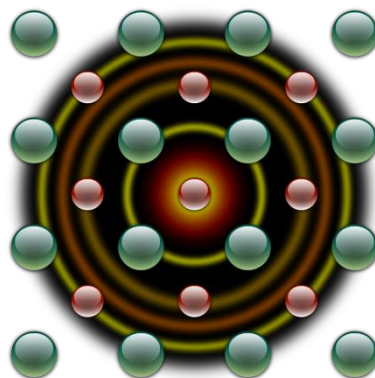




New Features in Profex 3.2

Nicola Döbelin
June 2014



New Toolbar Layout



1) Main Toolbar

- Open files
- Save files
- Close Project
- Copy Control File

2) Project Toolbar

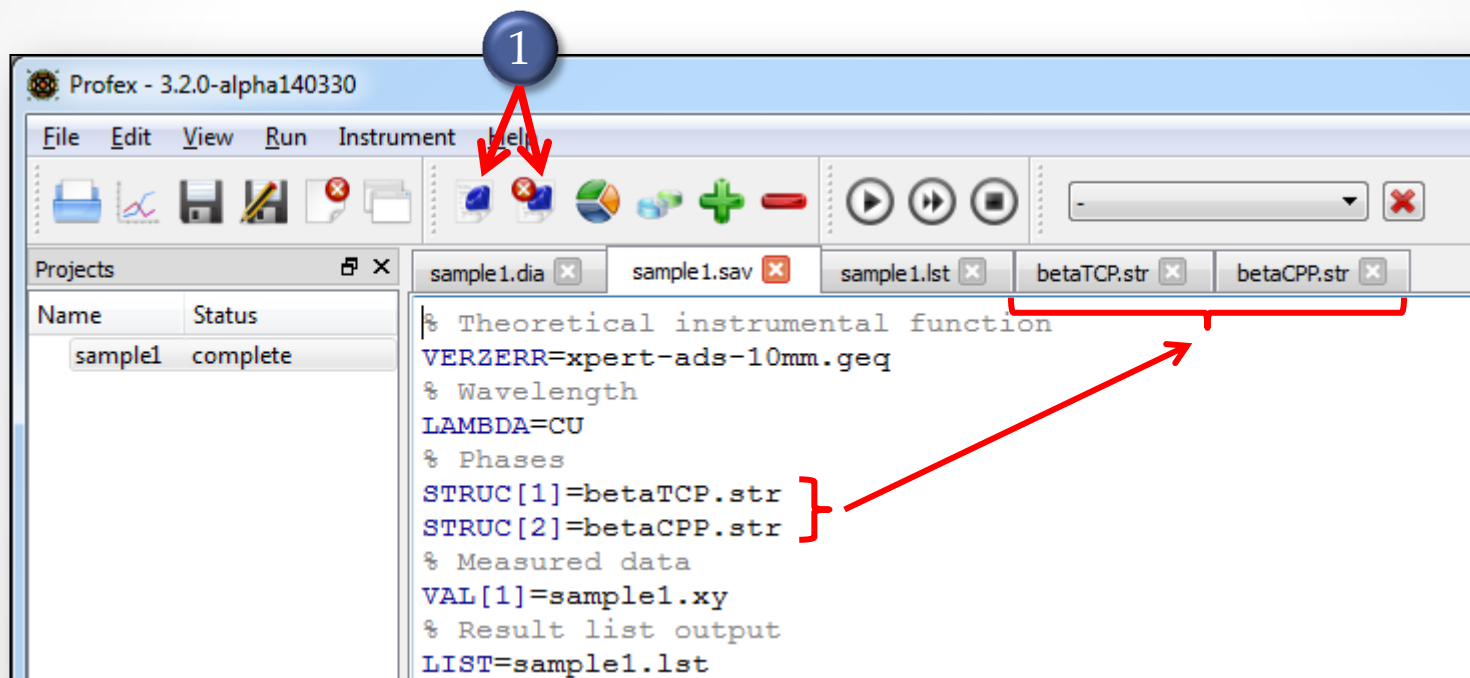
- Open / Close Project Str Files
- Export Global Parameters and GOALs
- Export Local Parameters
- Add / Remove Phase

3) Refinement Control

- Start Refinement
- Start Batch Refinement
- Stop Refinement

4) Reference Structures

Open / Close all Project STR files



1) Open / Close all STR files referenced in the Control File

New Output Tables

```
sample1.dia x sample1.sav x sample1.lst x
Rietveld refinement to file(s) sample1.xy
BGMN version 4.2.20, 4219 measured points, 592 peaks, 100 parameters
Start: Sun Mar 30 16:09:37 2014; End: Sun Mar 30 16:11:10 2014
44 iteration steps

Rp=7.31% Rpb=15.63% R=6.96% Rwp=8.99% Rexp=6.57%
Durbin-Watson d=1.07
1-rho=1.61%

Global parameters and GOALS
*****
betaTCP/sum=0.9900+-0.0019
betaCPP/sum=0.0100+-0.0019
CaPoverall=1.4405+-0.0017
EPS2=-0.0003198+-0.0000034
```

Global Parameters and GOALS		
C:\xrd\sample1.lst		
R _{wp} =8.99%, R _{exp} =6.57%, χ^2 =1.3683		
Parameter / Goal	Value	ESD
betaTCP/sum	0.9900	0.0019
betaCPP/sum	0.0100	0.0019
CaPoverall	1.4405	0.0017

Global Parameters and GOALS

New Output Tables

```

sample1.dia x sample1.sav x sample1.lst x
Local parameters and GOALs for phase betaTCP
*****
SpacegroupNo=161
HermannMauguin=R3c
XrayDensity=3.002
Rphase=8.29%
UNIT=NM
A=1.0474569+-0.0000096
C=3.739172+-0.000035
GrainSize(1,1,1)=280.6+-4.6
pCa4=0.121+-0.010
CaPbetaTCP=1.4459+-0.0015
MbetaTCP=305.84+-0.12
TDSca=0.01267+-0.00081
TDSP=0.0042+-0.0010
TDSO=0.0093+-0.0012
GEWICHT=SPHAR6, MeanValue(GEWICHT)
    
```

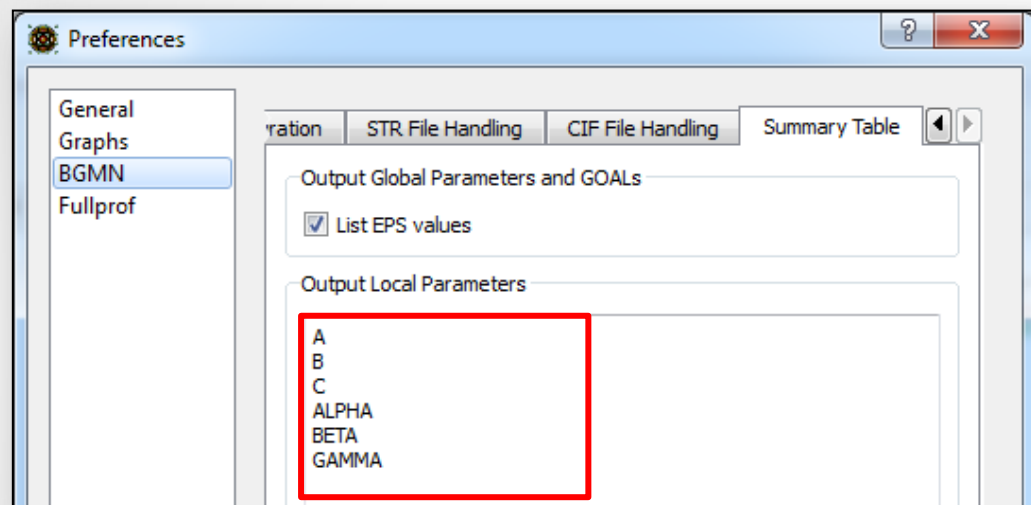
Local Parameters

C:/xrd/sample1.lst
 $R_{wp}=8.99\%$ $R_{exp}=6.57\%$ $\chi^2=1.36834$

Phase	A	ESD (A)	B	ESD (B)	C	ESD (C)	ALPHA	ESD (ALPHA)
betaTCP	1.0474569	0.0000096			3.739172	0.000035		
betaCPP	0.66906	0.00020			2.4192	0.0011		

Local Parameters and GOALs

New Output Tables

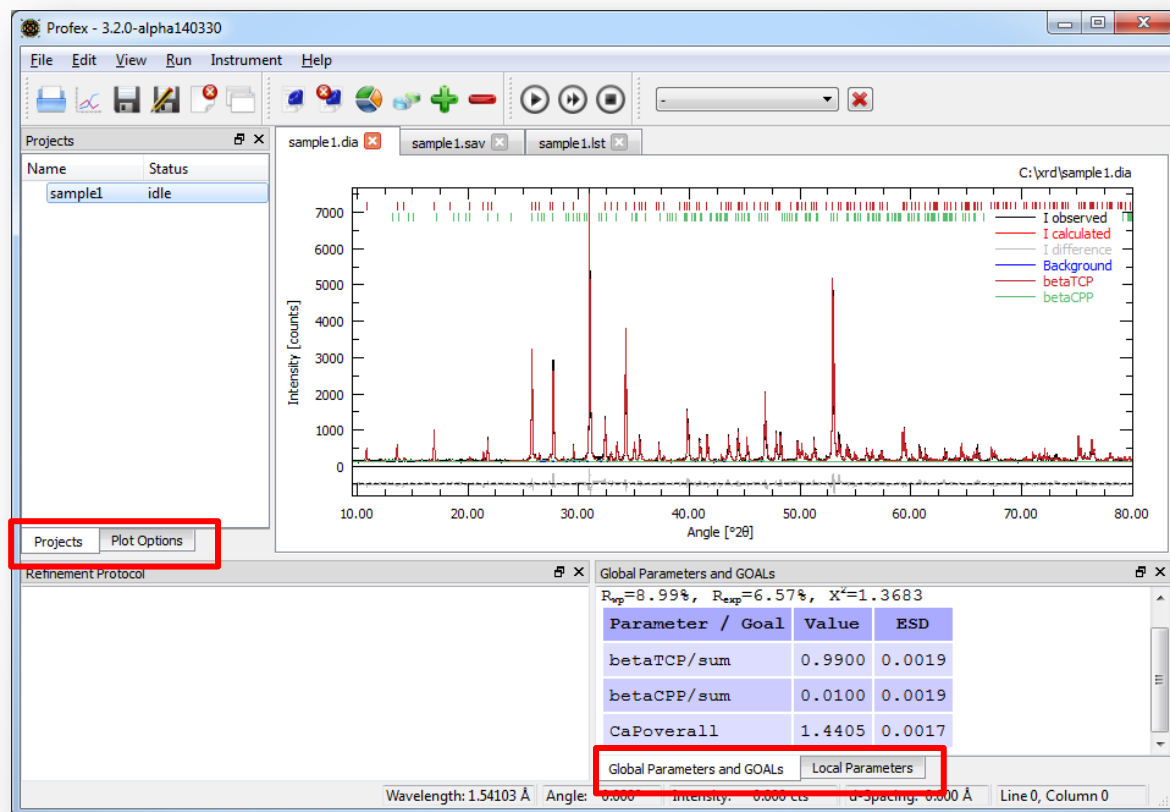


$R_w = 8.99\%$ $R_{exp} = 6.57\%$ $\chi^2 = 1.36834$

Phase	A	ESD (A)	B	ESD (B)	C	ESD (C)	ALPHA	ESD (ALPHA)
betaTCP	1.0474569	0.0000096			3.739172	0.000035		
betaCPP	0.66906	0.00020			2.4192	0.0011		

Customize Local Parameters Table

Recommended Layout



Stack Windows
Close unused Windows

Denominator («sum») for Phase Quantities



```

sample1.dia x sample1.sav x sample1.lst x
* Diagram output
DIAGRAMM=sample1.dia
WMIN=9.5
% Global parameters for zero point and sample displacement
EPS1=0
PARAM[1]=EPS2=0_-0.01^0.01
EPS3=0
betaratio=0.005
NTHREADS=2
PROTOKOLL=Y
ITMAX=10
expansion=1.0
CaPoverall=(2*CaPbetaTCP*GOAL[1]/MbetaTCP+2*GOAL[2]/MbetaCPP) / (2*GOAL[1]/
MbetaTCP+2*GOAL[2]/MbetaCPP)
SAVE=N

sum=betaTCP+betaCPP
GOAL[1]=betaTCP/sum
GOAL[2]=betaCPP/sum
    
```

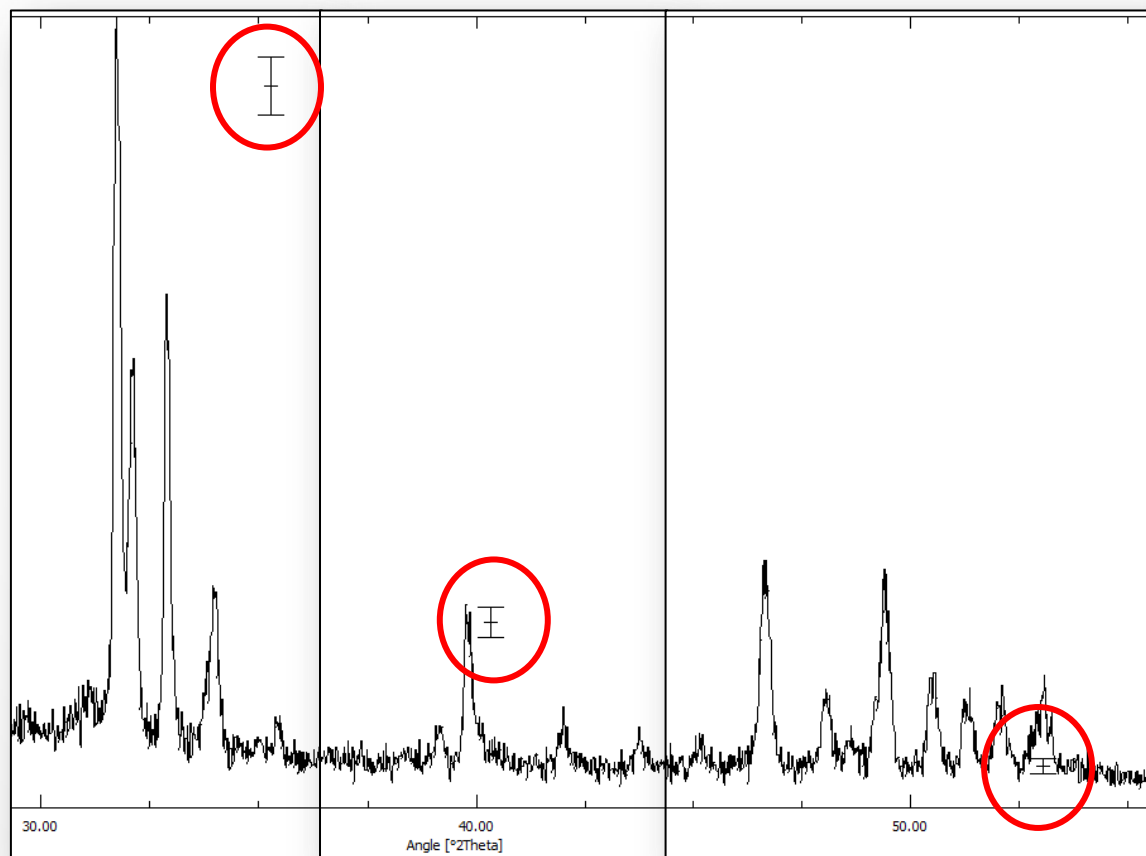
Global Parameters and GOALS

C:\xrd\sample1.lst
 $R_{wp}=8.99\%$, $R_{exp}=6.57\%$, $\chi^2=1.3683$

Parameter / Goal	Value	ESD
betaTCP/sum	0.9900	0.0019
betaCPP/sum	0.0100	0.0019

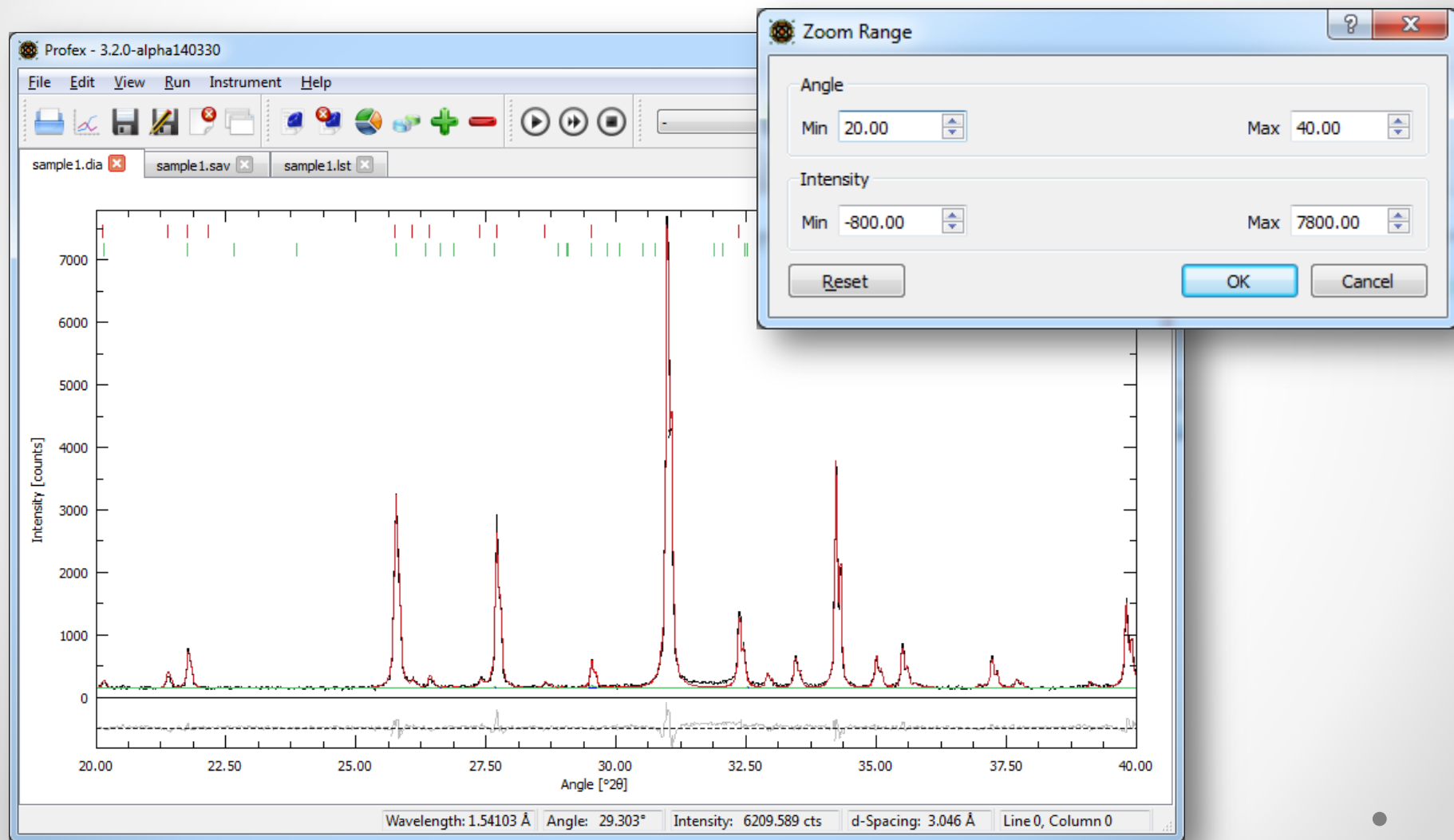
Easier manual editing
 Tidier output table

Cursor shows Counting Noise



Press «Shift» to show error bars = $\frac{1}{\sqrt{\text{counts}}}$

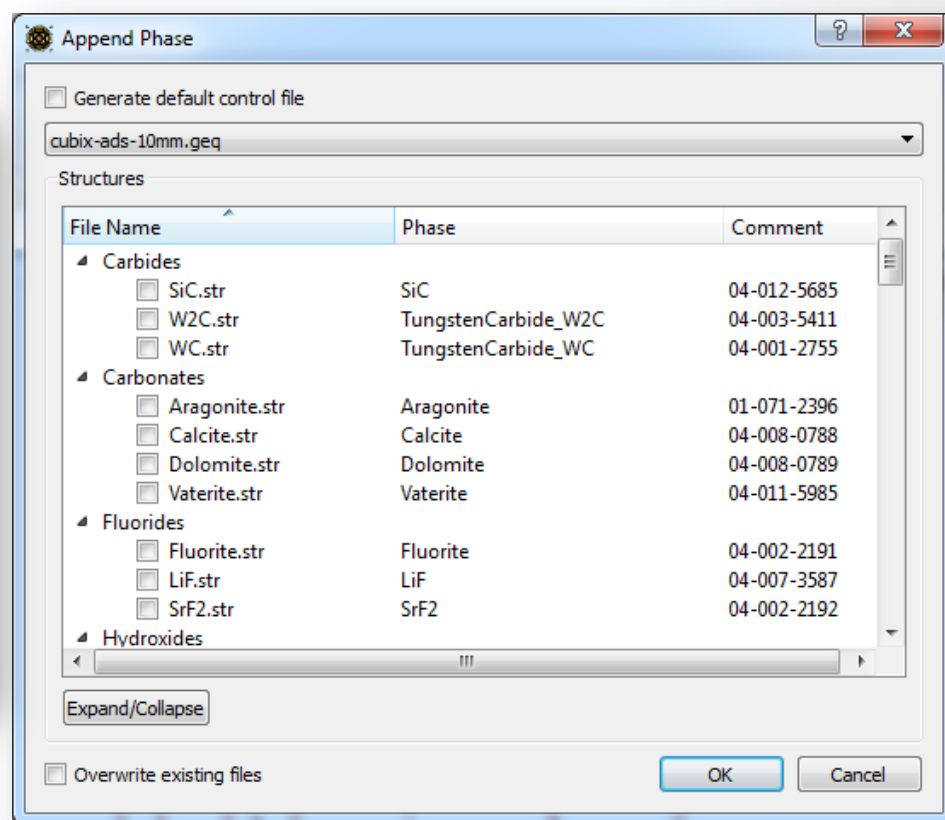
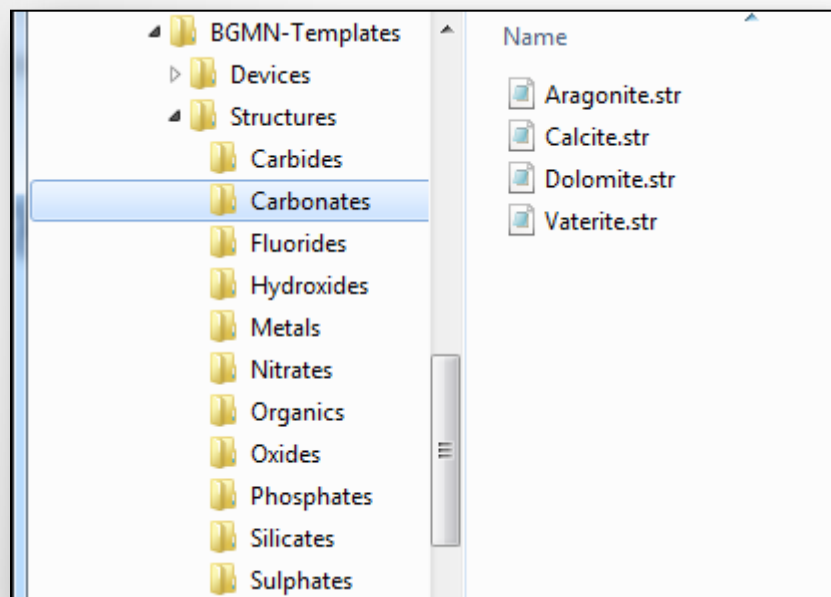
Dialog for Zoom Range



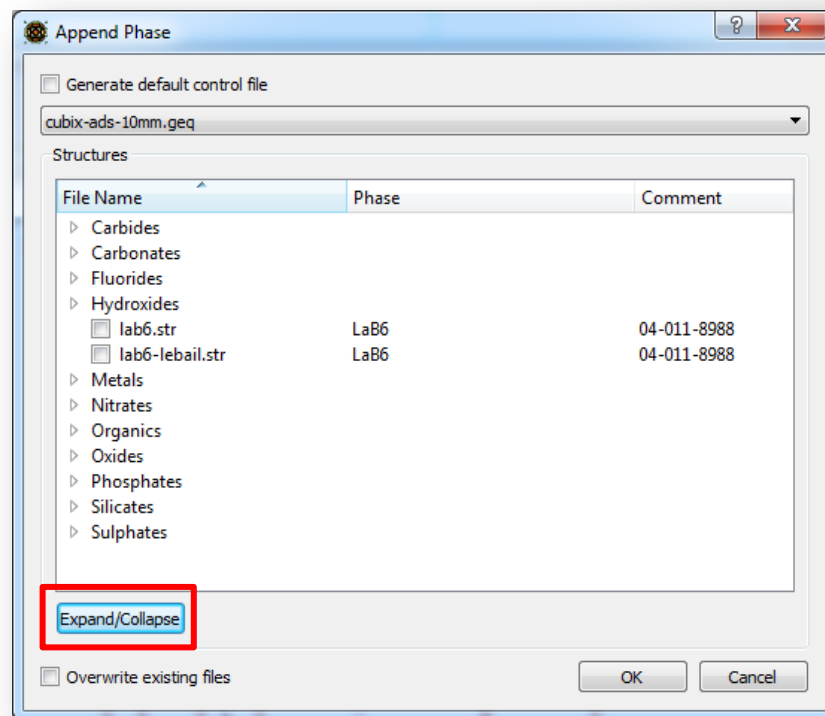
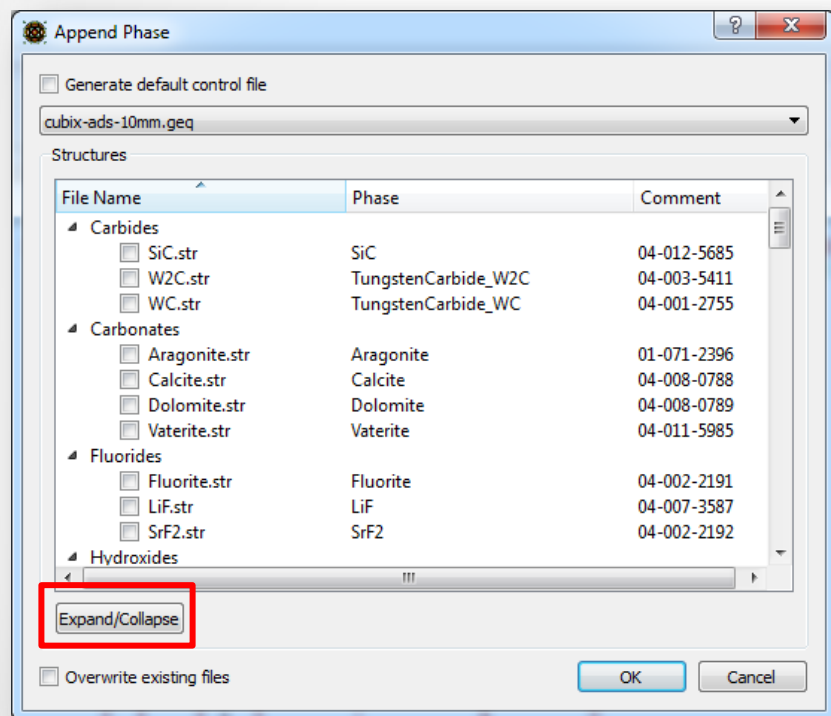
Categorize STR Files in Directories

Append Phase Dialog:

Directories:

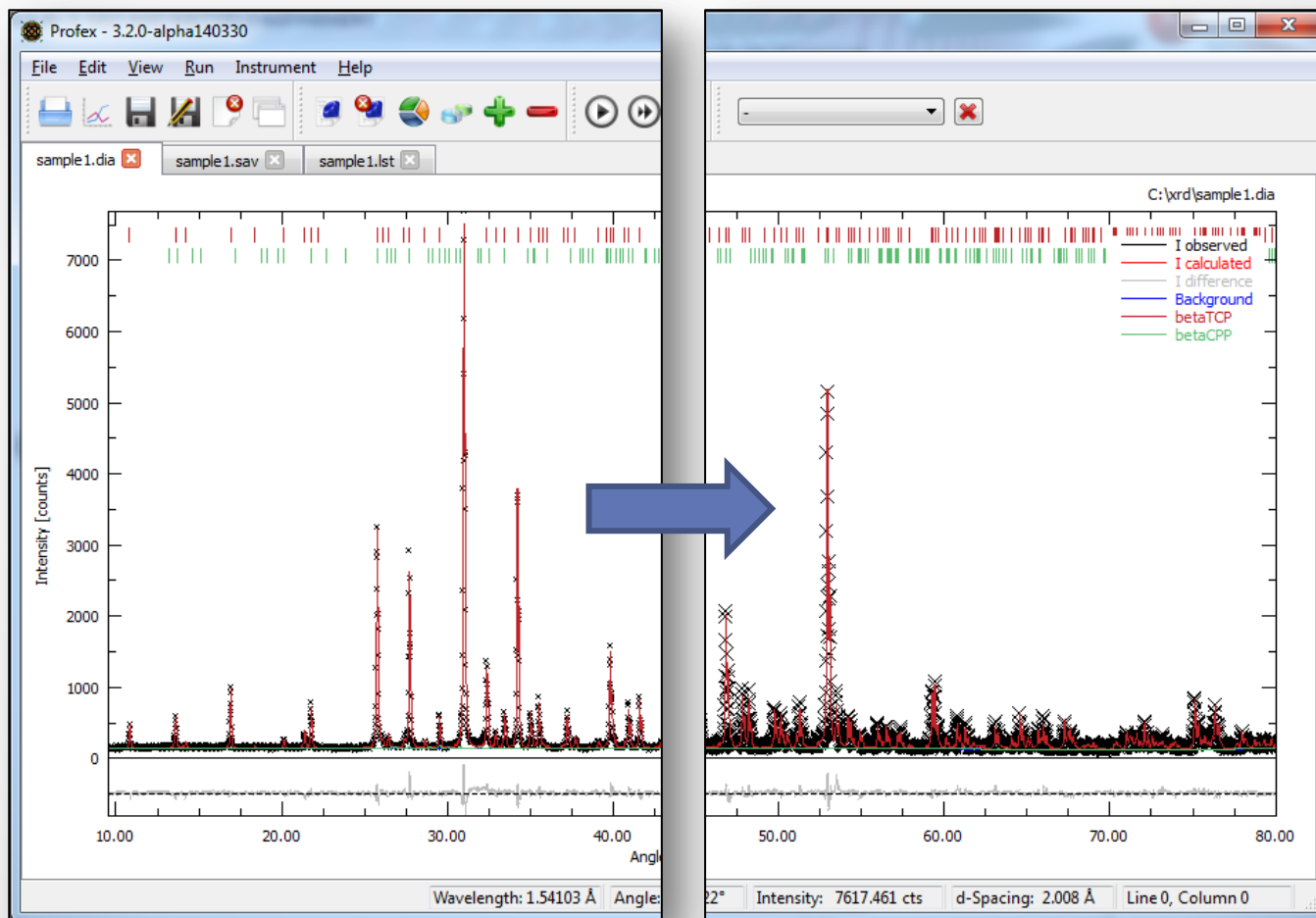


Categorize STR Files in Directories

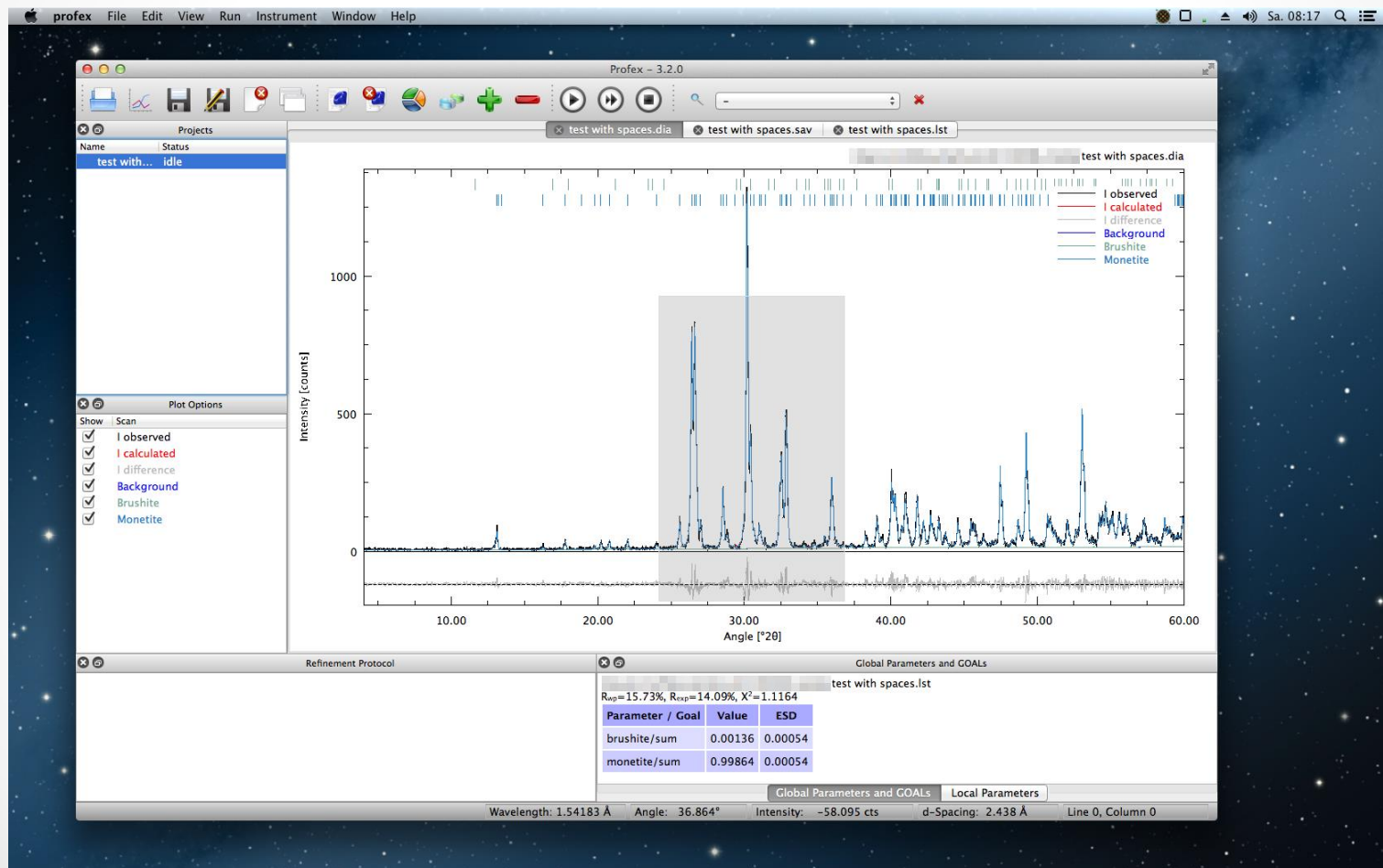


Expand / Collapse Categories

Change Symbol Size



Fixed Printing of Graphs and Opaque Zoom Area on Mac





+ many more

- DIA files can be used as input files
- major improvements for Bruker RAW version 4 files
- support for STOE Raw files (experimental)
- new export filter for Gnuplot
- new icons and toolbar layout
- new function to search and index new structure files
- write log file on OS X
- show/hide phase contributions and hkl indices was improved
- improved auto-recognition of VAL[] = files
- run batch refinement on selected projects only
- improved error handling
- new option to switch off automatic scan conversion
- fixed Save As function for text files to load the new file name
- fixed infinite loop in case of non-existent STR and Device file directories
- fixed asymmetric cross symbols for scans
- fixed crash with preferences dialog
- fixed bug in STR File Handling
- fixed bug in copyControlFile when convertToXy is deactivated
- fixed flickering of left y axis
- performance improvements