambda = 1.54060 \text{ \AA}$ | $2\theta = 0.000^\circ$ | $I = 0.000 \text{ cts}$ | $d = 0.000 \text{ \AA}$

Refinement Control Files (*.sav)

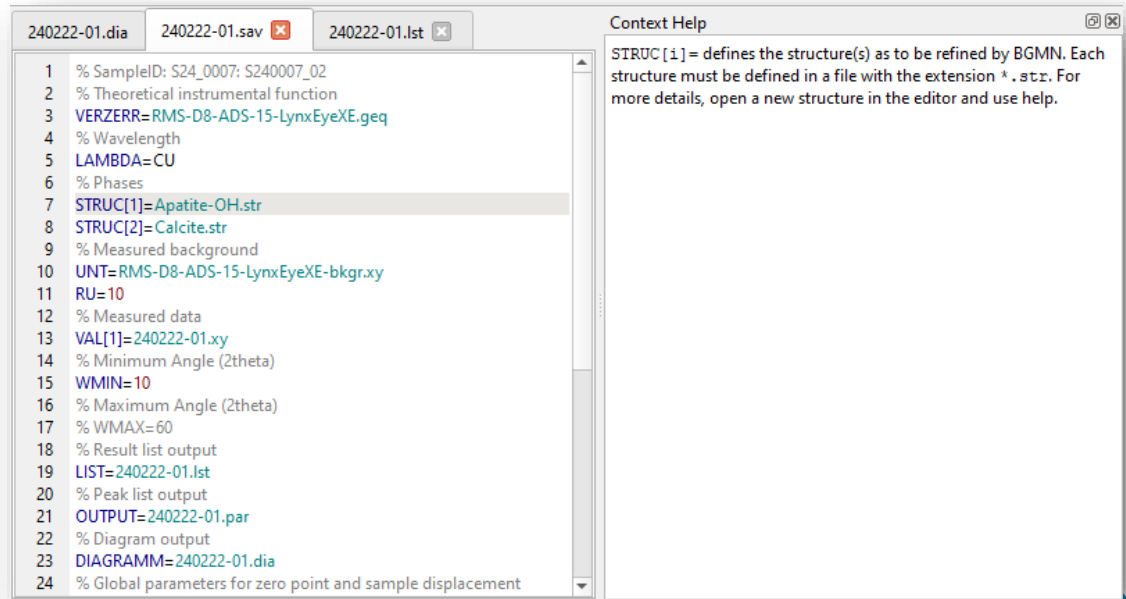
```
% SampleID: S24_0007: S240007_02
% Theoretical instrumental function
VERZERR=RMS-D8-ADS-15-LynxEyeXE.geq
% Wavelength
LAMBDA=CU
% Phases
STRUC[1]=Apatite-OH.str
STRUC[2]=Calcite.str
% Measured background
UNT=RMS-D8-ADS-15-LynxEyeXE-bkgr.xy
RU=10
% Measured data
VAL[1]=240222-01.xy
% Minimum Angle (2theta)
WMIN=10
% Maximum Angle (2theta)
% WMAX=60
% Result list output
LIST=240222-01.lst
% Peak list output
OUTPUT=240222-01.par
% Diagram output
DIAGRAMM=240222-01.dia
% Global parameters for zero point and
% sample displacement
EPS1=0
PARAM[1]=EPS2=0_-0.01^0.01
EPS3=0
alpha3ratio=0.020
betaratio=0.005
NTHREADS=8
PROTOKOLL=Y
SAVE=N

sum=Hydroxyapatite+Calcite
QHydroxyapatite=Hydroxyapatite/sum
QCalcite=Calcite/sum

GOAL[1]=QHydroxyapatite
GOAL[2]=QCalcite
```

% = comments (will be ignored by BGMN)
BLUE = variable name
Green = input / output file name
Red = numerical value

Window → Context help displays a description of variables.



Refinement Control Files (*.sav)

```
% SampleID: S24_0007: S240007_02
```

```
% Theoretical instrumental function
```

```
VERZERR=RMS-D8-ADS-15-LynxEyeXE.geq
```

```
% Wavelength
```

```
LAMBDA=CU
```

```
% Phases
```

```
STRUC[1]=Apatite-OH.str
```

```
STRUC[2]=Calcite.str
```

```
% Measured background
```

```
UNT=RMS-D8-ADS-15-LynxEyeXE-bkgr.xy
```

```
RU=10
```

```
% Measured data
```

```
VAL[1]=240222-01.xy
```

```
% Minimum Angle (2theta)
```

```
WMIN=10
```

```
% Maximum Angle (2theta)
```

```
% WMAX=60
```

```
% Result list output
```

```
LIST=240222-01.lst
```

```
% Peak list output
```

```
OUTPUT=240222-01.par
```

```
% Diagram output
```

```
DIAGRAMM=240222-01.dia
```

```
% Global parameters for zero point and
```

```
% sample displacement
```

```
EPS1=0
```

```
PARAM[1]=EPS2=0_-0.01^0.01
```

```
EPS3=0
```

```
alpha3ratio=0.020
```

```
betaratio=0.005
```

```
NTHREADS=8
```

```
PROTOKOLL=Y
```

```
SAVE=N
```

```
sum=Hydroxyapatite+Calcite
```

```
QHydroxyapatite=Hydroxyapatite/sum
```

```
QCalcite=Calcite/sum
```

```
GOAL[1]=QHydroxyapatite
```

```
GOAL[2]=QCalcite
```

Reference to instrument configuration file

Reference to wavelength distribution file

Reference to structure files (must be numbered)

Reference to measured background scan

Reference to measured diffraction pattern
(Profex will convert all formats to xy format)

Various output file names

Refinement of sample height error

Calculation of phase quantities

Refinement Control Files (*.sav)

Context menu (right mouse button) for many parameters:

240222-01.dia 240222-01.sav* 240222-01.lst

```
1 % SampleID: S24_0007: S240007_02
2 % Theoretical instrumental function
3 VERZERR=RMS-D8-ADS-15-LynxEyeXE.geq
4 % Wavelength
5 LAMBDA=CU
6 % Phases
7 STRUC[1]=Apatite-OH.str
8 STRUC[2]=Calcite.str
9 % Measured background
10 UNT=RMS-D8-ADS-15-LynxEyeXE-bkgr.xy
11 RU=10
12 % Measured data
13 VAL[1]=240222-01.xy
14 % Minimum Angle (2theta)
15 WMIN=10
16 % Maximum Angle (2theta)
17 % WMAX=60
18 % Result list output
19 LIST=240222-01.lst
20 % Peak list output
21 OUTPUT=240222-01.par
22 % Diagram output
23 DIAGRAMM=240222-01.dia
24 % Global parameters for zero point and sample displacement
```

Context menu for WMIN=10:

- Undo
- Redo Ctrl+Y
- Cut
- Copy
- Paste
- Delete
- Select All Ctrl+A
- Decrease value F5
- Increase value F6
- Comment line

240222-01.dia 240222-01.sav* 240222-01.lst

```
13 VAL[1]=240222-01.xy
14 % Minimum Angle (2theta)
15 WMIN=10
16 % Maximum Angle (2theta)
17 % WMAX=60
18 % Result list output
19 LIST=240222-01.lst
20 % Peak list output
21 OUTPUT=240222-01.par
22 % Diagram output
23 DIAGRAMM=240222-01.dia
24 % Global parameters for zero point and sample displacement
25 EPS1=0
26 PARAMETER=
27 EPS3=0
28 alpha3rd=
29 betaratio=
30 NTHREAF=
31 PROTOK=
32 SAVE=N
33 sum=Hydro
34 QHydro=
35 QCalcite=
```

Context menu for EPS1=0:

- Undo
- Redo Ctrl+Y
- Cut
- Copy
- Paste
- Delete
- Select All Ctrl+A
- Refine parameter
- Fix parameter
- Comment line

240222-01.dia 240222-01.sav* 240222-01.lst

```
1 % SampleID: S24_0007: S240007_02
2 % Theoretical instrumental function
3 VERZERR=RMS-D8-ADS-15-LynxEyeXE.geq
4 % Wavelength
5 LAMBDA=CU
6 % Phases
7 STRUC[1]=Apatite-OH.str
8 STRUC[2]=Calcite.str
9 % Measured background
10 UNT=RMS-D8-ADS-15-LynxEyeXE-bkgr.xy
11 RU=10
12 % Measured data
13 VAL[1]=240222-01.xy
14 % Minimum Angle (2theta)
15 WMIN=10
16 % Maximum Angle (2theta)
17 % WMAX=60
18 % Result list output
19 LIST=240222-01.lst
20 % Peak list output
21 OUTPUT=240222-01.par
22 % Diagram output
23 DIAGRAMM=240222-01.dia
24 % Global parameters for zero point and sample displacement
```

Context menu for UNT=RMS-D8-ADS-15-LynxEyeXE-bkgr.xy:

- Undo
- Redo Ctrl+Y
- Cut
- Copy
- Paste
- Delete
- Select All Ctrl+A
- Open file as text
- Open file as graph
- Comment line

Refinement Control Files (*.sav)

```
% Global parameters for zero point and  
% sample displacement  
EPS1=0  
PARAM[1]=EPS2=0_-0.01^0.01  
EPS3=0
```

How to refine parameters

Parameter fixed at 0 (not refined):

```
EPS1=0
```

Parameter refined:

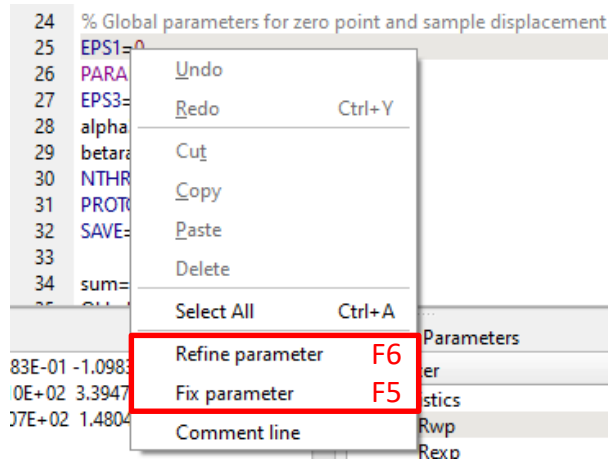
```
PARAM[n]=EPS1=0
```

Parameter refined with limits:

```
PARAM[n]=EPS1=0_-0.01^0.01
```

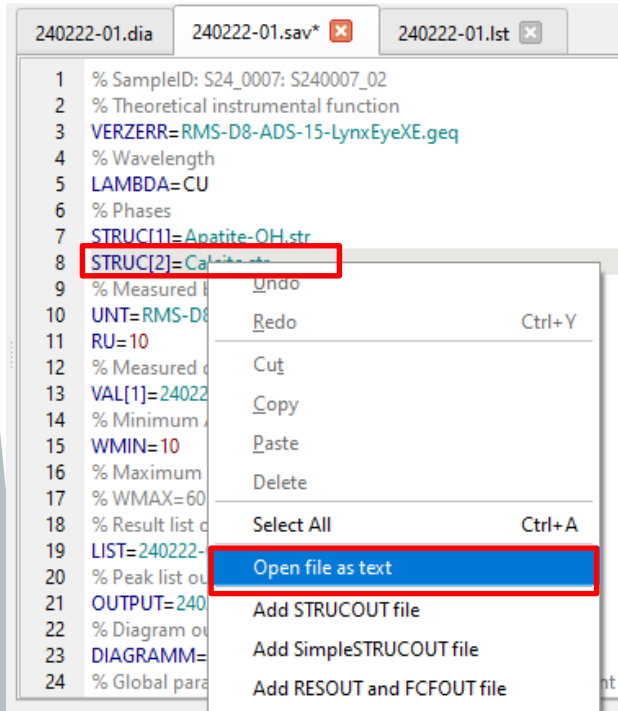
```
PARAM[n]= name= initial value _lower limit ^upper limit
```

n = consecutive number



Structure Files (*.str)

Opening structure files



or Ctrl+T on STRUC[n] line

```
PHASE=Calcite // 04-008-0788
MineralName=Calcite //
Formula=Ca_(CO3) //
SpacegroupNo=167 HermannMauguin=R-32/c //
PARAM=A=0.4991_0.4941^0.5041 PARAM=C=1.7062_1.6891^1.7233 //
RP=4 k1=0 k2=0 PARAM=B1=0_0^0.01 GEWICHT=SPHAR4 //
GOAL=GrainSize(1,1,1) //
GOAL:Calcite=GEWICHT*ifthenelse(ifdef(d),exp(my*d*3/4),1)
E=CA Wyckoff=b x=0.0000 y=0.0000 z=0.0000 TDS=0.00796938
E=C Wyckoff=a x=0.0000 y=0.0000 z=0.2500 TDS=0.00757986
E=O Wyckoff=e x=0.2573 y=0.0000 z=0.2500 TDS=0.01400168
```

// = comments (will be ignored by BGMN)
(trailing // are optional / used for historic reasons)

BLUE = variable name
Light blue = input / output file name
Red = numerical value
GREEN = GOAL declaration

Refined parameters in STR files are **not numbered**:
PARAM=name=value_lowerLimit^upperLimit

Structure Files (*.str)

PHASE=Calcite // 04-008-0788

Phase name (don't use spaces or special characters)
Database record (used by Profex)

MineralName=Calcite
Formula=Ca_(CO3)

Informative (not used by Profex or BGMN)

SpacegroupNo=167 **HermannMauguin**=R-32/c

Space group number and HM symbol

PARAM=A=0.4991_0.4941^0.5041 **PARAM=C**=1.7062_1.6891^1.7233

Cell parameters (A, B, C, ALPHA, BETA, GAMMA)

RP=4 **k1**=0 **k2**=0 **PARAM=B1**=0_0^0.01

Profile parameters (peak broadening)

GEWICHT=SPHAR4

Scale factor and texture refinement

GOAL=GrainSize(1,1,1)

Calculate crystallite size

GOAL:Calcite=**GEWICHT***ifthenelse(ifdef(d),exp(my*d*3/4),1)

Brindley correction for micro-absorption and assign corrected scale factor **GEWICHT** to variable „Calcite“

E=CA Wyckoff=b x=0.0000 **y**=0.0000 **z**=0.0000 **TDS**=0.00796938
E=C Wyckoff=a x=0.0000 **y**=0.0000 **z**=0.2500 **TDS**=0.00757986
E=O Wyckoff=e x=0.2573 **y**=0.0000 **z**=0.2500 **TDS**=0.01400168

Atomic sites (TDS = thermal displacement parameter)

Structure Files (*.str)

RP=4 k1=0 k2=0 PARAM=B1=0_0^0.01 GEWICHT=SPHAR4

RP=4

Profile function:

RP=2: no peak broadening

RP=3: only crystallite size peak broadening

RP=4: crystallite size + micro-strain peak broadening

k1=0

Crystallite size distribution

k2=0

Micro-strain related peak broadening (can be anisotropic)

PARAM=B1=0_0^0.01

Crystallite size related peak broadening (can be anisotropic)

GEWICHT=SPHAR4

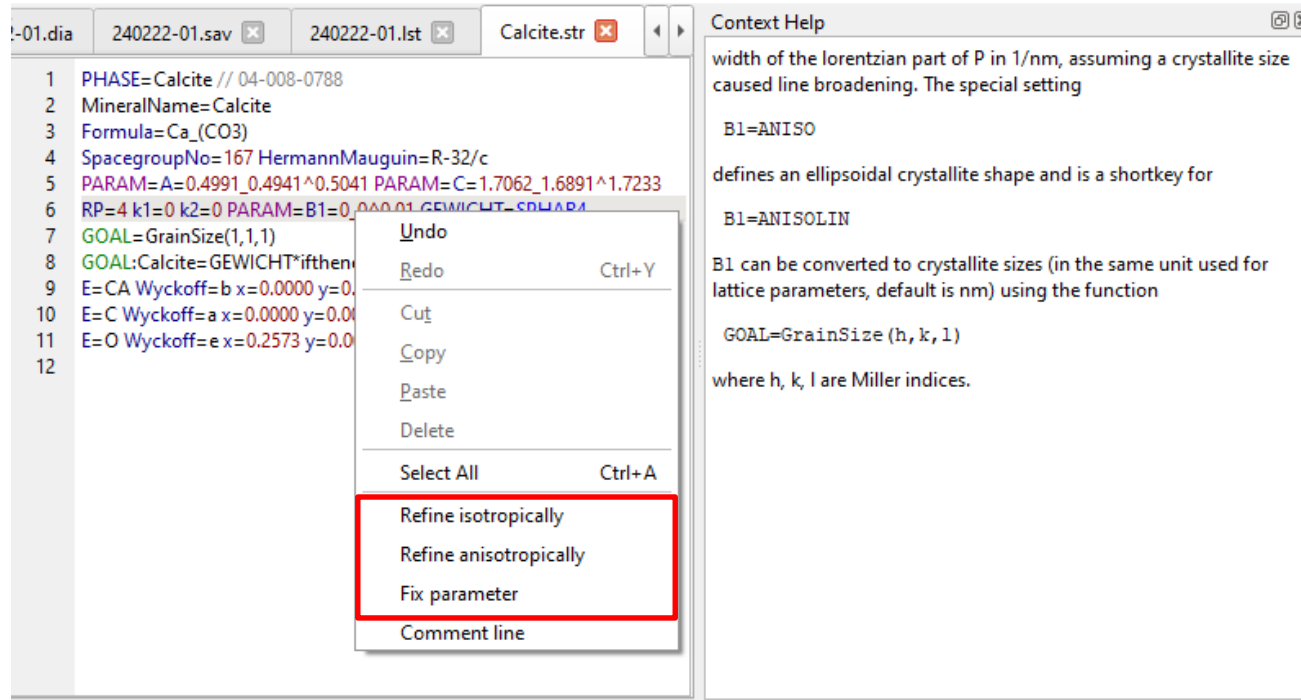
Scale factor corrected for unit cell density ($GEWICHT = S \cdot (Z \cdot M \cdot V)$)

SPHAR0: no texture

SPHAR>0: texture model activated

Structure Files (*.str)

Use the context help (Window → Context Help) for a description of the parameters, and the context menu (right mouse button) to toggle the refinement state:



The screenshot displays a software interface with a text editor on the left and a context help window on the right. The text editor shows a structure file named 'Calcite.str' with the following content:

```
1 PHASE= Calcite // 04-008-0788
2 MineralName= Calcite
3 Formula= Ca_(CO3)
4 SpacegroupNo= 167 HermannMauguin=R-32/c
5 PARAM=A=0.4991_0.4941^0.5041 PARAM=C= 1.7062_1.6891^1.7233
6 RP=4 k1=0 k2=0 PARAM=B1=0.00001 GEWICHT= SCHWARZ
7 GOAL=GrainSize(1,1,1)
8 GOAL:Calcite=GEWICHT*ifthen
9 E=CA Wyckoff=b x=0.0000 y=0.0000
10 E=C Wyckoff=a x=0.0000 y=0.0000
11 E=O Wyckoff=e x=0.2573 y=0.0000
12
```

The context help window, titled 'Context Help', provides a description of the parameter B1:

width of the lorentzian part of P in 1/nm, assuming a crystallite size caused line broadening. The special setting

B1=ANISO

defines an ellipsoidal crystallite shape and is a shortcut for

B1=ANISOLIN

B1 can be converted to crystallite sizes (in the same unit used for lattice parameters, default is nm) using the function

GOAL=GrainSize (h, k, l)

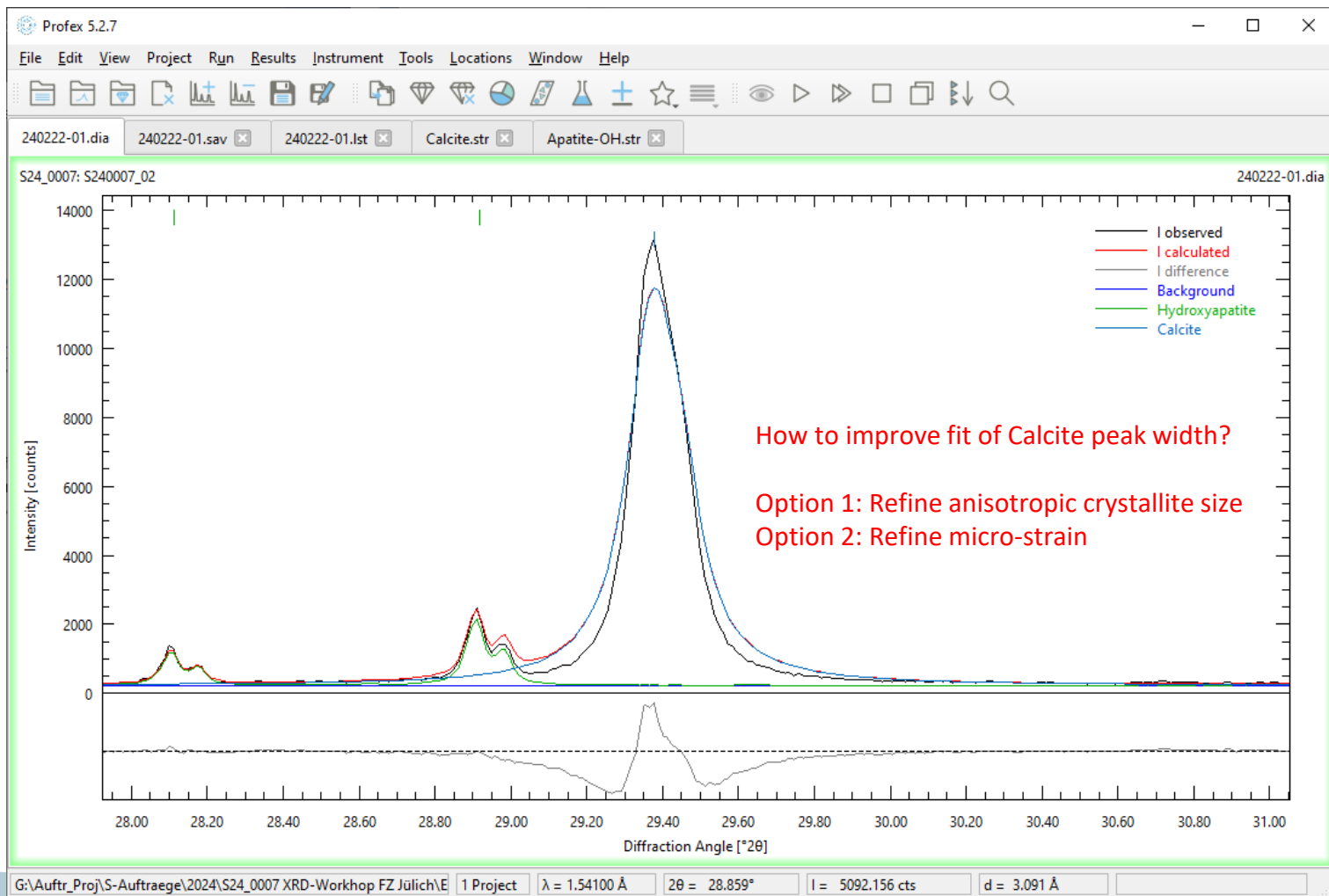
where h, k, l are Miller indices.

A context menu is open over the text editor, listing the following options:

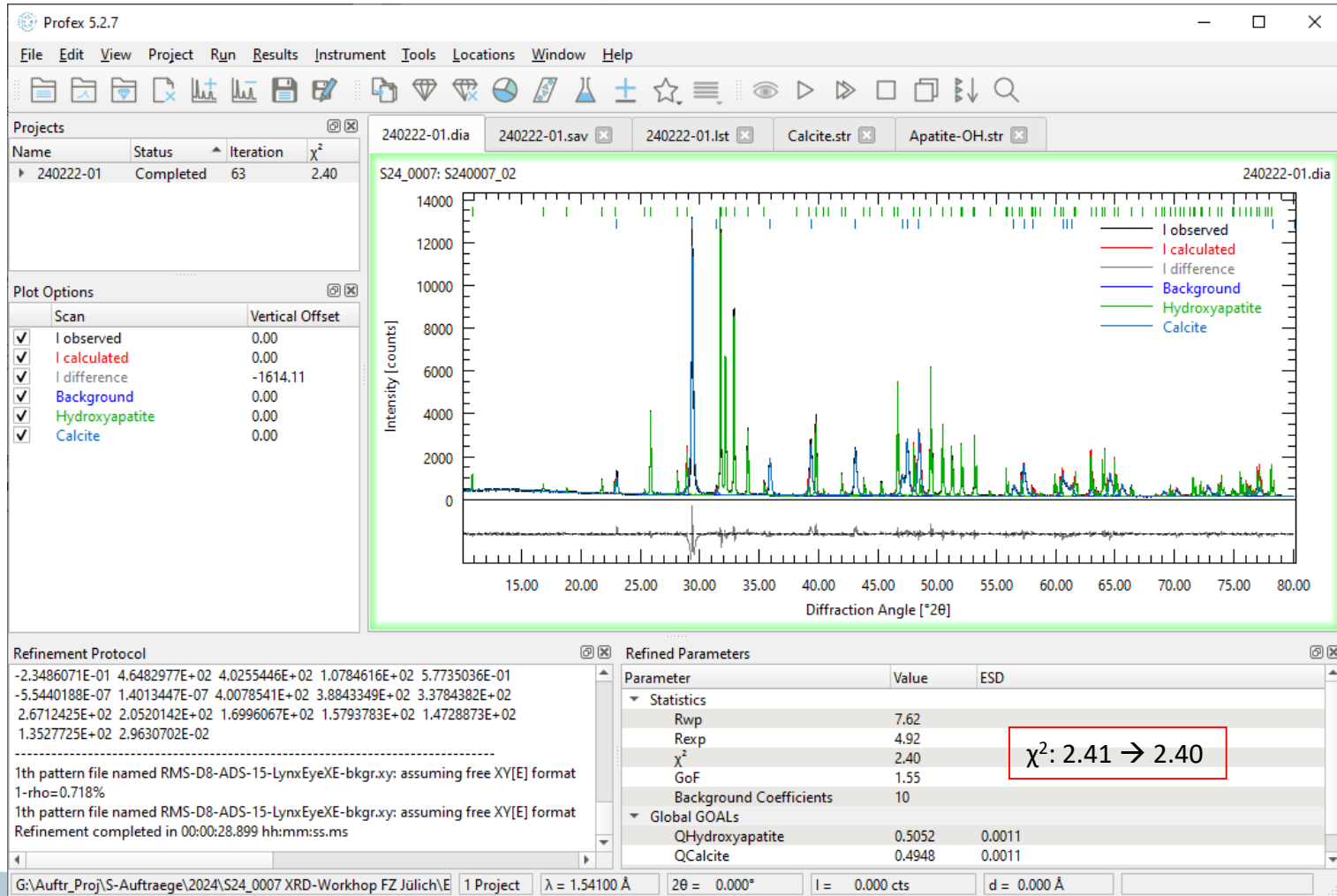
- Undo
- Redo Ctrl+Y
- Cut
- Copy
- Paste
- Delete
- Select All Ctrl+A
- Refine isotropically
- Refine anisotropically
- Fix parameter
- Comment line

The 'Refine isotropically', 'Refine anisotropically', and 'Fix parameter' options are highlighted with a red box.

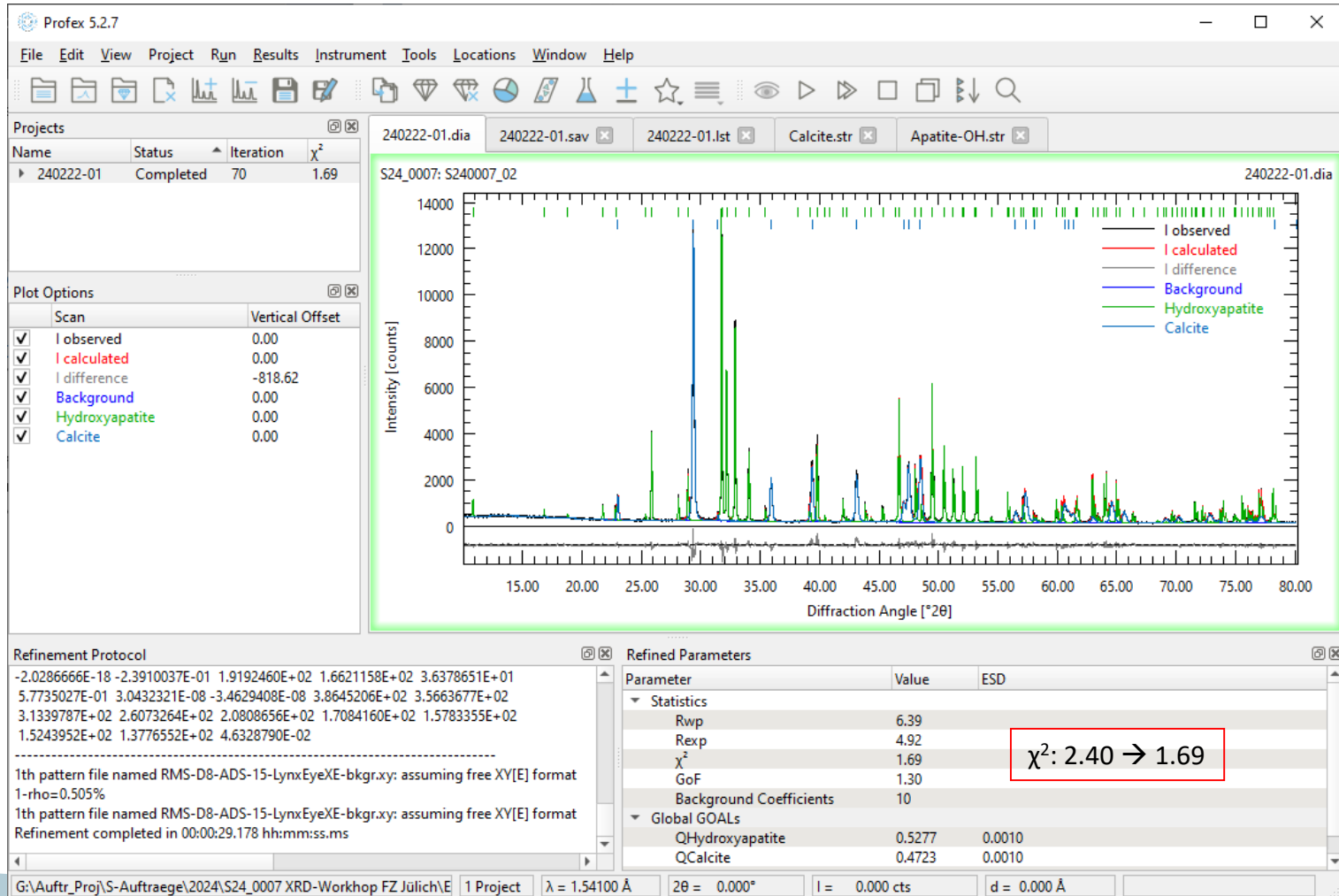
First Rietveld Refinement: Improving the Refinement



First Rietveld Refinement: Improving the Refinement



First Rietveld Refinement: Improving the Refinement



First Rietveld Refinement: Results

Profex 5.2.7

File Edit View Project Run Results Instrument Tools Locations Window Help

Projects

Name	Status	Iteration	χ^2
240222-01	Completed	70	1.69

Plot Options

Scan	Vertical Offset
<input checked="" type="checkbox"/> I observed	0.00
<input checked="" type="checkbox"/> I calculated	0.00
<input checked="" type="checkbox"/> I difference	-818.62
<input checked="" type="checkbox"/> Background	0.00
<input checked="" type="checkbox"/> Hydroxyapatite	0.00
<input checked="" type="checkbox"/> Calcite	0.00

240222-01.dia 240222-01.sav 240222-01.lst Calcite.str Apatite-OH.str

```
1 Rietveld refinement to file(s) 240222-01.xy
2 BGMN version 4.2.22, 5717 measured points, 148 peaks, 58 parameters
3 Start: Mon Feb 26 14:08:53 2024; End: Mon Feb 26 14:09:08 2024
4 74 iteration steps
5
6 Rp=5.43% Rpb=9.17% R=5.64% Rwp=6.39% Rexp=4.92%
7 Durbin-Watson d=1.00
8 1-rho=0.505%
9
10 Global parameters and GOALS
11 *****
12 QHydroxyapatite=0.5277+-0.0010
13 QCalcite=0.4723+-0.0010
14 EPSZ=-0.0000153+-0.0000016
15
16 Local parameters and GOALS for phase Hydroxyapatite
17 *****
18 SpacegroupNo=176
19 HermannMauguin=P6_3/m
20 XrayDensity=3.150
21 Rphase=6.04%
22 UNIT=NM
23 A=0.9425490+-0.0000036
24 C=0.6883865+-0.0000033
```

Phase quantities (normalized to 1.0)

Refinement Protocol

```
-2.0286666E-18 -2.3910037E-01 1.9192460E+02 1.6621158E+02 3.6378651E+01
5.7735027E-01 3.0432321E-08 -3.4629408E-08 3.8645206E+02 3.5663677E+02
3.1339787E+02 2.6073264E+02 2.0808656E+02 1.7084160E+02 1.5783355E+02
1.5243952E+02 1.3776552E+02 4.6328790E-02
-----
1th pattern file named RMS-D8-ADS-15-LynxEyeXE-bkgr.xy: assuming free XY[E] format
1-rho=0.505%
1th pattern file named RMS-D8-ADS-15-LynxEyeXE-bkgr.xy: assuming free XY[E] format
Refinement completed in 00:00:29.178 hh:mm:ss.ms
```

Refined Parameters

Parameter	Value	ESD
Statistics		
Rwp	6.39	
Rexp	4.92	
χ^2	1.69	
GoF	1.30	
Background Coefficients		
10		
Global GOALS		
QHydroxyapatite	0.5277	0.0010
QCalcite	0.4723	0.0010

G:\Auftr_Proj\S-Auftraege\2024\524_0007 XRD-Workhop FZ Jülich\ 1 Project $\lambda = 1.54060 \text{ \AA}$ $2\theta = 0.000^\circ$ $I = 0.000 \text{ cts}$ $d = 0.000 \text{ \AA}$ Line: 9, Column: 1

First Rietveld Refinement: Results

Profex 5.2.7

File Edit View Project Run Results Instrument Tools Locations Window Help

Projects

Name	Status	Iteration	χ^2
240222-01	Completed	70	1.69

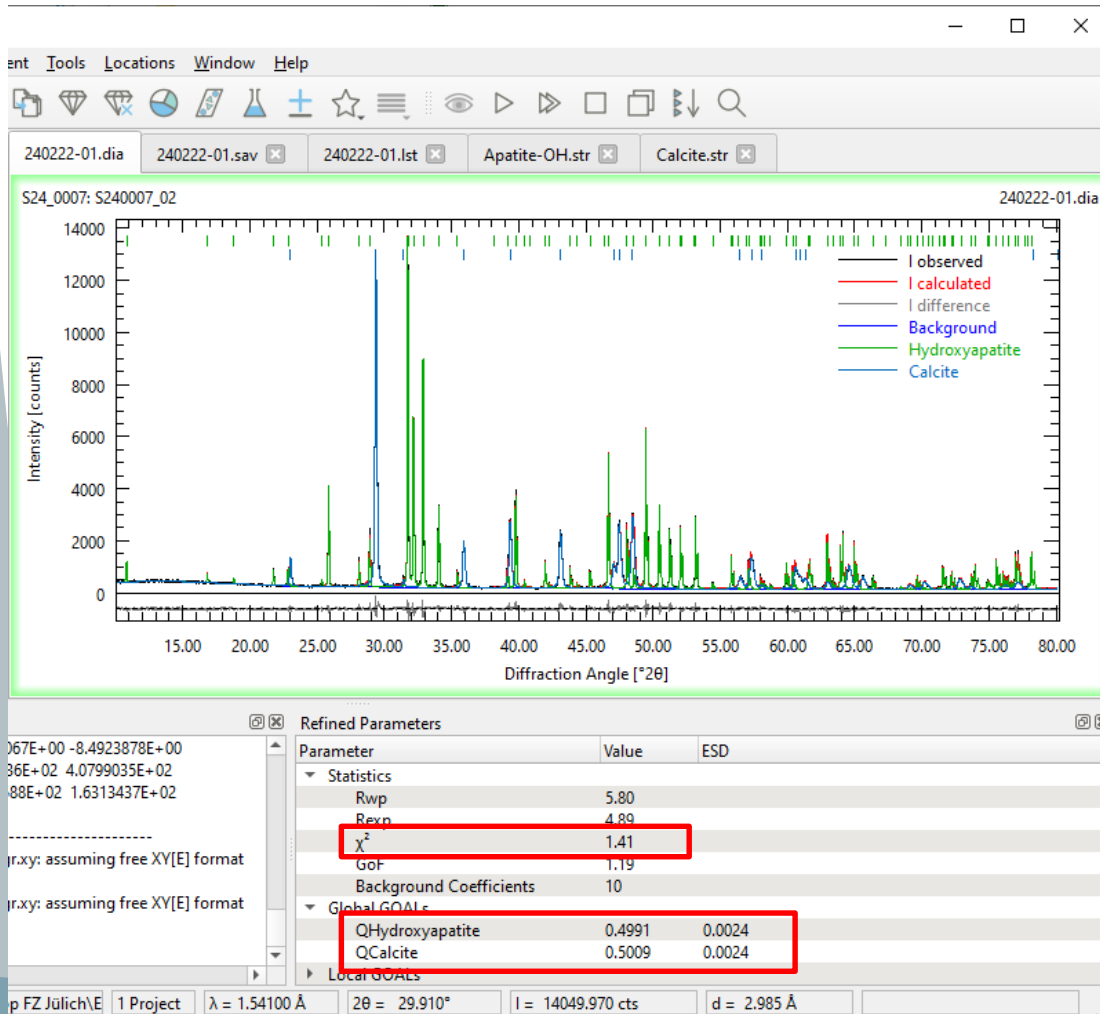
Rietveld refinement to file(s) 240222-01.xy
2 BGMN version 4.2.22, 5717 measured points, 148 peaks, 58 parameters
3 Start: Mon Feb 26 14:08:53 2024; End: Mon Feb 26 14:09:08 2024
4 74 iteration steps

results-ex1.csv - Excel

File Start Einfügen Seitenlayout Formeln Daten Überprüfen Ansicht Hilfe Sie wünschen... Freigeben

File	Sample	Sample ID	Parameter, Goal	Value	ESD
240222-01	S24_0007: S240007_02	QHydroxyapatite	0.5277	0.001	
240222-01	S24_0007: S240007_02	QCalcite	0.4723	0.001	
240222-01	S24_0007: S240007_02	Rwp	6.39		
240222-01	S24_0007: S240007_02	Rexp	4.92		
240222-01	S24_0007: S240007_02	Chi2	1.6868		
240222-01	S24_0007: S240007_02	GOF	1.2988		

First Rietveld Refinement: Outlook



My best fit (with additional tweaks):

- Anisotropic k2 and B1 for both phases
- Texture SPHAR6 for both phases
- Bimodal crystallite size for Calcite
- Substitution Ca \rightarrow Mg for Calcite
- Substitution Ca \rightarrow Na for Apatite-OH

The sample is a synthetic mixture of 50.0 wt-% Calcite + 50.0 wt-% Apatite-OH