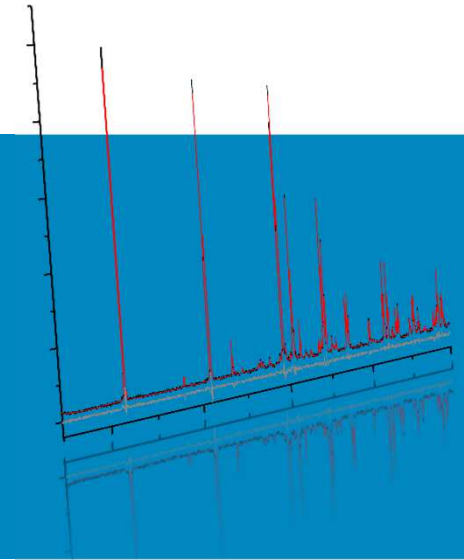


Lesson 5

BGMN & Profex



Nicola Döbelin
RMS Foundation, Bettlach, Switzerland

Repetition: BGMN

BGMN:

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

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

Program Description

Site map

Up Program Description BGMN FAQ Download Page

Instrumental Function The following pages serve as a short introduction into the BGMN Rietveld software. A description of an example (plaster) makes your test runs easier.

Tube Tails and size/strain estimation First, the generation of the instrumental function is described.

Structure Description Second, the construction of structure files is explained. In an extra topic the handling of preferred orientation is mentioned in detail.

Download Structures Third, the calculation control during a problem specific control file is shown.

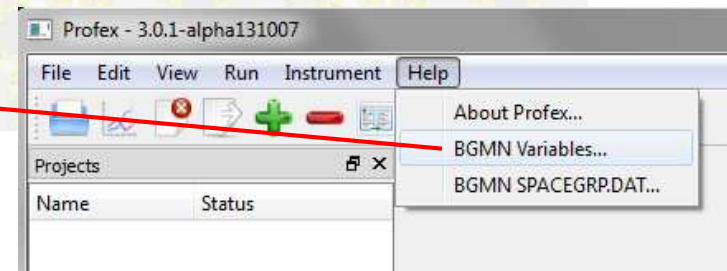
Preferred Orientation Last, we have a look at the different result files.

Calculation Control A somewhat extended explanation of the used variables is also available.

Result Output

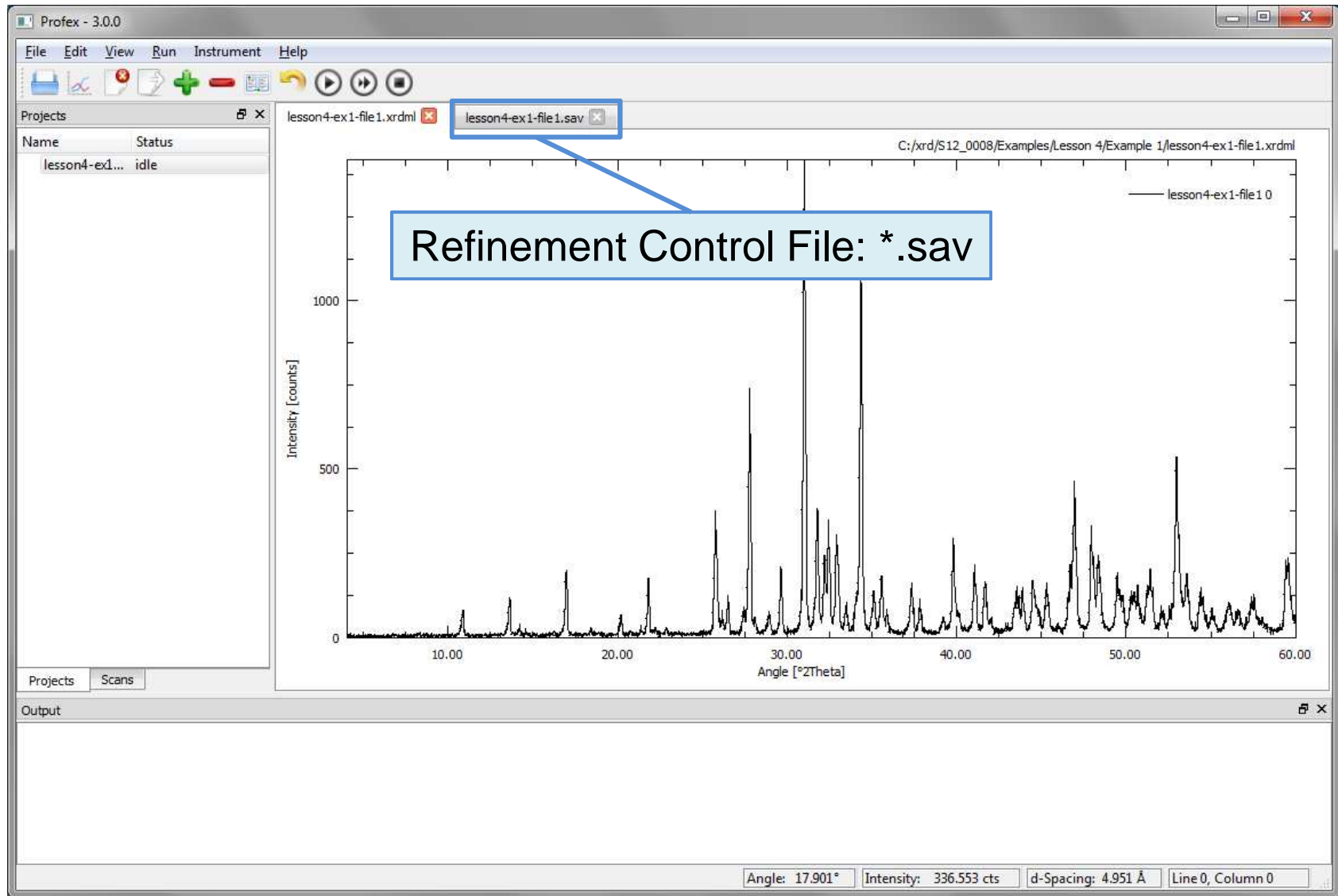
BGMN Variables

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

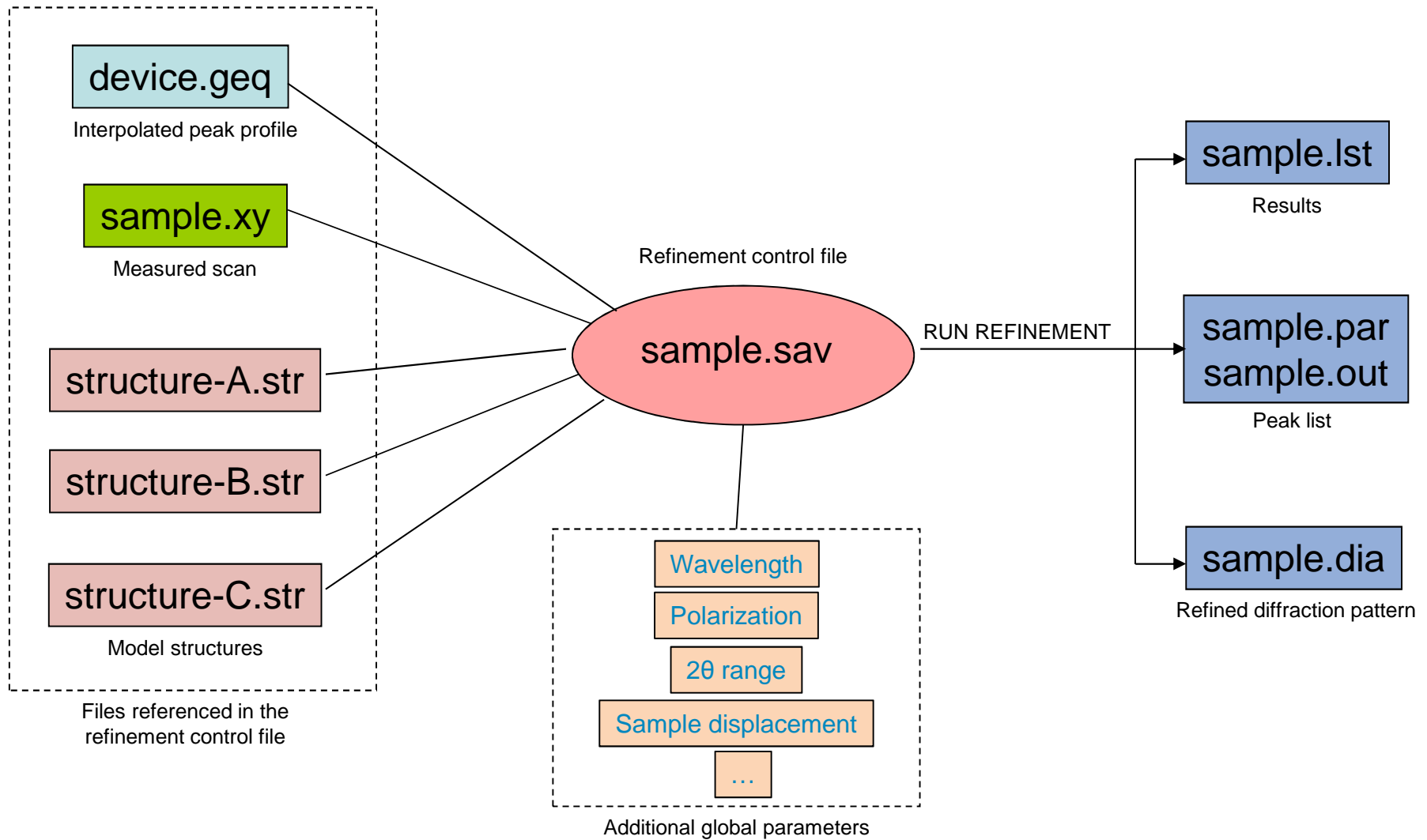


opens website

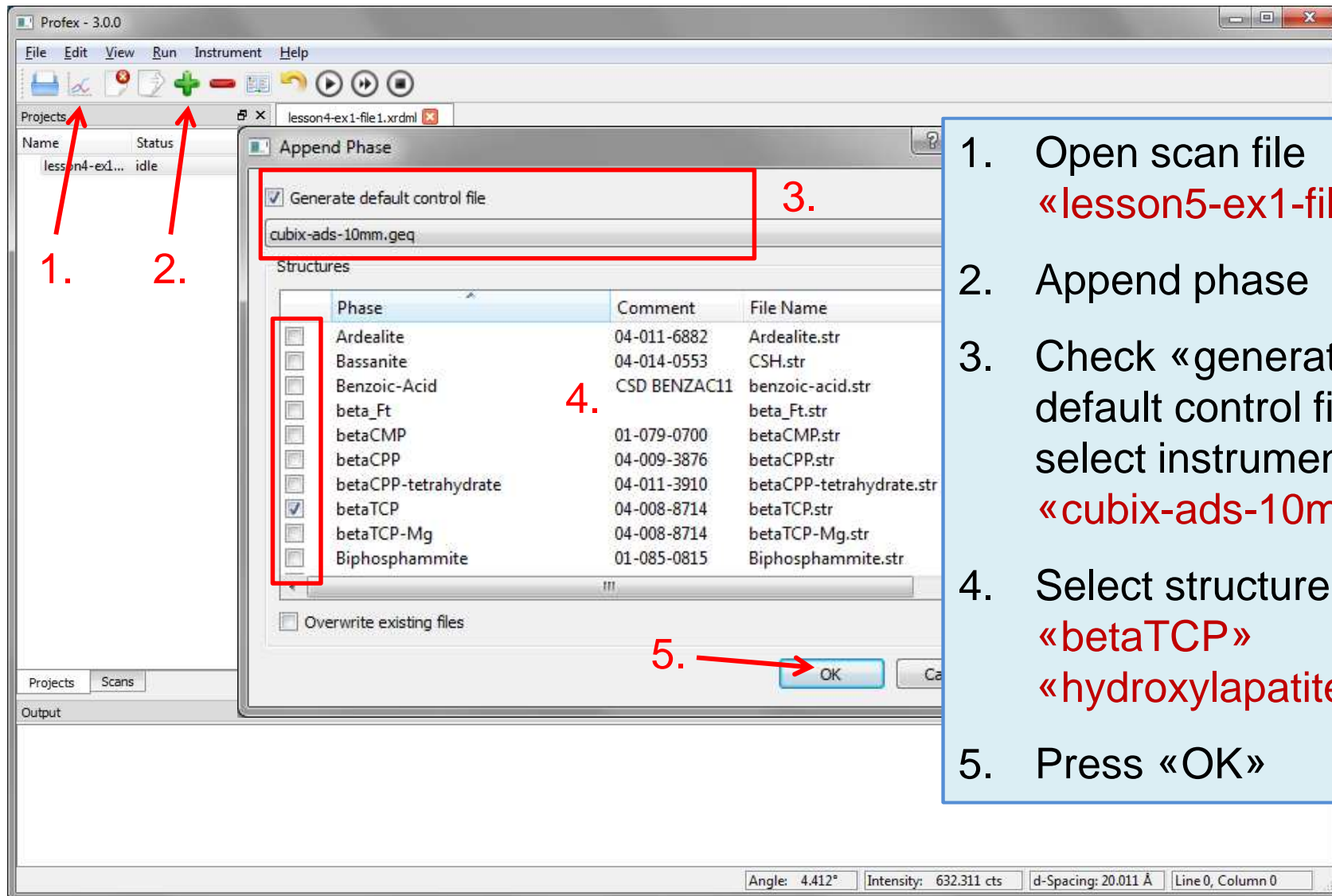
BGMN Program Structure



BGMN Control File (*.sav)

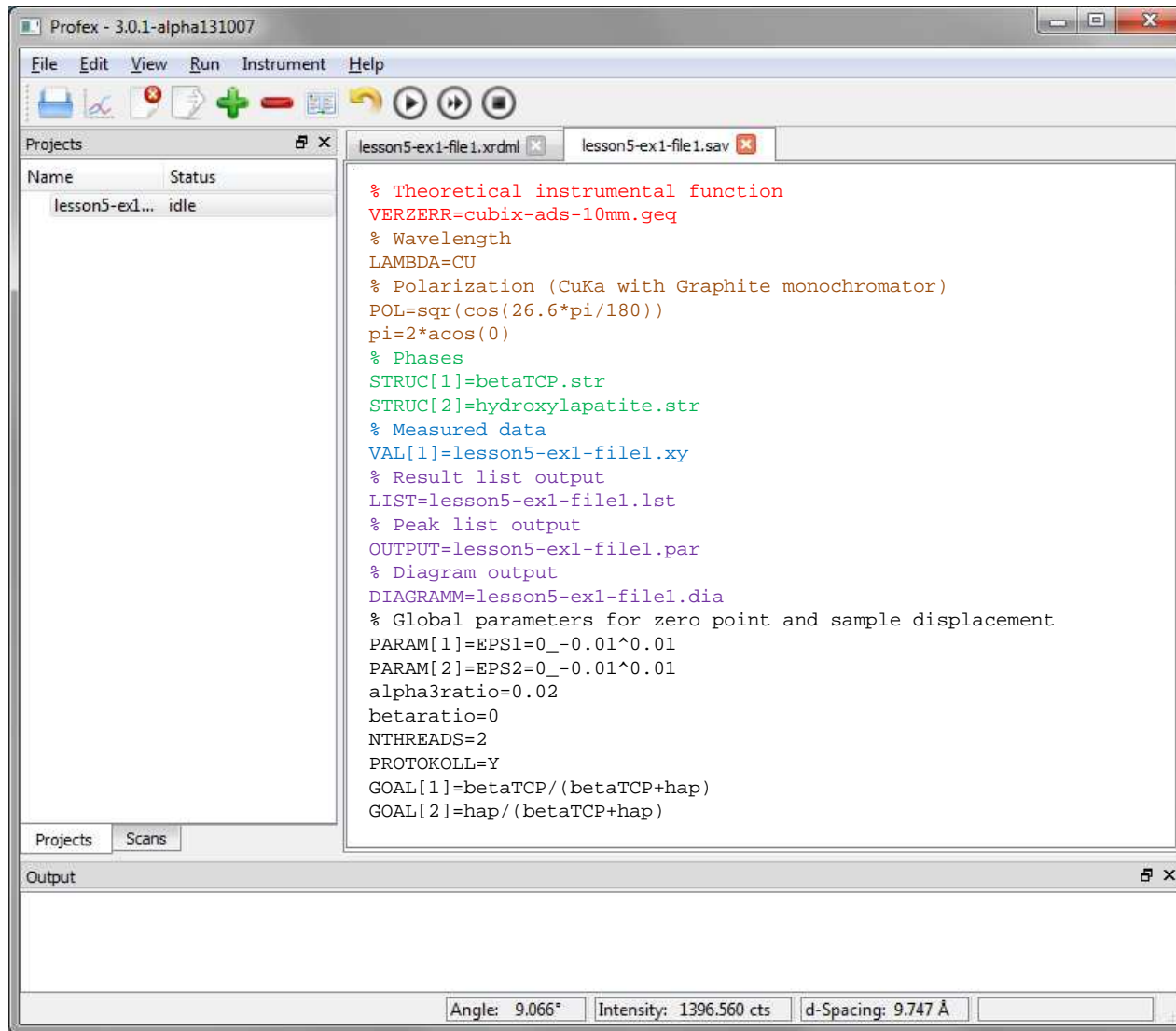


Lesson 5: Example 1



1. Open scan file «lesson5-ex1-file1»
2. Append phase
3. Check «generate default control file», select instrument «cubix-ads-10mm»
4. Select structure files «betaTCP» «hydroxylapatite»
5. Press «OK»

Lesson 5: Example 1



Instrument profile

Wavelength and polarization

Refined phases

Measured scan

Various output files
(may be empty before running BGMN)

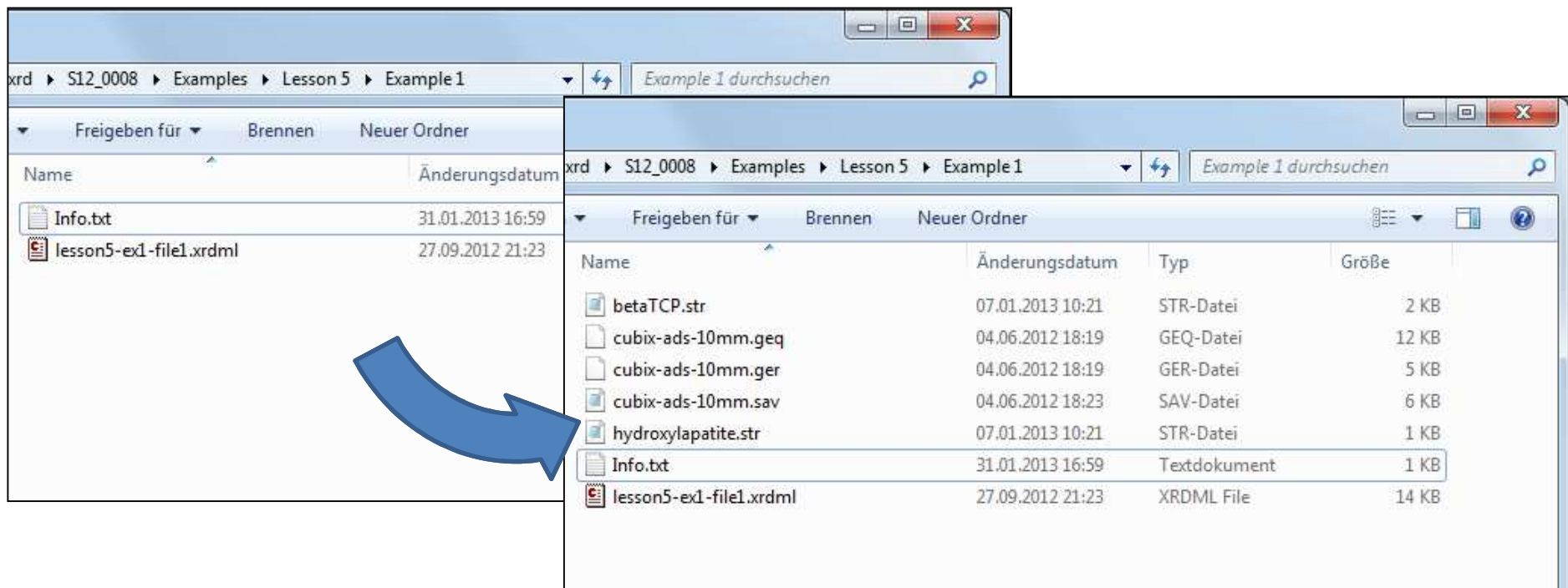
Various global parameters

- Zero-shift (EPS1)
- Sample displacement (EPS2)
- Sample transparency (EPS3)
- Calculation of phase quantities (GOAL[x])

BGMN Control File (*.sav)

What Profex does in the background:

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



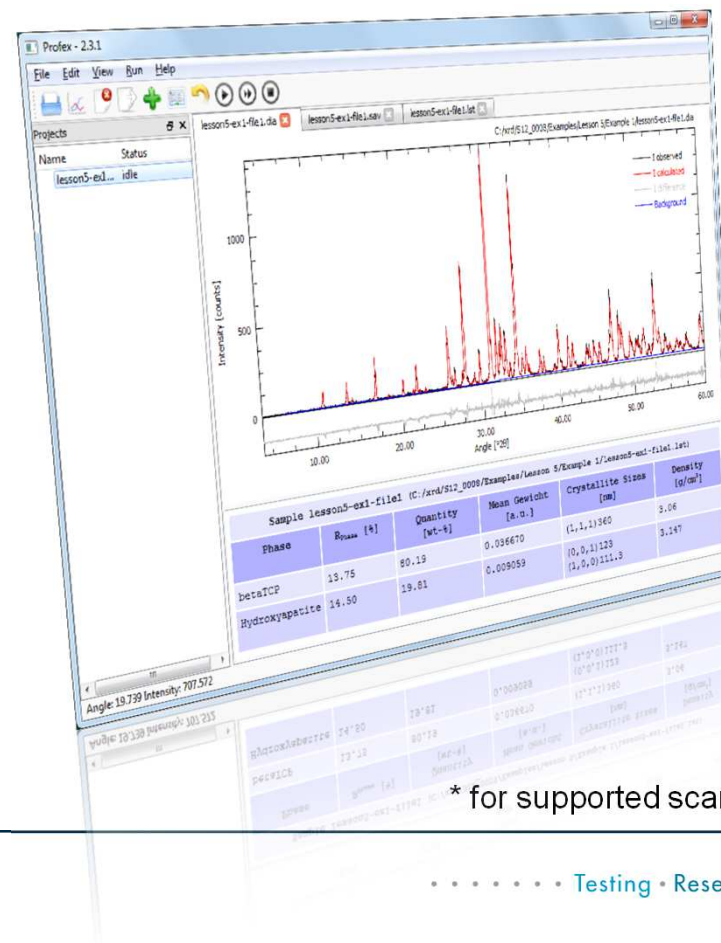
Profex

With Profex:

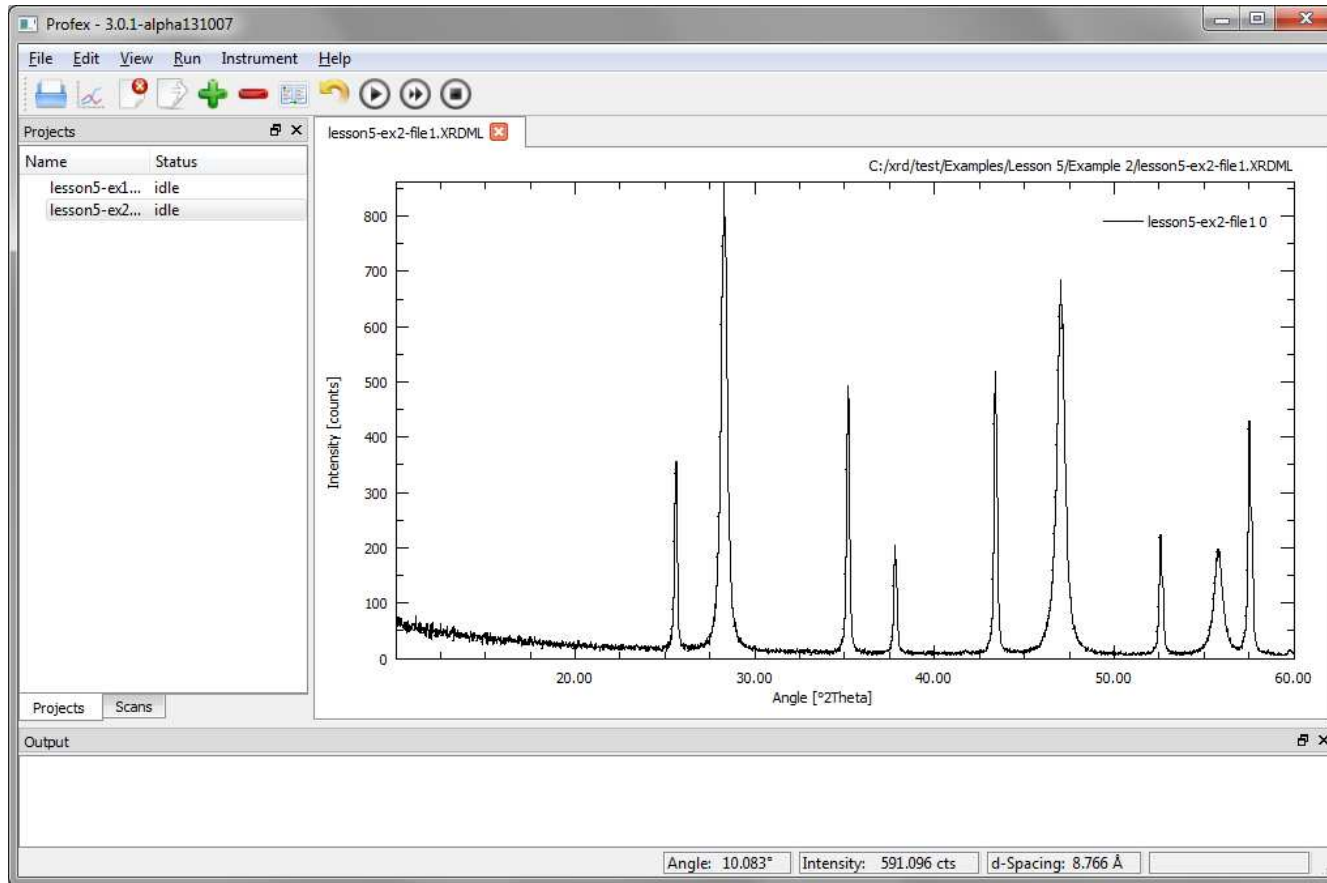
1. Load scan file
2. Use «Append phase» dialog to select phases, instrument, and generate control file
3. Run refinement

No need to:

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



Lesson 5: Example 2



Instrument:

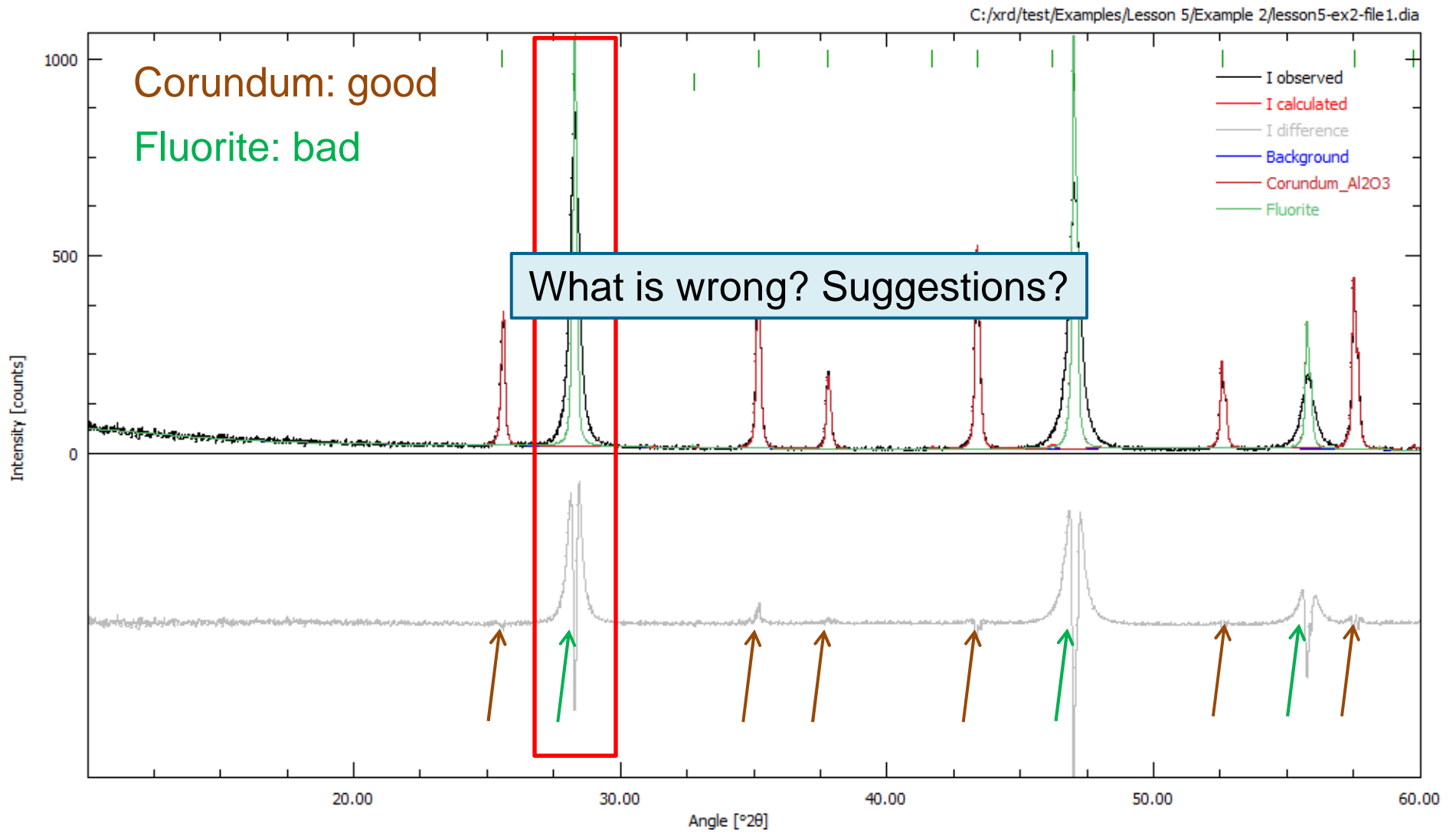
«pw1800-fds-0250»

Phases:

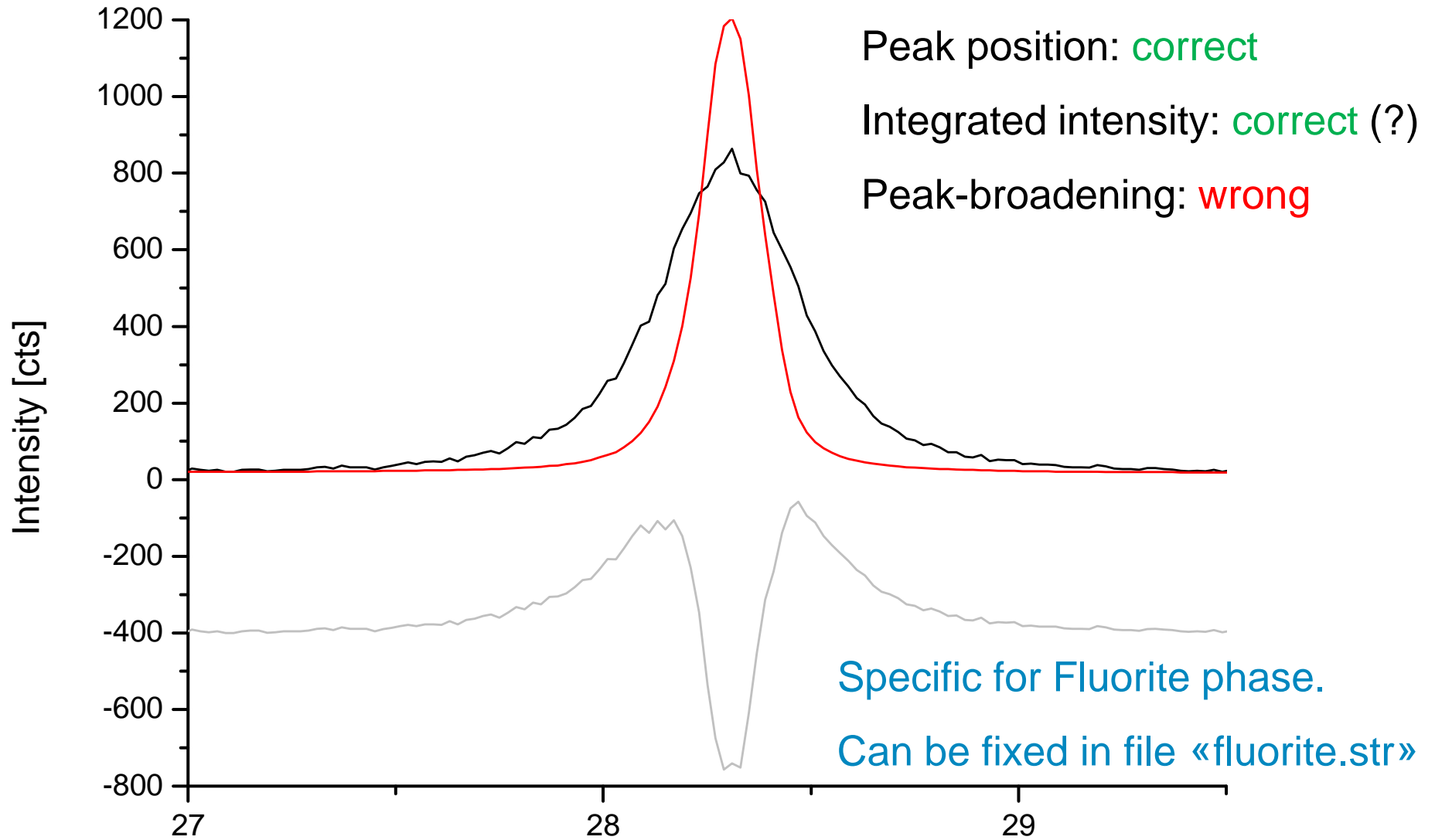
«Corundum_AL2O3»

«Fluorite»

Lesson 5: Example 2

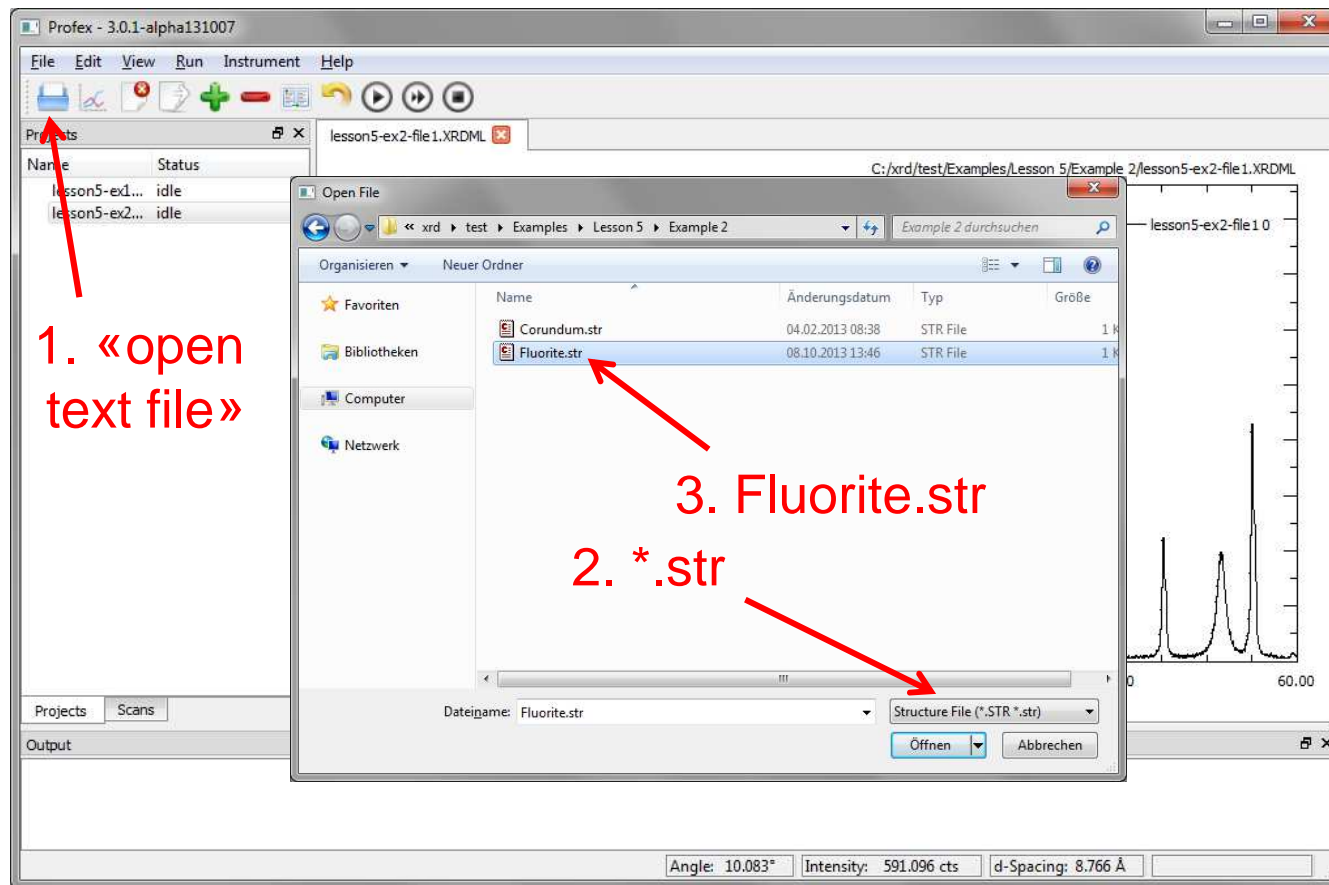


Lesson 5: Example 2



BGMN Structure Files (*.str)

Structure files contain a description of the crystal structure.
Similar to CIF files, but different file format.



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
    
```

Phase name // PDF code
 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

Full notation:

E=CA+2(1) Wyckoff=a x=0.0 y=0.0 z=0.0 TDS=0.0041

Element

Wyckoff sequence

Thermal displacement parameter
(B_{iso} [nm²])

Site occupancy

Fractional coordinates

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
    
```

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

Lesson 5: Example 2

```
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
```

In Lesson 5, Example 2,
peak broadening was not
fitted correctly

Peak profile is
controlled here

RP=4: usage of both Lorentzian and squared Lorentzian broadening

B1: lorentzian broadening caused by size effects

k1: gaussian-like part of the size effects

k2: micro strain effect

<http://www.bgm.de/variables.html#real>

Lesson 5: Example 2

```
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
```

RP=4: uses all possible broadening contributions (**good**)

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

k1: gaussian size effect: not refined (**bad**)

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

Lesson 5: Example 2

Change:

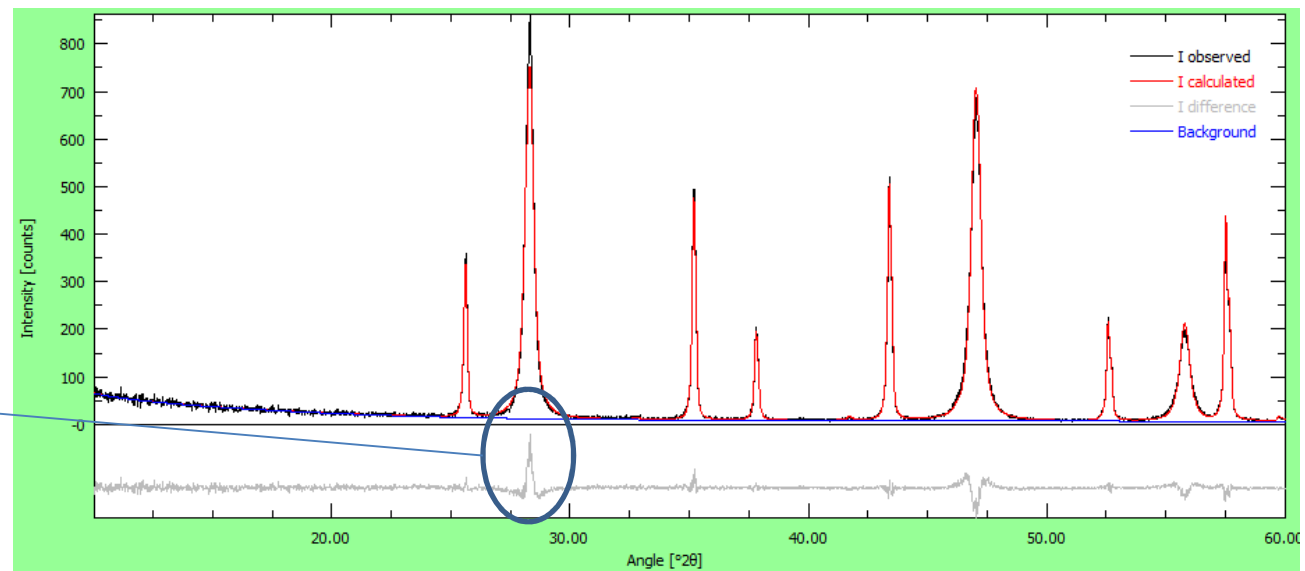
```
RP=4 k1=0 k2=0 PARAM=B1=0_0^0.003 PARAM=GEWICHT=0.1_0 //
```

To:

```
RP=4 PARAM=k1=0_0^1 k2=0 PARAM=B1=0_0^0.03 PARAM=GEWICHT=0.1_0 //
```

Repeat Refinement

Better, but not perfect.
Is there microstrain?



Lesson 5: Example 2

Change:

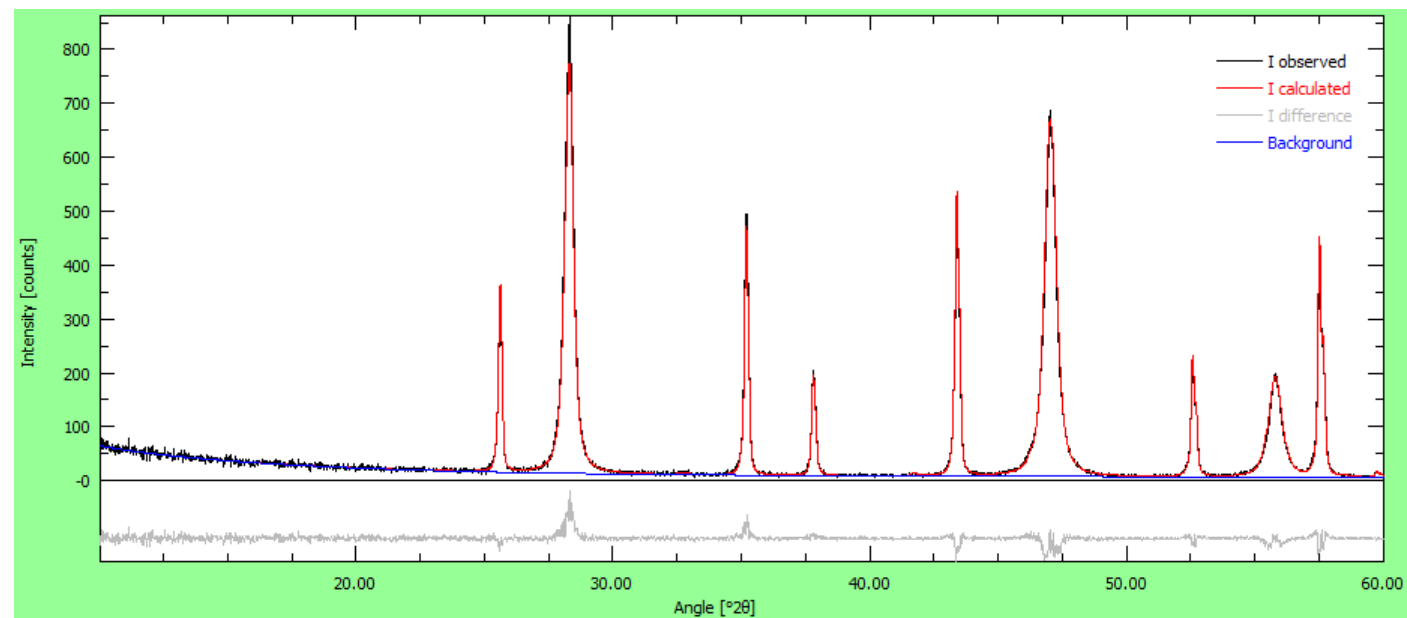
```
RP=4 PARAM=k1=0_0^1 k2=0 PARAM=B1=0_0^0.03 PARAM=GEWICHT=0.1_0 //
```

To:

```
RP=4 PARAM=k1=0_0^1 PARAM=k2=0_0 PARAM=B1=0_0^0.03 PARAM=GEWICHT=0.1_0 //
```

Repeat Refinement

Better, but **still**
not perfect.



Lesson 5: Example 2

Preferred Orientation:

- Refine «GEWICHT» as «SPHAR6»
- Remove «PARAM=»
- Explanation follows later

Change:

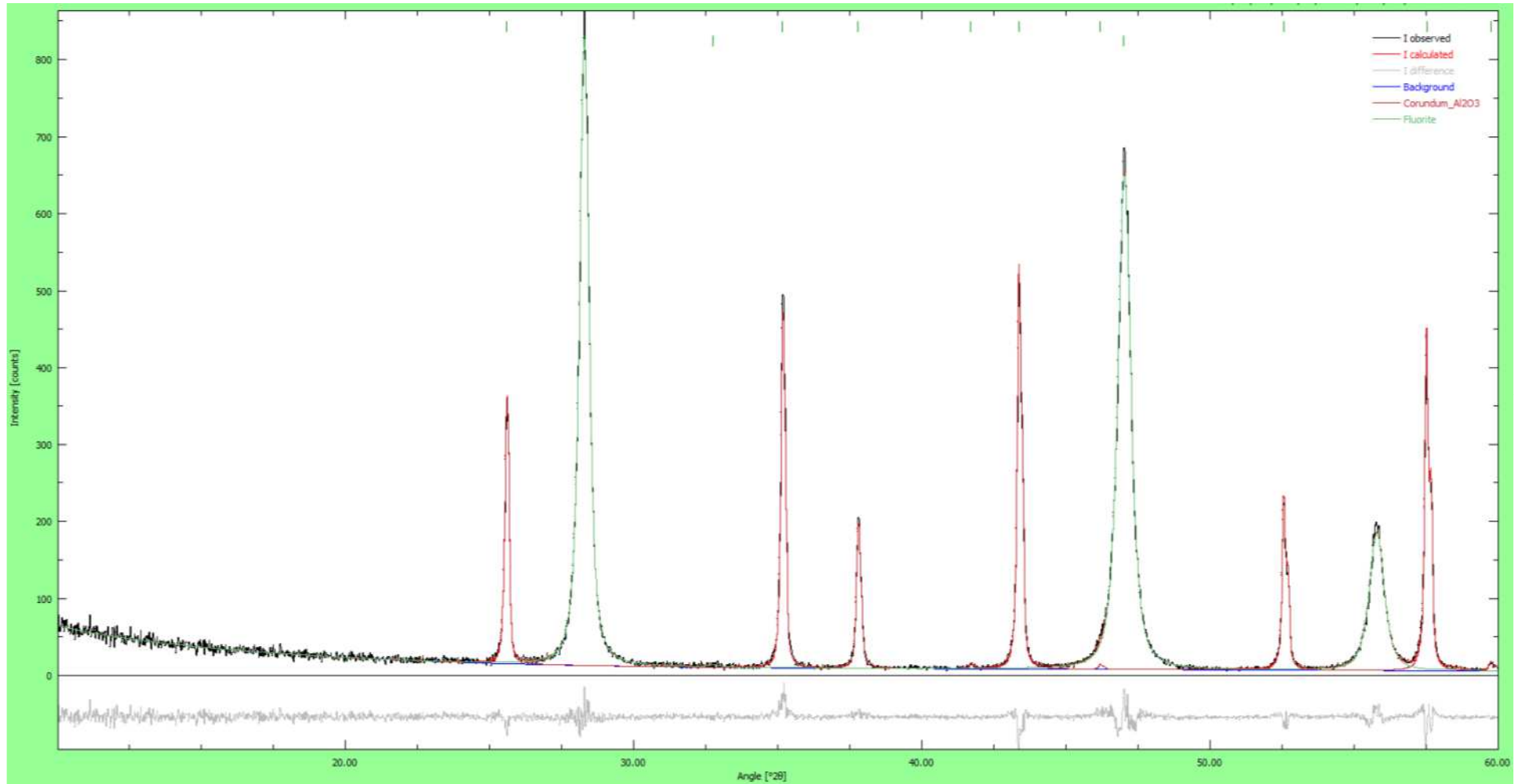
```
RP=4 PARAM=k1=0_0^1 PARAM=k2=0_0 PARAM=B1=0_0^0.03 PARAM=GEWICHT=0.1_0 //
```

To:

```
RP=4 PARAM=k1=0_0^1 PARAM=k2=0_0 PARAM=B1=0_0^0.03 GEWICHT=SPHAR6 //
```

Repeat Refinement

Lesson 5: Example 2



Summary: Structure Files (*.str)

- Structure file database (*.str) is stored in C:\Program Files\Profex-x.y.z\Structures
- Copied by Profex to the location of the scan file
- They contain:
 - Space group information
 - Unit cell dimensions
 - Profile parameters
 - Scaling (weight)
 - 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)

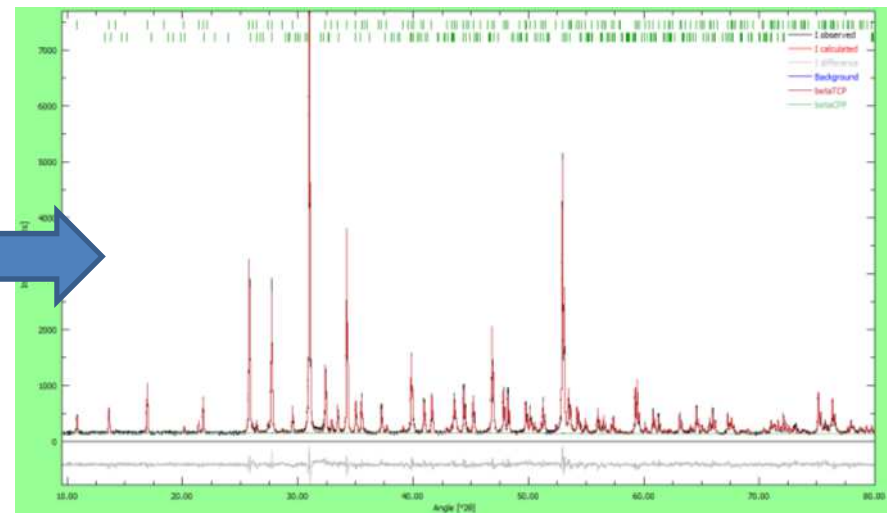
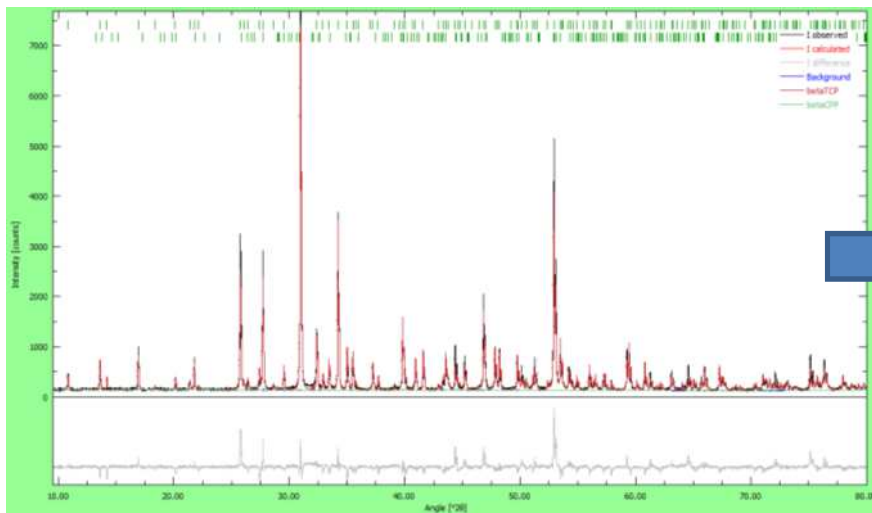
Refinements are «fine tuned» by editing Structure Files:

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 shipped with Profex (created manually by Nicola Doebelin)
- <http://www.bgm.de/download-structures.html>
- Create manually from:
 - ICSD (<http://www.fiz-karlsruhe.de/icsd.html>)
 - PDF-4+ (<http://www.icdd.com/>)
 - American Mineralogist Structure Database (<http://rruff.geo.arizona.edu/AMS/amcsd.php>)
 - Crystallography Open Database COD (<http://www.crystallography.net/>)
 - Cambridge Crystallographic Data Centre (<http://beta-www.ccdc.cam.ac.uk/pages/Home.aspx>)

Creating Structure Files

Official Documentation:

<http://www.bgm.de/variables.html>

Control File (*.sav)

Structure File (*.str)

Device Conf. File (*.sav)

Variables for use with BGMN

The expression interpreter

- standard functions
- multiple equation symbols in assignments
- user-defined string functions

Variables in the task description SAV file for BGMN

NTHREADS, VAL, VERZERR, STRUC, STRUCOUT, SimpleSTRUCOUT, PDBOUT, RESOUT, FCFOUT, OUTPUT, LIST, RU, UNT, UNTC, DDM, PARAM, LAMBDA, SYNCHROTRON, EPS1, EPS2, EPS3, EPS4, POL, PROTOKOLL, ONLYISO, ITMAX, DIAGRAMM, PLAN, STANDALONEPLAN, GOAL, WMIN, WMAX, CUT, LIMIT2, LIMIT4, LIMIT6, LIMIT8, LIMIT10, ANISOLIMIT, ANISO4LIMIT

Items in the structure description *.str-file

Definition of the lattice

SpacegroupNo, HermannMauguin, GeneralCondition, A, B, C, ALPHA, BETA, GAMMA, UNIT

Anisotropic variables

ANISO, ANISOLIN, ANISOSQR, ANISO4

Scaling factor/prefered orientation

GEWICHT, SPHAR0, SPHAR2, SPHAR4, SPHAR6, SPHAR8, SPHAR10

Real structure

B1, B2, k1, k2, k3, sk, H, h, k, l, zweiTheta, RP

Peak deselection

GeneralCondition

Atomic positions

E=, Wyckoff, x, y, z, TDS, B, betaij, U, Uij

GOAL's quant analysis

GOAL, GEWICHT

BGMN-specific functions

PHASE, sk, B1, k2, ANISO, GEWICHT(h,k,l), GrainSize, TDS.

Advanced feature: subphases

RefMult, iref, GEWICHT[i], B1[i], B2[i], k1[i], k2[i], k3[i], DELTAsk, DELTAzweiTheta, LeBail, FPARAM

Advanced feature: Structure amplitudes etc

F, Finv, H

Advanced feature: User calculated structure amplitudes

FMult, F[i], phi[i], Finv[i], phiinv[i]

Advanced feature: molecules

set, setgitter, cross, diffvec, normvec, skalpro, distance, angle, cpXYZ, T, D, X, Y, Z, WW, WWalt, Straf, Theory, Bondings, BondLevel

Micro absorption correction according to Brindley

my, my[i]

X ray density

density, density[i]

Variables in the task description SAV file for computation of standard profiles

NTHREADS, VERZERR, TubeTails, R, FocusH, FocusW, HSlitR, HSlitW, RoundSlitR, RoundSlitD, PColl, PCollA, VSlitR, VSlitH, SamplD, SamplW, SamplH, DeltaOmega, SCollA, SSlitW, SSlitR, SColl, SCollA, DetW, DetH, DetArrayW, MonR, MonH, EPSG, zweiTheta[i], GSUM, TSlitR, TSlitH, FocusS, FocusA, GEOMETRY, WMIN, WMAX, WSTEP, GEQ, D, T, STANDARDPAR, VAL.

Results Files (*.lst)

The screenshot shows the Profex software interface. The main window displays the contents of a results file named 'lesson5-ex2-file1.lst'. The text includes refinement statistics and parameters for the 'Corundum_Al2O3' phase. A red box highlights the file name in the 'Projects' pane. Two callout boxes with red arrows point to specific parts of the output: 'More detailed Results' points to the refinement statistics, and 'Summary' points to the table at the bottom.

More detailed Results

Rietveld refinement to file(s) lesson5-ex2-file1.xy
 BGMN version 4.2.20, 2500 measured points, 14 peaks, 50 parameters
 Start: Tue Oct 8 13:42:39 2013; End: Tue Oct 8 13:42:40 2013
 15 iteration steps

Rp=6.31% Rpb=9.32% R=4.85% Rwp=8.80% Rexp=14.36%
 Durbin-Watson d=1.60
 1-rho=0.697%

Global parameters and GOALS

 corundum/(corundum+fluorite)=0.4838+-0.0029
 fluorite/(corundum+fluorite)=0.5162+-0.0029
 EPS2=-0.000529+-0.000018

Local parameters and GOALS for phase Corundum_Al2O3

SpacegroupNo=167
 HermannMauguin=R-32/c
 XrayDensity=3.982
 Rphase=7.24%
 UNIT=NM
 A=0.476109+-0.000028
 C=1.299598+-0.000073
 B1=0.00300000
 GEWICHT=0.02297+-0.00015
 GrainSize(1,1,1)=141.471
 my=0.0126075+-0.0000016
 d=12.0000
 Atomic positions for phase Corundum_Al2O3

Summary

Phase	R _{phase} [%]	Rel. Weight Fraction [wt-%]	Mean Gewicht [a.u.]	Crystallite Sizes [nm]	Density [g/cm ³]
Corundum_Al2O3	7.24	48.38	0.025730	(1,1,1)141.471	3.982
Fluorite	5.51	51.62	0.027453	(1,1,1)38.8	3.172

Sample lesson5-ex2-file1 (C:/xrd/test/Examples/Lesson 5/Example 2/lesson5-ex2-file1.lst)

Angle: 20.456° Intensity: 861.535 cts d-Spacing: 4.341 Å Line 0, Column 0

Results Files (*.lst)

Rietveld refinement to file(s) lesson5-ex2-file1.xy
BGMN version 4.2.20, 2500 measured points, 14 peaks, 50 parameters
Start: Tue Oct 8 13:42:39 2013; End: Tue Oct 8 13:42:40 2013
15 iteration steps

Rp=6.31% Rpb=9.32% R=4.85% Rwp=8.80% Rexp=14.36%
Durbin-Watson d=1.60
1-rho=0.697%

Global parameters and GOALs

corundum/(corundum+fluorite)=0.4838+-0.0029
fluorite/(corundum+fluorite)=0.5162+-0.0029
EPS2=-0.000529+-0.000018

...

General information

Statistical Information
(Goodness of fit)

Phase quantities (rel. Wt-%)

Sample displacement (EPS2)

$$\text{Displacement [mm]} = R * \text{EPS2} / 2 = -0.0458 \text{ mm}$$

R = goniometer radius [mm] = 173 mm

Results Files (*.lst)

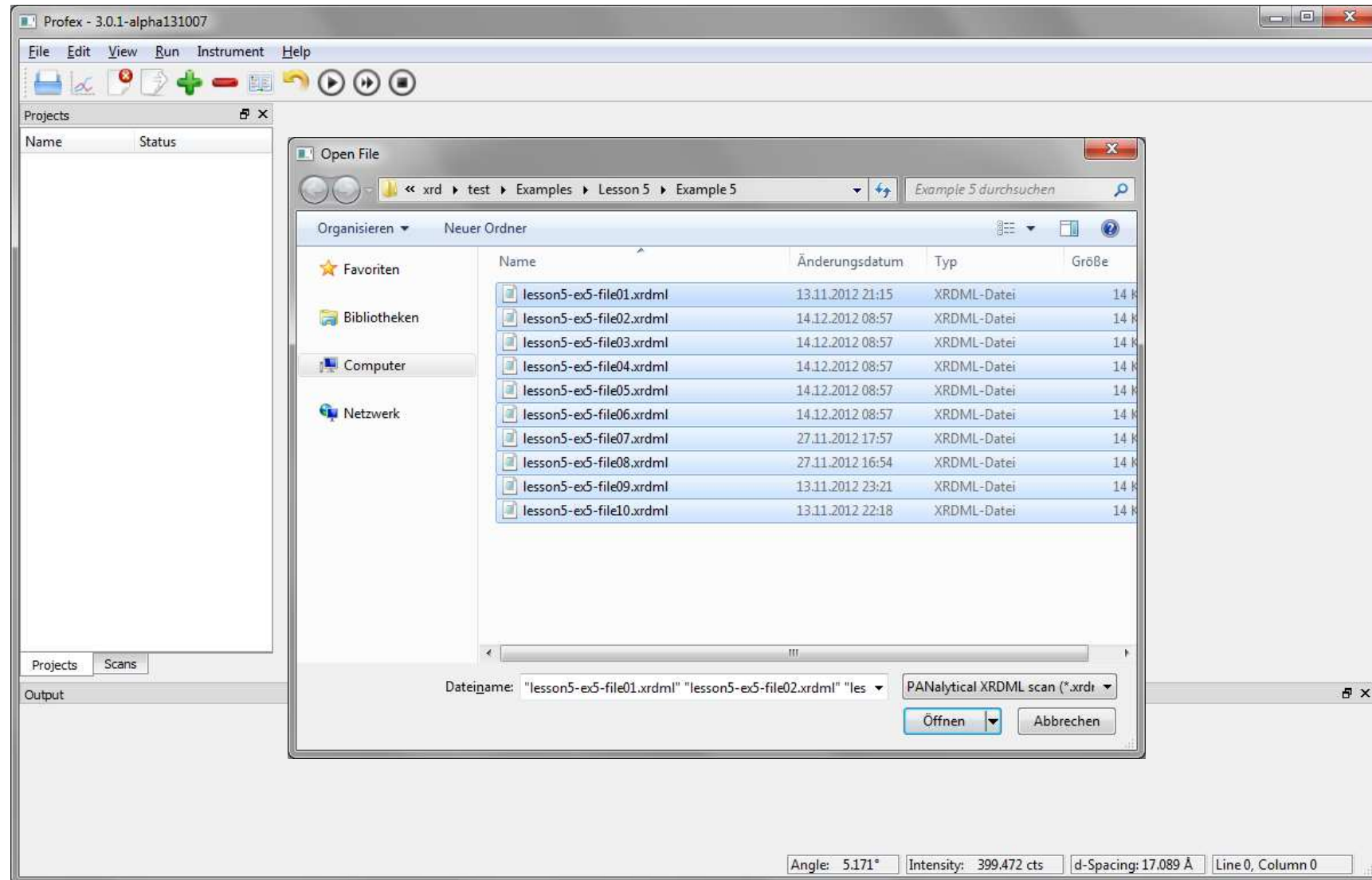
```
...
Local parameters and GOALs for phase Corundum_Al2O3
*****
SpacegroupNo=167
HermannMauguin=R-32/c
XrayDensity=3.981
Rphase=5.76%
UNIT=NM
A=0.47615+-0.00032
C=1.29972+-0.00090
k1=0
k2=0.000000073+-0.000000071
B1=0.00344+-0.00014
GrainSize(1,1,1)=123.4+-4.9
my=0.012604+-0.000025
d=12.0000
GEWICHT=SPHAR4, MeanValue(GEWICHT)=0.0241631
Atomic positions for phase Corundum_Al2O3
-----
12 0.0000 0.0000 0.3522 E=(AL(1.0000))
18 0.3062 0.0000 0.2500 E=(O-2(1.0000))
...
```

That's why the upper limit of 0.003
was too restrictive!

Refined Parameters & Goals

```
...
Local parameters and GOALs for phase Fluorite
*****
SpacegroupNo=225
HermannMauguin=F4/m-32/m
XrayDensity=3.171
Rphase=5.44%
UNIT=NM
A=0.54682+-0.00037
k1=0
k2=0.0000223+-0.0000014
B1=0.01090+-0.00035
GrainSize(1,1,1)=38.9+-1.2
my=0.030116+-0.000061
d=10.0000
GEWICHT=SPHAR6, MeanValue(GEWICHT)=0.0220520
Atomic positions for phase Fluorite
-----
4 0.0000 0.0000 0.0000 E=(CA+2(1.0000))
8 0.2500 0.2500 0.2500 E=(F-1(1.0000))
```

Lesson 5: Example 5 - Batch Refinement



Lesson 5: Example 5 - Batch Refinement

The screenshot shows the Profex software interface. A dialog box titled 'Append Phase' is open, allowing the user to select a phase for refinement. The 'Generate default control file' checkbox is checked, and the control file name is 'cubix-ads-10mm.geq'. The 'Structures' list includes various phases, with 'Hydroxyapatite' selected. The background shows an XRD pattern plot with 'Intensity [counts]' on the y-axis and 'Angle' on the x-axis. A status bar at the bottom displays 'Angle: 5.817°', 'Intensity: 303.111 cts', 'd-Spacing: 15.180 Å', and 'Line 0, Column 0'.

Create control file for first scan

Instrument: cubix-ads-10mm
Phase 1: betaTCP
Phase 2: hydroxylapatite

Phase	Comment	File Name
<input type="checkbox"/> Fluorite	04-002-2191	Fluorite.str
<input type="checkbox"/> Graphite-2H	04-014-0362	graphite-2h.str
<input type="checkbox"/> Graphite-3R	04-007-2076	graphite-3r.str
<input type="checkbox"/> Gypsum	04-010-9409	CSD.str
<input type="checkbox"/> Hematite	04-003-2900	hematite.str
<input type="checkbox"/> Hydrogen_Hydrazinium_Phosphate	04-012-6227	HHP.str
<input checked="" type="checkbox"/> Hydroxyapatite	01-074-0565	hydroxylapatite.str
<input type="checkbox"/> Hydroxylapatite-M	01-076-0694	hydroxylapatite-monoclinic.str
<input type="checkbox"/> inh_benzoic_cocrystal		inh_benzoic_cocrystal.str
<input type="checkbox"/> Isoniazid		isoniazid.str

Lesson 5: Example 5 - Batch Refinement

The screenshot shows the Profex software interface. The 'Projects' panel on the left lists ten projects, all with a status of 'idle'. The main window displays the refinement file 'lesson5-ex5-file01.xrdml' with the following content:

```
% 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[2]=hydroxylapatite.str
% Measured data
VAL[1]=lesson5-ex5-file01.xy
% Result list output
LIST=lesson5-ex5-file01.lst
% Peak list output
OUTPUT=lesson5-ex5-file01.out
% Diagram output
DIAGRAMM=lesson5-ex5-file01.dia
% Global parameters for zero point and sample displacement
EPS1=0
PARAM[1]=EPS2=0_-0.01^0.01
PARAM[2]=B1global=0_0^0.01
alpha3ratio=0.02
betaratio=0
NTHREADS=8
PROTOKOLL=Y
GOAL[1]=betaTCP/(betaTCP+hap)
GOAL[2]=hap/(betaTCP+hap)
```

Annotations in the image include:

- A green box with the text "Sav file created for first scan" and a green arrow pointing to the first project in the list.
- A red box with the text "But not for the other scans" and a red arrow pointing to the remaining nine projects in the list.

The status bar at the bottom of the window shows: Angle: 14.027° Intensity: 1360.632 cts d-Spacing: 6.309 Å Line 0, Column 0

Lesson 5: Example 5 - Batch Refinement

The screenshot shows the Profex software interface with a main window displaying a list of projects and a central text area containing refinement parameters. A 'Copy Control File' dialog box is open, listing projects lesson5-ex5-file02 through lesson5-ex5-file10. A callout box points to the 'Copy Control File' button in the main interface.

«Copy Control File»

```
% 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.s
STRUC[2]=hydroxylate
% Measured data
VAL[1]=lesson5-ex5-file01.xrdml
% Result list output
LIST=lesson5-ex5-file01.sav
% Peak list output
OUTPUT=lesson5-ex5-file01.psf
% Diagram output
DIAGRAMM=lesson5-ex5-file01.pdf
% Global parameters
EPS1=0
PARAM[1]=EPS2=0.01
PARAM[2]=B1global=0.01
alpha3ratio=0.02
betaratio=0
NTHREADS=8
PROTOKOLL=Y
GOAL[1]=betaTCP/(betaTCP+betaHAP)
GOAL[2]=hap/(betaTCP+betaHAP)
```

Projects

Name	Status
lesson5-ex5...	idle
lesson5-ex5...	idle
lesson5-ex5...	idle
lesson5-ex5...	idle
lesson5-ex5...	idle
lesson5-ex5...	idle
lesson5-ex5...	idle
lesson5-ex5...	idle
lesson5-ex5...	idle
lesson5-ex5...	idle
lesson5-ex5...	idle
lesson5-ex5...	idle

Copy Control File

Project
<input checked="" type="checkbox"/> lesson5-ex5-file02
<input checked="" type="checkbox"/> lesson5-ex5-file03
<input checked="" type="checkbox"/> lesson5-ex5-file04
<input checked="" type="checkbox"/> lesson5-ex5-file05
<input checked="" type="checkbox"/> lesson5-ex5-file06
<input checked="" type="checkbox"/> lesson5-ex5-file07
<input checked="" type="checkbox"/> lesson5-ex5-file08
<input checked="" type="checkbox"/> lesson5-ex5-file09
<input checked="" type="checkbox"/> lesson5-ex5-file10

Toggle all OK Cancel

Output

Angle: 14.027° Intensity: 1360.632 cts d-Spacing: 6.309 Å Line 0, Column 0

Lesson 5: Example 5 - Batch Refinement

The screenshot shows the Profex software interface with a control file loaded. The control file contains the following text:

```
% 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[2]=hydroxylapatite.str
% Measured data
VAL[1]=lesson5-ex5-file01.xy
% Result list output
LIST=lesson5-ex5-file01.lst
% Peak list output
OUTPUT=lesson5-ex5-file01.out
% Diagram output
DIAGRAMM=lesson5-ex5-file01.dia
% Global parameters for zero point and sample displacement
EPS1=0
PARAM[1]=EPS2=0_-0.01^0.01
PARAM[2]=B1global=0_0^0.01
alpha3ratio=0.02
betaratio=0
NTHREADS=8
PROTOKOLL=Y
GOAL[1]=betaTCP/(betaTCP+hap)
GOAL[2]=hap/(betaTCP+hap)
```

A callout box on the right contains the following text:

- Copies the control file to all projects
- Adjusts all input/output file names

Arrows point from the callout box to the following lines in the control file: VAL[1]=lesson5-ex5-file01.xy, LIST=lesson5-ex5-file01.lst, OUTPUT=lesson5-ex5-file01.out, and DIAGRAMM=lesson5-ex5-file01.dia.

Lesson 5: Example 5 - Batch Refinement

The screenshot displays the Profex software interface. On the left, a 'Batch List' window shows a table of project names and their statuses. The 'lesson5-ex5...' entry is highlighted with a blue selection bar, and a red box encloses the entire list. A blue callout box with the text 'Start Batch Refinement' points to the 'Run' button in the software's toolbar. The main window shows an XRD plot with 'Intensity [counts]' on the y-axis (0 to 1000) and 'Angle [°2θ]' on the x-axis (10.00 to 60.00). The plot includes 'I observed' (black line), 'I calculated' (red line), 'Difference' (green line), 'Background' (blue line), 'aTCP' (purple line), and 'Hydroxyapatite' (green vertical lines). The 'Output' window at the bottom displays a table of numerical data.

Name	Status
lesson5-ex5...	complete
lesson5-ex5...	complete
lesson5-ex5...	complete
lesson5-ex5...	running...
lesson5-ex5...	scheduled
lesson5-ex5...	scheduled
lesson5-ex5...	scheduled
lesson5-ex5...	scheduled
lesson5-ex5...	scheduled
lesson5-ex5...	scheduled

1.4492643E-20	-4.2777890E+00	-5.4058265E+00	1.6005900E-20	-1.5534723E+00
1.4492643E-20	-2.3617814E+00	5.0130792E-20	-1.1188819E+01	2.6764399E-20
-3.2457247E+00	2.1760055E-20	-4.2776844E+00	5.0130792E-20	-3.1126646E+01
1.2928624E+02	1.1196517E+02	1.4615027E+02	5.7735027E-01	3.7023089E-11
4.7793684E-11	4.0277782E+00	4.3340548E+00	4.2898072E+00	4.9371445E+00
5.5233179E+00	6.3773299E+00	7.7818434E+00	9.3523302E+00	1.1904932E+01
1.6044565E+01	1.6534777E+01			

Angle: 11.992° Intensity: 852.128 cts d-Spacing: 7.374 Å Line 0, Column 0

Lesson 5: Example 5 - Batch Refinement

Export Summary of all Projects to Spread Sheet

The screenshot shows the Profex software interface. A 'Save Results' dialog box is open, allowing the user to save the results of the refinement. The dialog shows the file name 'result.csv' and the file type 'CSV File (*.CSV *.csv)'. The background shows a list of projects, all with a status of 'complete', and a plot of intensity versus angle. The plot includes curves for 'I observed', 'I calculated', 'I difference', 'Background', 'betaTCP', and 'Hydroxyapatite'. The x-axis ranges from 50.00 to 60.00 degrees.

Sample lesson5-ex5-file10 (C:/xrd/test/Examples/Lesson 5/Example 5/lesson5-ex5-file10.lst)					
Phase	R _{phase} [%]	Rel. Weight Fraction [wt-%]	Mean Gewicht [a.u.]	Crystallite Sizes [nm]	Density [g/cm ³]
betaTCP	75.41	28.98	0.014312	(1,1,1)187.7	3.085
Hydroxyapatite	83.07	71.02	0.035066	(0,0,1)110.0 (1,0,0)87.4	3.151

Angle: 19.198° Intensity: 503.549 cts d-Spacing: 4.623 Å Line 0, Column 0

Lesson 5: Example 5 - Batch Refinement

results.csv - Microsoft Excel

Start Einfügen Seitenlayout Formeln Daten Überprüfen Ansicht

Calibri 11 Standard

Einfügen Bedingte Formatierung Einfügen Σ Sortieren und Filtern Suchen und Auswählen Bearbeiten

Zwischenab... Schrifart Ausrichtung Zahl Formatvorlagen Zellen

A1 Sample

	A	B	C	D	E	F	G	H	I	J	K	L	M
1	Sample	lesson5-ex5-file01											
2	Phase	Rphase [%]	Quantity [wt Mean Gewic	Crystallite Si	Density [g/ccm]								
3	betaTCP	15.4	28.03	0.013846	(1,1,1)426	3.083							
4	Hydroxyapat	14.05	71.97	0.035543	(0,0,1)136.1 (3.149							
5													
6	Sample	lesson5-ex5-file02											
7	Phase	Rphase [%]	Quantity [wt Mean Gewic	Crystallite Si	Density [g/ccm]								
8	betaTCP	24.9	27.75	0.014067	(1,1,1)334	3.082							
9	Hydroxyapat	19.87	72.25	0.036634	(0,0,1)146 (1,	3.149							
10													
11	Sample	lesson5-ex5-file03											
12	Phase	Rphase [%]	Quantity [wt Mean Gewic	Crystallite Si	Density [g/ccm]								
13	betaTCP	14.24	27.8	0.01395	(1,1,1)460	3.088							
14	Hydroxyapat	12.1	72.2	0.036234	(0,0,1)122.6 (3.155							
15													
16	Sample	lesson5-ex5-file04											
17	Phase	Rphase [%]	Quantity [wt Mean Gewic	Crystallite Si	Density [g/ccm]								
18	betaTCP	14.59	28.5	0.014226	(1,1,1)341	3.083							
19	Hydroxyapat	12.58	71.5	0.035689	(0,0,1)132.0 (3.149							
20													

results

Bereit 100%