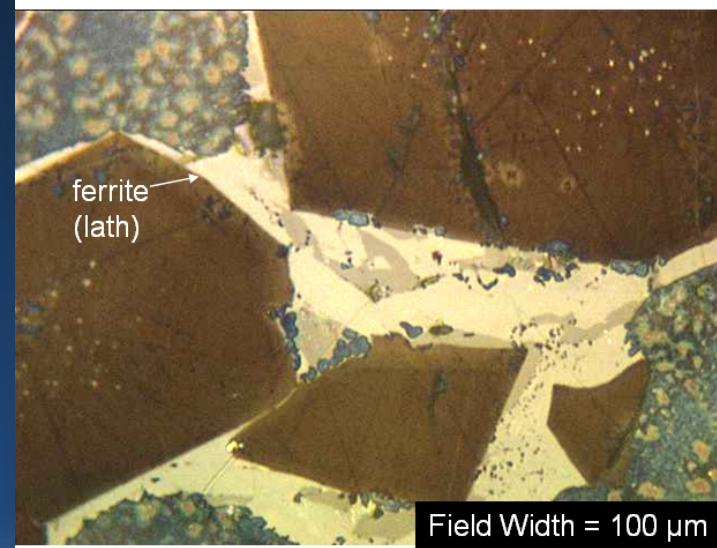
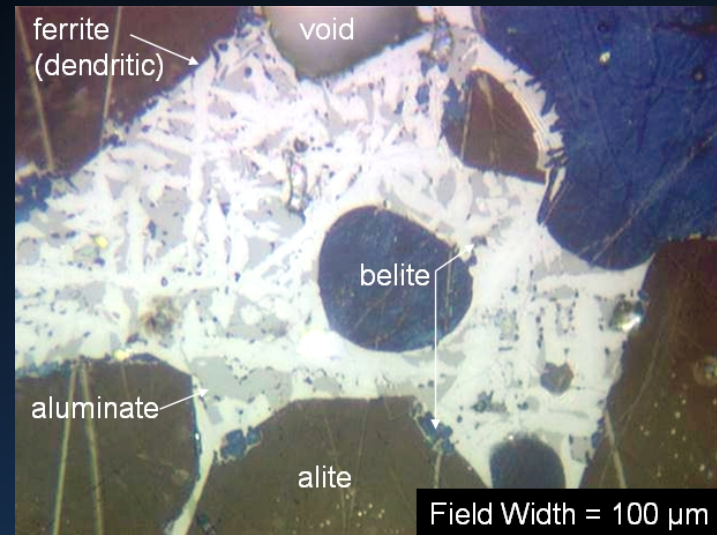


Single Phase Example

Ferrite Phase from SRM2686a

Nitric acid/methanol extraction



We will be using only a subset of the features provided by Profex/BGMN to run a basic refinement for quantitative analysis; we leave it to you to explore the more advanced refinement features after you have had some experience.

Introduction to the Rietveld Method, R.A. Young

- Provides background on the method, its historical development and subsequent application to laboratory X-ray diffraction
- Refining parameters in models for the structure, specimen and instrument effects on the diffraction pattern
- Least-squares refinements are carried out until the best fit is obtained between the entire observed powder diffraction pattern and calculated pattern based upon simultaneously refined models for crystal structures and instrument effects
- Potential systematic errors include preferred orientation, background, anisotropic peak broadening, profile shapes, absorption, specimen displacement, specimen transparency, extinction, 2-theta-Zero error, graininess, beam instability

Profex and BGMN*

BGMN Author: Dr. Joerg Bergmann

<http://www.bgmn.de>

Profex Author: Nicola Doebelin

<http://profex.doebelin.org>

GPL Open Source, Windows, OS X, Linux; front end for BGMN and for Fullprof 2k
Fundamental Parameters, adaptable to different instruments, multi-platform, robust

Profex

Creates a control (input) file

Copies structure models to working folder

Copies the instrument configuration files

(they allow calculation of the instrument contribution to the diffraction peak shapes based upon the X-ray optics)

Allows editing of the working versions of the structure files and saves changes/refined values

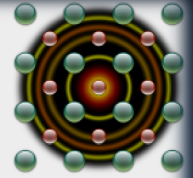
Döbelin, N., Kleeberg, R., "Profex: a graphical user interface for the Rietveld refinement program *BGMN*", *Journal of Applied Crystallography* 48 (2015), 1573-1580.

DOI: doi:10.1107/S1600576715014685

Profex

Version 3.9.1

(c) 2003-2016 by Nicola Doebelin

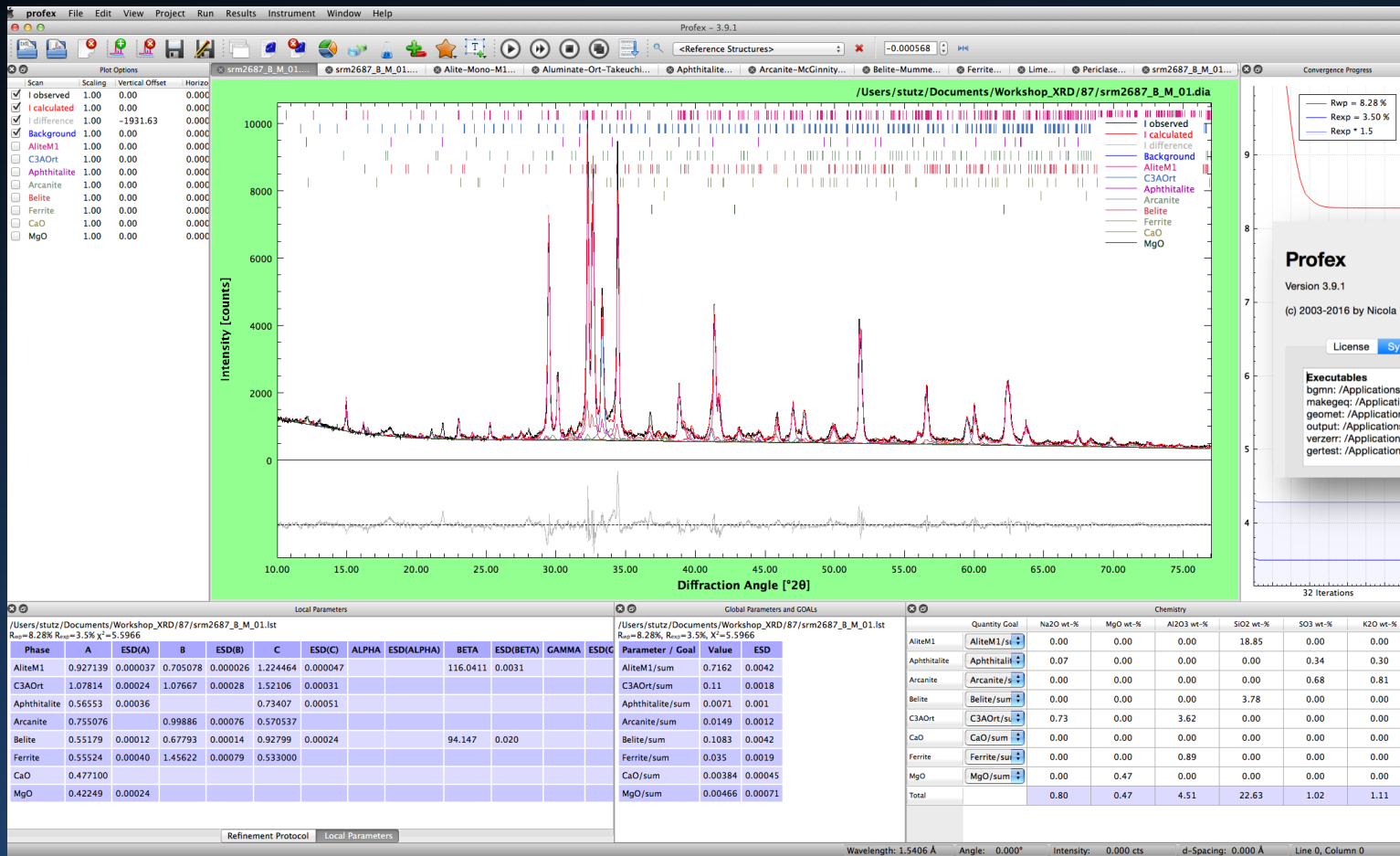


License System Information Acknowledgements

Executables

```
bgmn: /Applications/Profex-BGMN/BGMNwin/bgmn
makegeq: /Applications/Profex-BGMN/BGMNwin/makegeq
geomet: /Applications/Profex-BGMN/BGMNwin/geomet
output: /Applications/Profex-BGMN/BGMNwin/output
verzerr: /Applications/Profex-BGMN/BGMNwin/verzerr
gertest: /Applications/Profex-BGMN/BGMNwin/gertest
```

Profex/BGMN



Profex
Version 3.9.1
(c) 2003-2016 by Nicola Doebelin

License System information Acknowledgements

Executables
bgmn: /Applications/Profex-BGMN/BGMNwin/bgmn
makegeq: /Applications/Profex-BGMN/BGMNwin/makegeq
geomet: /Applications/Profex-BGMN/BGMNwin/geomet
output: /Applications/Profex-BGMN/BGMNwin/output
verzerr: /Applications/Profex-BGMN/BGMNwin/verzerr
gerstest: /Applications/Profex-BGMN/BGMNwin/gerstest

In place of actual powder reference specimens for calibration, crystal structure models allow calculation of phase diffraction patterns. These models include space group, lattice parameters, atomic positions, atomic site occupancies, atomic vibrational parameters.

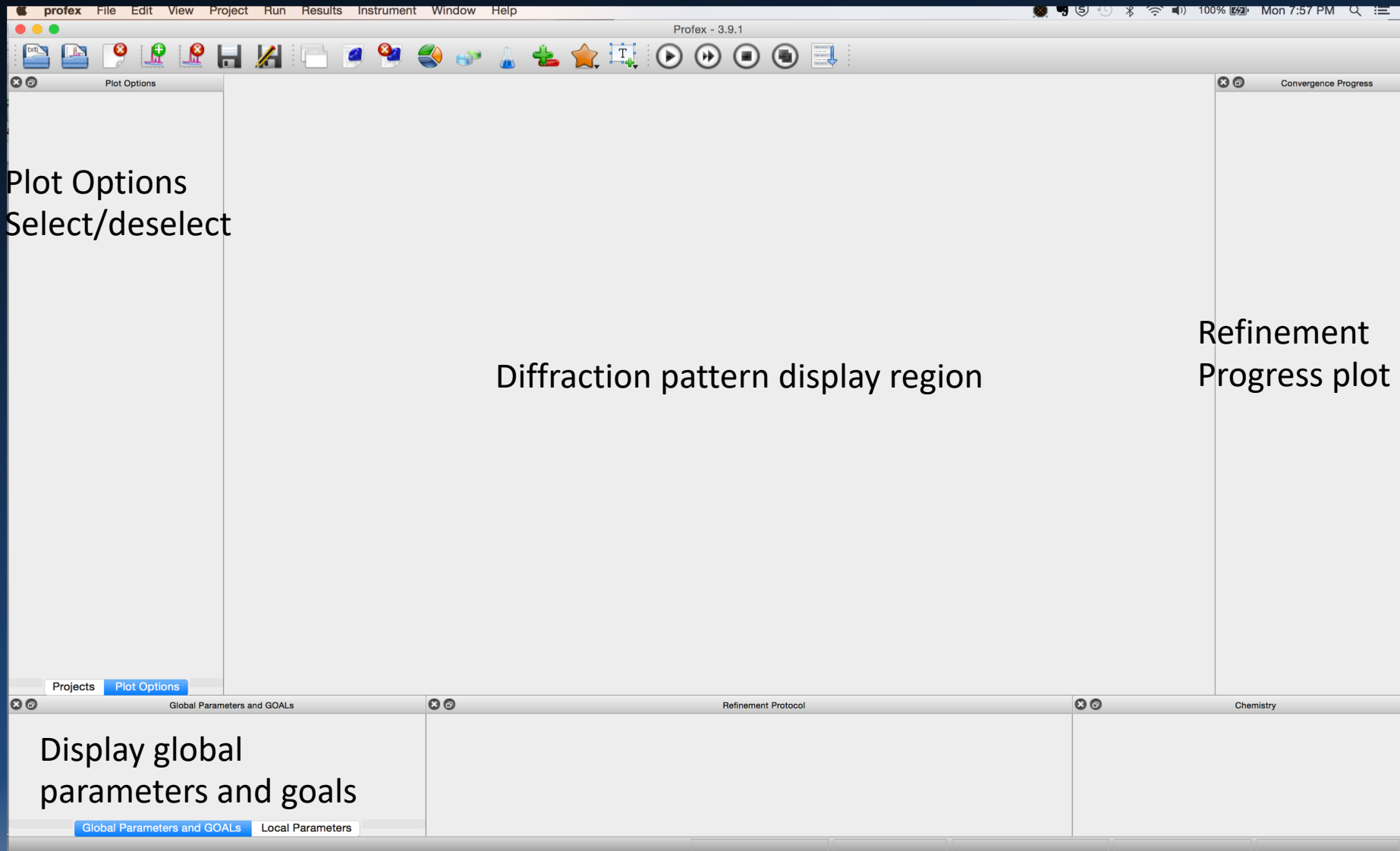
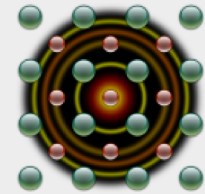
The code fits a multivariable model of structure, peak profile [°2θ], background to the observed data

Initialize Profex

Profex

Version 3.9.1

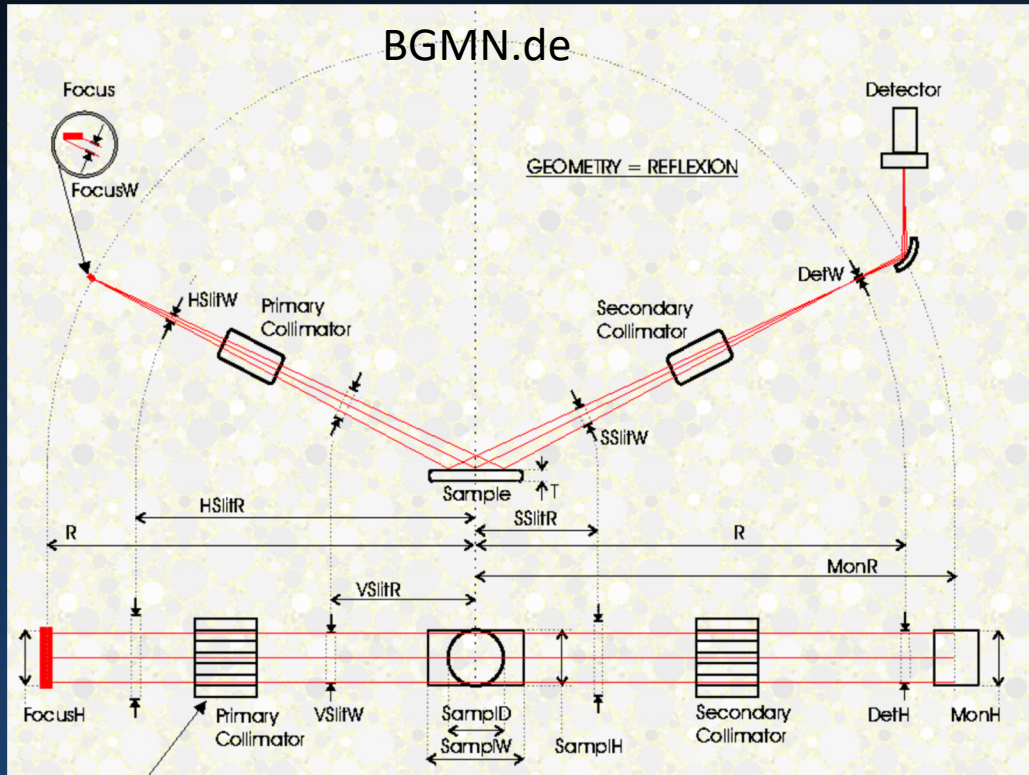
(c) 2003-2016 by Nicola Doebelin



The screenshot displays the Profex software interface with the following components:

- Menu Bar:** profex File Edit View Project Run Results Instrument Window Help
- Title Bar:** Profex - 3.9.1
- Toolbar:** Contains icons for file operations (open, save, print), editing (undo, redo, delete), and simulation (run, stop, refresh).
- Plot Options Panel (Left):** Labeled "Plot Options Select/deselect".
- Convergence Progress Panel (Right):** Labeled "Refinement Progress plot".
- Main Display Area:** Labeled "Diffraction pattern display region".
- Bottom Panels:**
 - Global Parameters and GOALS:** Labeled "Display global parameters and goals". Includes sub-tabs for "Global Parameters and GOALS" and "Local Parameters".
 - Refinement Protocol:** A panel for configuring the refinement process.
 - Chemistry:** A panel for entering chemical information.

Profex/BGMN Instrument Configuration



```
% BGMN Device Configuration File for Bruker D8
% -----
% Created by Nicola Doebelin, RMS Foundation,
% Switzerland
% November 12, 2012
%
% Device Configuration:
% - Detector: LynxEye
% - Radiation: CuK $\alpha$ , Ni-filtered
% - Soller Slits: 2.5 degrees
% - Divergence Slit: fixed, 0.6 mm
% - Anti-Scatter Slit: fixed, 6.76 mm
% -Goniometer Radius: 217.5 mm
```

We will use File=D8_6div_4SS.geq or D8-06mm.geq, modifications of the D8 file provided.

Device functions are available for a wide variety of instruments and configurations, though some may require editing and re-saving. Different configurations will require a new device file!

Profex Configuration

Control file (.SAV)

- References model structures from the Cement_Structures Folder
- A copy of the structure is stored in the same folder as the data

```
% SampleID: SRM2688, 1b, micronized 0.6 divergence, 4 deg SS, 11-80 30 min, rep. 2
% Theoretical instrumental function
VERZERR=D8-06mm.geq
% Wavelength
LAMBDA=cu
% Phases
STRUC[1]=Alite-Mono_M1.str
STRUC[2]=Aluminate-Ort-Takeuchi.str
STRUC[3]=Belite_Beta_Mumme.str
STRUC[4]=Ferrite.str
STRUC[5]=Periclase.str
% Measured data
VAL[1]=88_1b_2.xy
% Minimum Angle (2theta)
% WMIN=10
% Maximum Angle (2theta)
% WMAX=60
% Result list output
LIST=88_1b_2.lst
% Peak list output
OUTPUT=88_1b_2.par
% Diagram output
DIAGRAMM=88_1b_2.dia
% Global parameters for zero point and sample displacement
EPS1=0
PARAM[1]=EPS2=0_-0.01^0.01
NTHREADS=8
PROTOKOLL=Y

sum=AliteM1+C3AOrt+Belite+Ferrite+MgO
GOAL[1]=AliteM1/sum
GOAL[2]=C3AOrt/sum
GOAL[3]=Belite/sum
GOAL[4]=Ferrite/sum
GOAL[5]=MgO/sum
```

Instrument profile

Wavelength

Refined Phases

Data File

Set two-theta angles for refinement
(remove the leading “%”)

Zero-Error (really *should* be zero)

Sample Displacement Parameter

Phase Quantity Calculation

Profex Configuration

.LST file: Refinement Summary

Rietveld refinement to file(s) 88_1b_2.xy
 BGMN version 4.2.22, 4420 measured points, 1295 peaks, 35 parameters
 Start: Wed Jun 29 17:24:42 2016; End: Wed Jun 29 17:25:18 2016
 63 iteration steps

Rp=5.00% Rpb=17.21% R=6.29% Rwp=6.24% Rexp=3.78%
 Durbin-Watson d=0.74
 1-rho=1.88%

Global parameters and GOALS

AliteM1/sum=0.6680+-0.0034
 C3AOrt/sum=0.0322+-0.0019
 Belite/sum=0.1407+-0.0032
 Ferrite/sum=0.1576+-0.0027
 MgO/sum=0.00147+-0.00057
 EPS2=0.0002031+-0.0000098

Local parameters and GOALS for phase AliteM1

SpacegroupNo=7
 HermannMauguin=P1c1
 XrayDensity=3.144
 Rphase=6.83%

UNIT=NM
 A=0.929734+-0.000036
 B=0.708015+-0.000025
 C=1.223895+-0.000045
 BETA=116.0856+-0.0032
 B1=0.003124+-0.000037
 GrainSize(1,1,1)=135.9+-1.6
 GEWICHT=0.16634+-0.00078

Atomic positions for phase AliteM1

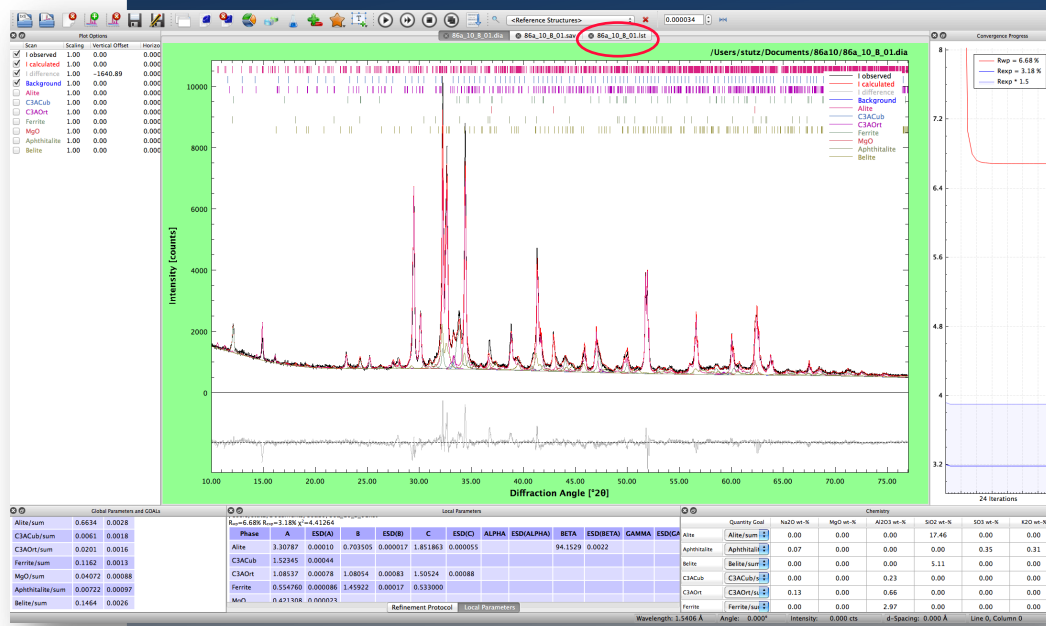
2	0.0067	0.9987	0.0210	E=(CA+2(1.0000))
2	0.0046	0.5002	0.0088	E=(CA+2(1.0000))
2	0.3316	0.4694	0.7907	E=(CA+2(1.0000))
2	0.3447	0.9982	0.7810	E=(CA+2(1.0000))
2	0.6881	0.7566	0.4851	E=(CA+2(1.0000))
2	0.0043	0.7268	0.2516	E=(CA+2(1.0000))
2	0.3333	0.7524	0.0482	E=(CA+2(1.0000))
2	0.6736	0.4852	0.7255	E=(CA+2(1.0000))
2	0.6766	0.0348	0.7350	E=(CA+2(1.0000))
2	0.8921	0.7611	0.3827	E=(O-2(1.0000))
2	0.1109	0.7281	0.1056	E=(O-2(1.0000))

- File, refinement details

- refinement statistic measures

- refinement global parameter (shift) and phase fraction goals

- refinement data, by phase



Profex Structure Files (.str)

Provided with the installation but may also be transcribed from databases

```
PHASE=Ferrite //  
Formula=Ca2_Fe_Al2_O5 //  
SpacegroupNo=46 Setting=2 HermannMauguin=Ibm2 Lattice=Orthorhombic //  
PARAM=A=0.5557_0.551^0.563 PARAM=B=1.4543_1.43^1.465 PARAM=C=0.53616_0.533^0.542 //  
RP=4 k1=0 k2=0 PARAM=B1=0_0^0.01 GEWICHT=SPHARO //  
GOAL=GrainSize(1,1,1) //  
GOAL:Ferrite=GEWICHT*ifthenelse(ifdef(d),exp(my*d*3/4),1) //  
E=CA+2 Wyckoff=c x=0.02730000 y=0.10870000 z=0.49200000 TDS=0.00971169  
E=FE+3(0.6400) Wyckoff=a x=0.00000000 y=0.00000000 z=0.00000000 TDS=0.00971169  
E=AL+3(0.8300) Wyckoff=b x=0.92830000 y=0.25000000 z=0.95330000 TDS=0.00971169  
E=O-2 Wyckoff=c x=0.25230000 y=0.98610000 z=0.24910000 TDS=0.00971169  
E=O-2 Wyckoff=c x=0.06800000 y=0.14390000 z=0.02460000 TDS=0.00971169  
E=O-2 Wyckoff=b x=0.86070000 y=0.25000000 z=0.61930000 TDS=0.00971169  
E=AL+3(0.3600) Wyckoff=a x=0.00000000 y=0.00000000 z=0.00000000 TDS=0.00971169  
E=FE+3(0.1700) Wyckoff=b x=0.92830000 y=0.25000000 z=0.95330000 TDS=0.00971169
```

$$\text{GEWICHT (mass)} = S * (Z * M * V)$$

E = CA+2(1) Wyckoff=c x=0.0273 y=0.1087 z=0.4920 TDS=0.00971169

Element Occupancy Wyckoff Position Fractional Coordinates Thermal Displacement Parameter

Profex Structure Files (.str)

Provided with the installation but may also be transcribed from databases

```
PHASE=Ferrite //
Formula=Ca2_Fe_Al2_O5 //
SpacegroupNo=46 Setting=2 HermannMauguin=Ibm2 Lattice=Orthorhombic //
PARAM=A=0.5557_0.551^0.563 PARAM=B=1.4543_1.43^1.465 PARAM=C=0.53616_0.533^0.542 //
RP=4 k1=0 k2=0 PARAM=B1=0_0^0.01 GEWICHT=SPHARO //
GOAL=GrainSize(1,1,1) //
GOAL:Ferrite=GEWICHT*ifthenelse(ifdef(d),exp(my*d*3/4),1) //
E=CA+2 Wyckoff=c x=0.02730000 y=0.10870000 z=0.49200000 TDS=0.00971169
E=FE+3(0.6400) Wyckoff=a x=0.00000000 y=0.00000000 z=0.00000000 TDS=0.00971169
E=AL+3(0.8300) Wyckoff=b x=0.92830000 y=0.25000000 z=0.95330000 TDS=0.00971169
E=O-2 Wyckoff=c x=0.25230000 y=0.98610000 z=0.24910000 TDS=0.00971169
E=O-2 Wyckoff=c x=0.06800000 y=0.14390000 z=0.02460000 TDS=0.00971169
E=O-2 Wyckoff=b x=0.86070000 y=0.25000000 z=0.61930000 TDS=0.00971169
E=AL+3(0.3600) Wyckoff=a x=0.00000000 y=0.00000000 z=0.00000000 TDS=0.00971169
E=FE+3(0.1700) Wyckoff=b x=0.92830000 y=0.25000000 z=0.95330000 TDS=0.00971169
```

Fixed Parameter

A=0.5557

Name Value

Refined Parameter

PARAM=A=0.5557

Refine Name Value

Refined Parameter With Limits

PARAM=A=0.5557_0.551^0.563

Refine Name Value Lower Upper

B1: peak broadening from crystallite size (diffracting domains)

GEWICHT = Scale, Weight

Microabsorption correction, (ifthenelse(ifdef(d),exp(my*d*3/4),1), is not being used

Sources of Crystal Structure Data

American Mineralogist Crystal Structure Database

<http://rruff.geo.arizona.edu/AMS/amcsd.php>

Mincryst

<http://database.iem.ac.ru/mincryst/>

Crystallography Open Database

<http://www.crystallography.net/cod/>

Cements Crystal Structure Database

http://www.nist.gov/el/building_materials/inorganic/gsas1.cfm

Commercial:

ICDD

<https://icdd.com>

ICSD

<https://icsd.fiz-karlsruhe.de/>

.CIF File: Ferrite

```
data_cif
_audit_creation_date          'Monday, August 13, 2007 2:46 PM'
_audit_creation_method        'MDI-jPOWD'
_chemical_name_common         Brownmillerite
_chemical_formula_sum          'Ca2Al0.72Fe1.28O5'
_publ_section_references      A.A.Colville & S.Geller, Crystal structures of Ca2Fe1.43Al0.57O5 and
Ca2Fe1.28Al0.72O5 , Acta Cryst. B28, 3196, 1972
Ibm2 (46) [PS oI36] |
_symmetry_cell_setting        Orthorhombic
_symmetry_space_group_name_H-M Ibm2
_symmetry_Int_Tables_number   46

_cell_length_a                 5.583
_cell_length_b                 14.58
_cell_length_c                 5.374
_cell_angle_alpha              90
_cell_angle_beta               90
_cell_angle_gamma              90
_cell_volume                   437.444
_cell_formula_units_Z          4

loop_
_atom_site_type_symbol
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_thermal_displace_type
_atom_site_U_iso_or_equiv
_atom_site_symmetry_multiplicity
Ca Ca(1) 0.27 0.1084 0.4907 1.0 Uiso 0.01230 8
Fe Fe(1) 0.0 0.0 0.0 0.83 Uiso 0.01230 4
Al Al(1) 0.0 0.0 0.0 0.17 Uiso 0.01230 4
Al Al(2) 0.9291 0.25 0.952 0.55 Uiso 0.01230 4
Fe Fe(2) 0.9291 0.25 0.952 0.45 Uiso 0.01230 4
O O(1) 0.2525 0.9859 0.2503 1.0 Uiso 0.01230 8
O O(2) 0.0683 0.1429 0.0256 1.0 Uiso 0.01230 8
O O(3) 0.8653 0.25 0.6133 1.0 Uiso 0.01230 4
```

American Mineralogist Crystal Structure Database

American Mineralogist Crystal Structure Database

This site is an interface to a crystal structure database that includes every structure published in the American Mineralogist, The Canadian Mineralogist, European Journal of Mineralogy and Physics and Chemistry of Minerals, as well as selected datasets from other journals. The database is maintained under the care of the Mineralogical Society of America and the Mineralogical Association of Canada, and financed by the National Science Foundation.

Search interface with fields for Mineral, Author, Chemistry Search, Cell Parameters and Symmetry, Diffraction Search, and General Search. Includes a search button and a reset button.

Logic interface: AND or OR. Viewing options: amc long form, amc short form, or diffraction data.

Download options: amc, cif, or diffraction data.

Navigation icons for People, Home, and other resources.

Number of Files downloaded since Apr 1, 2003: 516504022
Data Last Updated: June 04, 2016
Web Page Last Updated: May 05, 2014
This page has been accessed 2204102 times.

Also see our complete list of minerals and complete list of authors.

This material is based upon work supported by the National Science Foundation under Grant Nos. EAR-0112782, and EAR-0622371. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the National Science Foundation.

Should the use of the database require a citation, then please use: Downs, R.T. and Hall-Wallace, M. (2003) The American Mineralogist Crystal Structure Database. American Mineralogist 88, 247-250. (pdf file)

Contact Robert T. Downs for suggestions and corrections.

American Mineralogist Crystal Structure Database

14 matching records for this search.

- Bassanite
- Ballirano P, Maras A, Meloni S, Caminiti R
European Journal of Mineralogy 13 (2001) 985-993
The monoclinic I2 structure of bassanite, calcium sulphate hemihydrate
_database_code_amcsd 0006909

a	b	c
12.0350	6.9294	12.6705

x	y	z
0.0000	0.5000	0.0000
0.0000	0.0000	0.5000
0.5000	0.0000	0.0000
0.5000	0.5000	0.0000
0.0000	0.5000	0.5000
0.5000	0.5000	0.5000

- Schmidt H, Paschke I, Freyer D, Voigt W
Acta Crystallographica B67 (2011) 467-475
Water channel structure of bassanite at high air humidity:
crystal structure of CaSO4·0.625H2O

- Search by a number of criteria
 - Get a listing of structure data
 - Download .CIF file
 - Import into Profex *
- *Use Vesta to view structure and get the Wyckoff positions*

<http://ruff.geo.arizona.edu/AMS/amcsd.php>

<http://jp-minerals.org/vesta/en/>

Vesta software interface showing a 3D ball-and-stick model of a crystal structure. The model is displayed in a 3D coordinate system with axes x, y, and z. The structure consists of various colored spheres representing atoms, arranged in a complex lattice. The interface includes a toolbar with various tools for manipulating the model, a list of atoms, and a status bar.

Structure name: Langbeinite
Formula: K2 Mg2 S12 O28
Space group: I2/m (No. 12)
Cell parameters: a=12.0350, b=6.9294, c=12.6705
Angles: alpha=90.0000, beta=90.0000, gamma=90.0000

Atom	x	y	z
K1	0.0000	0.0000	0.0000
Mg1	0.0000	0.5000	0.0000
S1	0.0000	0.0000	0.5000
O1	0.5000	0.0000	0.0000
O2	0.5000	0.5000	0.0000
O3	0.0000	0.5000	0.5000
O4	0.5000	0.5000	0.5000

Import CIF Example

Profex->File->Import Structure File

- Point toward selected .CIF file
- At the same time, open that CIF file using VESTA
 - necessary to get the Wyckoff position notation 😊
- Add PHASE name: PHASE=Ferrite // 😊
- Add phase name to GOAL: GOAL:Ferrite=GEWICHT ... 😊
- Add atom charge (CA+2, AL+3, FE+3, O-2) 😊
- Save to Structures Folder; include extension .str

Profex

Vesta

The image shows two software windows side-by-side. The left window is Profex, displaying the 'Import Structure Files' dialog with a list of files including 'c4af2_jp.cif'. Below the list, the CIF file content is shown, including phase and goal information. The right window is VESTA, showing a 3D ball-and-stick model of the structure. The VESTA interface includes a toolbar, a 'Tools' panel with 'Show models' and 'Show dot surface' options, and a 'Style' panel with 'Ball-and-stick' selected. The main display area shows the structure and a coordinate system. Below the structure, technical details like OpenGL version, video configuration, and CIF file path are visible. A table of structure parameters is also present, with the 'Site' column circled in red.

Files

STR File Source File XML File

c4af2_jp.cif

```
PHASE= //
Formula=Ca2[Fe0.76Al0.24](Fe0.24Al0.76)AlO5 //
SpacegroupNo=46 Setting=2 HermannMauguin=Ibm2 Lattice=Orthorhombic //
PARAM=A=0.558400_0.552816^0.563984 PARAM=B=1.460000_1.445400^1.474600 PARAM=C=0.537400_0.532026^0.542774 //
RP=4 k1=0 k2=0 PARAM=B1=0_0^0.01 GEWICHT=SPHARO //
GOAL:=GEWICHT*ifthenelse(ifdef(d),exp(my*d*3/4),1) //
E=CA Wyckoff= x=0.02730000 y=0.10870000 z=0.49200000 TDS=0.00971169
E=FE(0.7600) Wyckoff= x=0.00000000 y=0.00000000 z=0.00000000 TDS=0.00971169
E=AL(0.7600) Wyckoff= x=0.92830000 y=0.25000000 z=0.95330000 TDS=0.00971169
E=O Wyckoff= x=0.25230000 y=0.98610000 z=0.24910000 TDS=0.00971169
E=O Wyckoff= x=0.06800000 y=0.14390000 z=0.02460000 TDS=0.00971169
E=O Wyckoff= x=0.86070000 y=0.25000000 z=0.61930000 TDS=0.00971169
E=AL(0.2400) Wyckoff= x=0.00000000 y=0.00000000 z=0.00000000 TDS=0.00971169
E=FE(0.2400) Wyckoff= x=0.92830000 y=0.25000000 z=0.95330000 TDS=0.00971169
```

Warning: No Wyckoff information found for atom number 0.
Warning: No Wyckoff information found for atom number 1.
Warning: No Wyckoff information found for atom number 2.
Warning: No Wyckoff information found for atom number 3.
Warning: No Wyckoff information found for atom number 4.
Warning: No Wyckoff information found for atom number 5.
Warning: No Wyckoff information found for atom number 6.
Warning: No Wyckoff information found for atom number 7.

Add Files Save STR Close

OpenGL version: 2.1 NVIDIA-10.4.2 310.41.35f01
Video configuration: NVIDIA GeForce GT 650M OpenGL Engine
Maximum supported width and height of the viewport: 16384 x 16384
OpenGL depth buffer bit: 16

/Users/stutz/Documents/XRD/Cements_XRD_Database/CIF_Files/c4af2_jp.cif

Title

Lattice type I
Space group name I b m 2
Space group number 46
Setting number 2

Lattice parameters

a b c alpha beta gamma
5.58400 14.60000 5.37400 90.0000 90.0000 90.0000

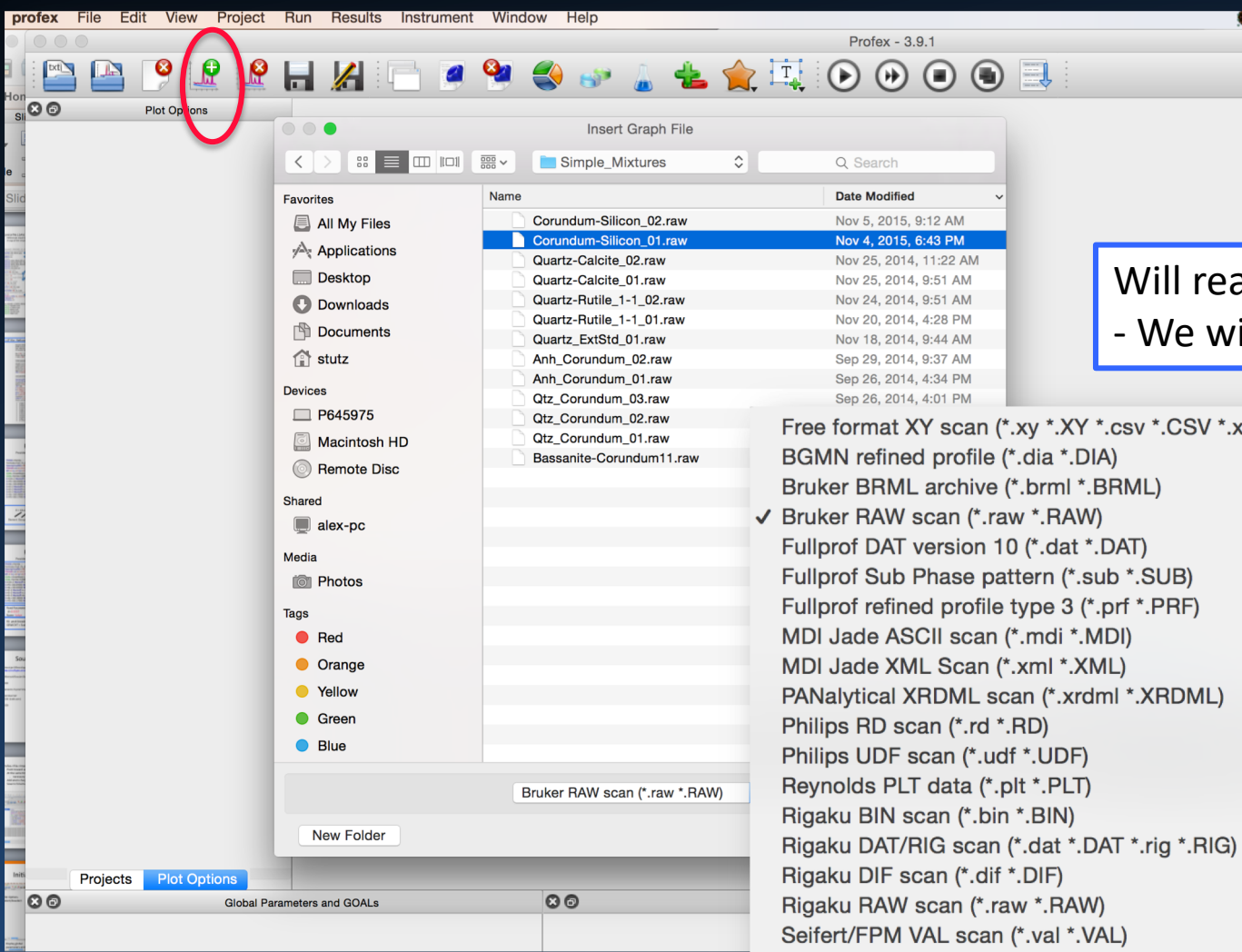
Unit-cell volume = 438.122900 Å³

Structure parameters

x y z Occ. U Site Sym.
1 Ca Ca(1) 0.02730 0.10870 0.49200 1.000 0.012 8c 1
2 Fe Fe(1) 0.00000 0.00000 0.00000 0.760 0.012 4a ..2
3 Al Al(2) 0.92830 0.25000 0.95330 0.760 0.012 4b m..
4 O O(1) 0.25230 0.98610 0.24910 1.000 0.012 8c 1
5 O O(2) 0.06800 0.14390 0.02460 1.000 0.012 8c 1
6 O O(3) 0.86070 0.25000 0.61930 1.000 0.012 4b m..
7 Al Al(1) 0.00000 0.00000 0.00000 0.240 0.012 4a ..2
8 Fe Fe(2) 0.92830 0.25000 0.95330 0.240 0.012 4b m..

Number of polygons and unique vertices on isosurface = 0 (0)
47 atoms, 0 bonds, 0 polyhedra; CPU time = 4 ms

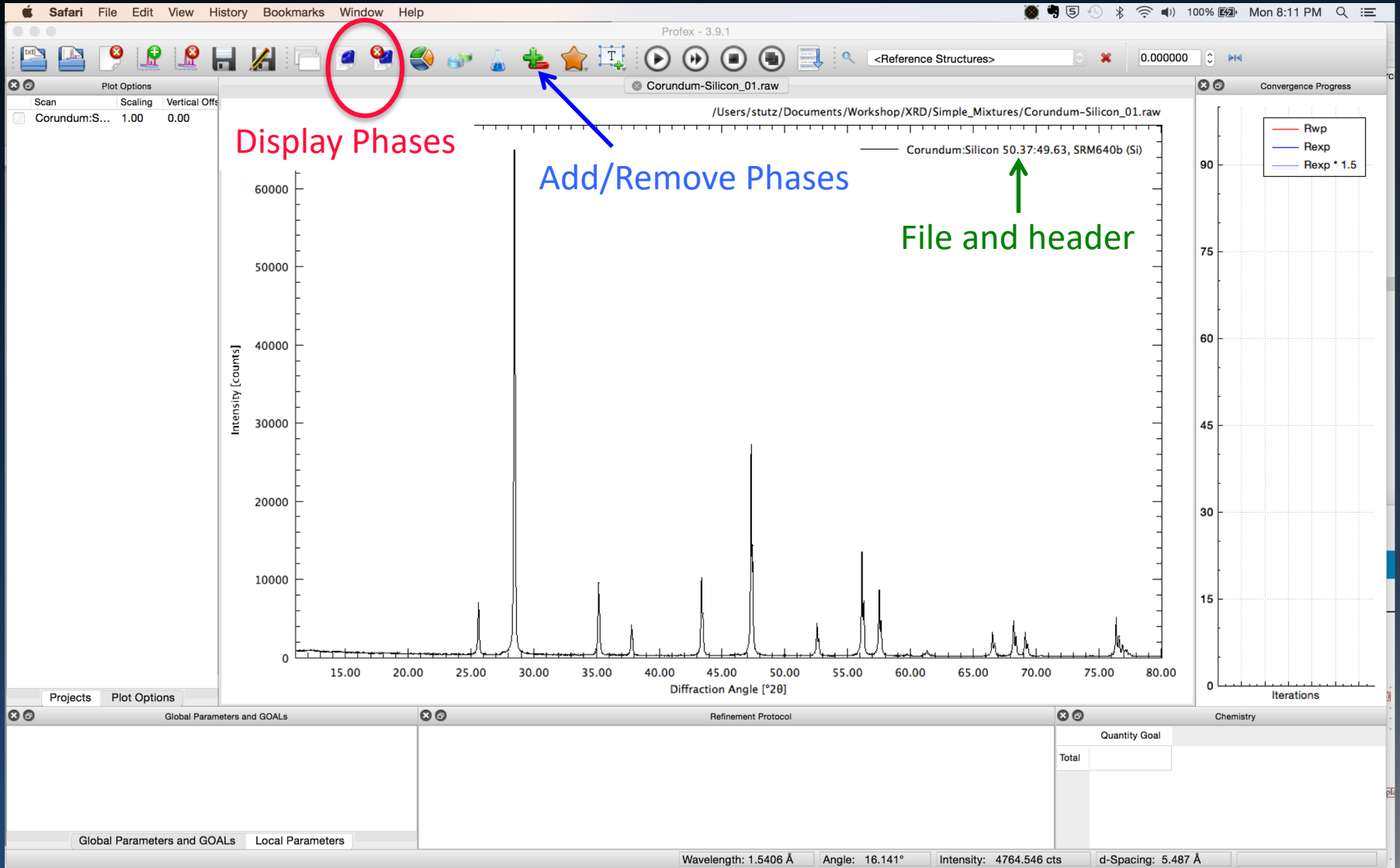
Load Data File: File->Insert Scan



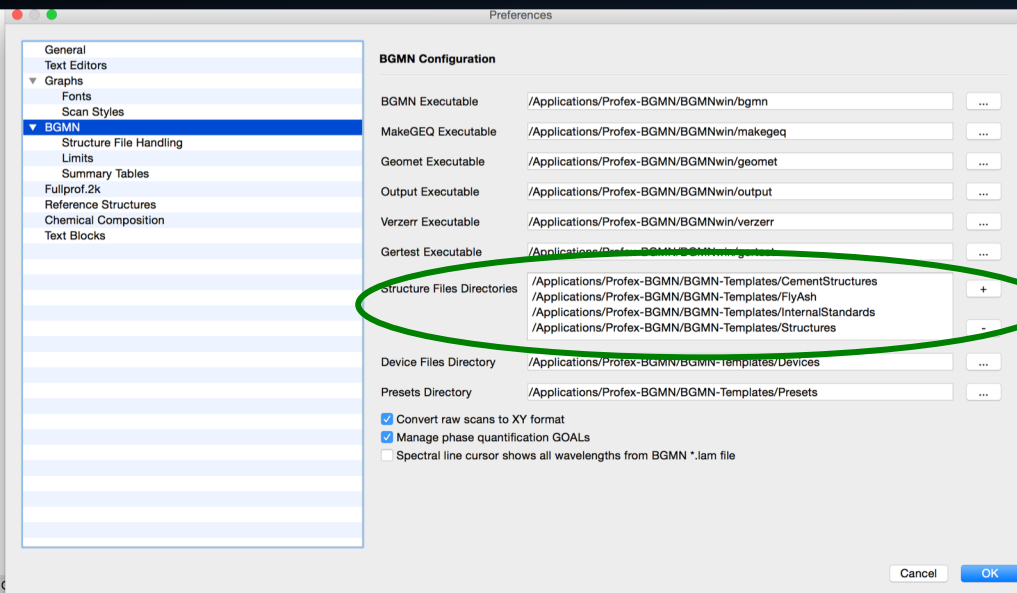
Will read numerous formats
- We will use the Bruker .RAW

Free format XY scan (*.xy *.XY *.csv *.CSV *.xyp *.XYP *.dat *.DAT *.asc *.ASC *.txt *.TXT)
BGMN refined profile (*.dia *.DIA)
Bruker BRML archive (*.brml *.BRML)
✓ Bruker RAW scan (*.raw *.RAW)
Fullprof DAT version 10 (*.dat *.DAT)
Fullprof Sub Phase pattern (*.sub *.SUB)
Fullprof refined profile type 3 (*.prf *.PRF)
MDI Jade ASCII scan (*.mdi *.MDI)
MDI Jade XML Scan (*.xml *.XML)
PANalytical XRDML scan (*.xrdml *.XRDML)
Philips RD scan (*.rd *.RD)
Philips UDF scan (*.udf *.UDF)
Reynolds PLT data (*.plt *.PLT)
Rigaku BIN scan (*.bin *.BIN)
Rigaku DAT/RIG scan (*.dat *.DAT *.rig *.RIG)
Rigaku DIF scan (*.dif *.DIF)
Rigaku RAW scan (*.raw *.RAW)
Seifert/FPM VAL scan (*.val *.VAL)
Stoe PRO scan (*.pro *.PRO)
Stoe RAW scan (*.raw *.RAW)
TexturePlus corrected rocking curve (*.ovl *.OVL)
All Files (*.*)

Corundum-Silicon File Added



Structure Files

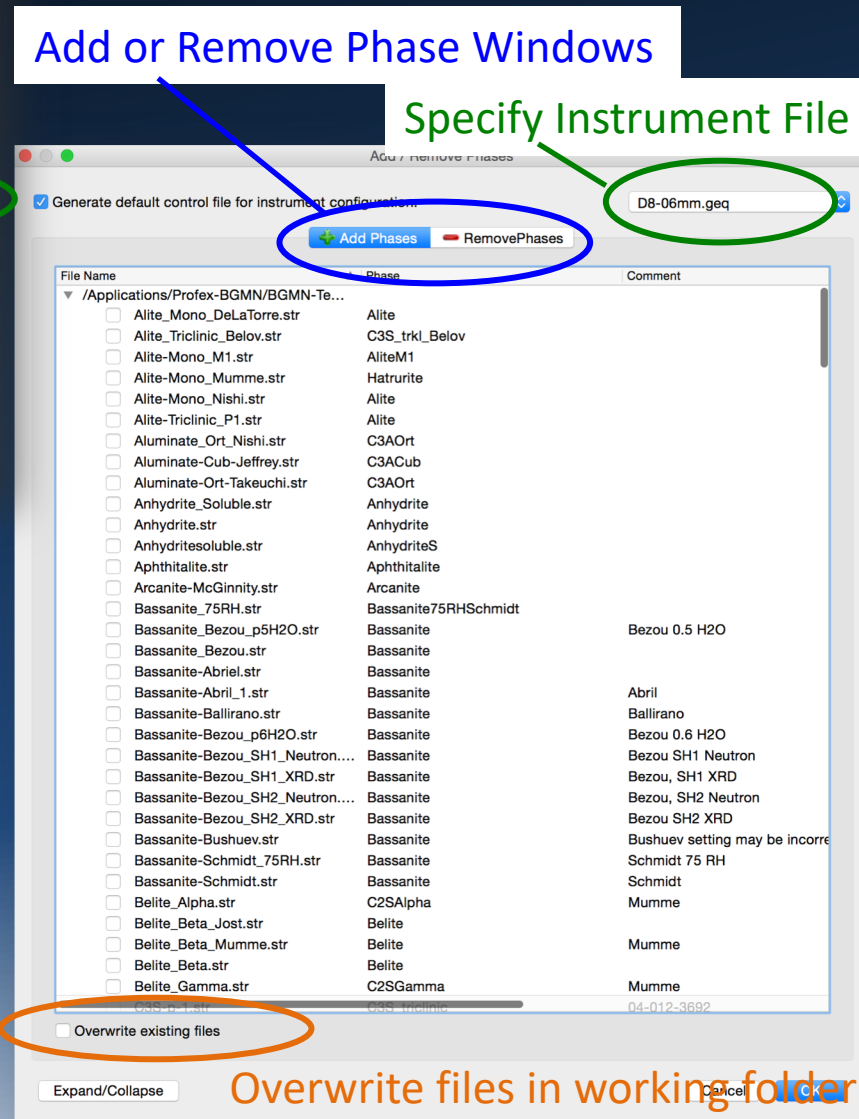


Profex->Preferences

- Paths to structure files
- Will list according to list order

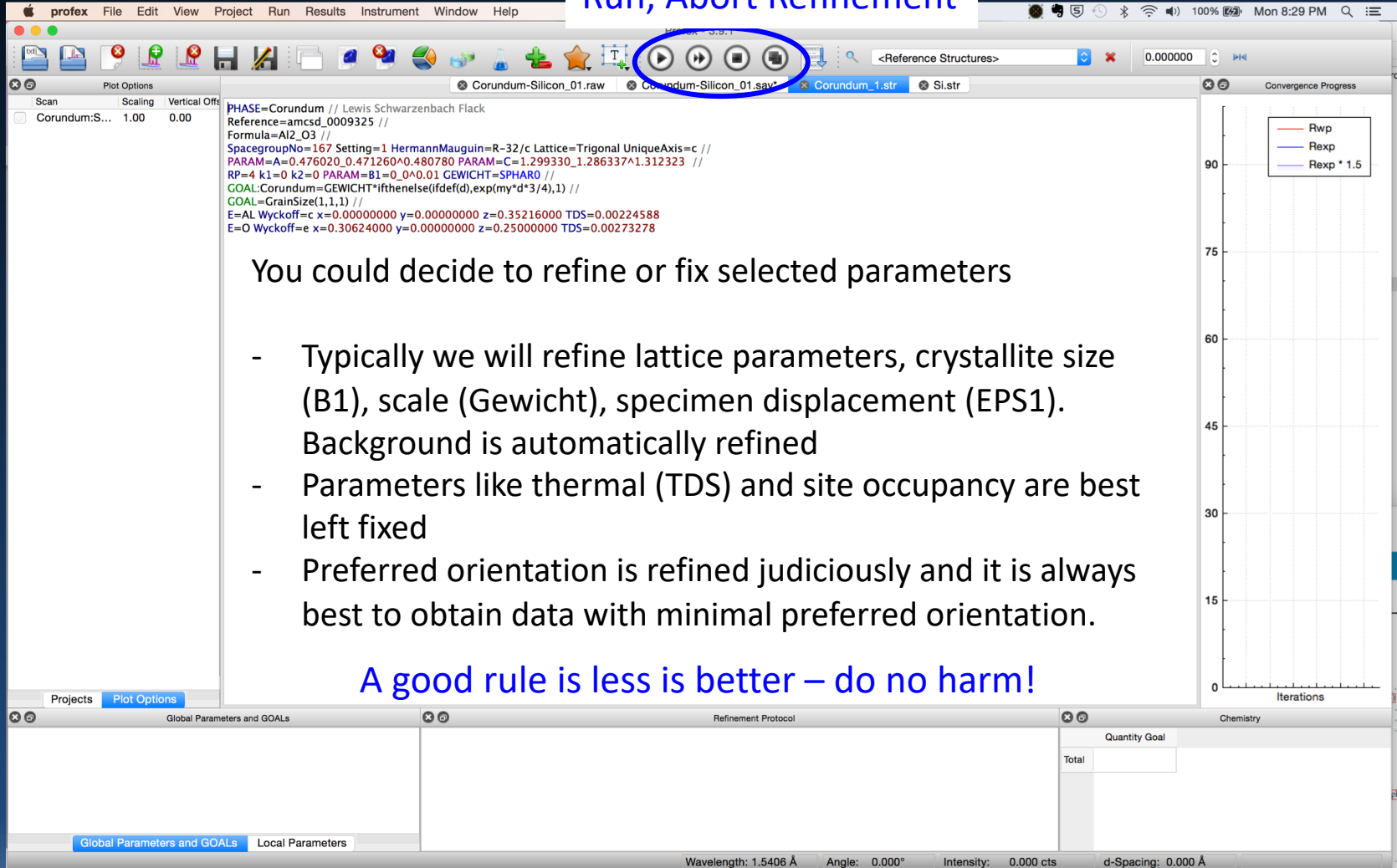
- CementStructures
- FlyAsh
- InternalStandards
- Structures

- Once added, select Display to see the copied data, make changes if desired



Profex: .raw, .sav, .str display

Run, Abort Refinement



The screenshot shows the Profex software interface. At the top, a menu bar includes 'profex', 'File', 'Edit', 'View', 'Project', 'Run', 'Results', 'Instrument', 'Window', and 'Help'. Below the menu bar is a toolbar with various icons, including a play button and a stop button, which are circled in blue. The main window displays a refinement protocol for Corundum-Silicon. The protocol includes parameters such as PHASE, Reference, Formula, SpacegroupNo, Setting, HermannMauguin, Lattice, UniqueAxis, PARAM, RP, k1, k2, GOAL, GrainSize, E=AL Wyckoff, and E=O Wyckoff. A 'Convergence Progress' plot is visible on the right side of the window, showing the convergence of Rwp, Rexp, and Rexp * 1.5 over iterations. The plot shows Rwp (red line) and Rexp (blue line) decreasing over iterations, while Rexp * 1.5 (purple line) remains relatively constant. The x-axis is labeled 'Iterations' and ranges from 0 to 90. The y-axis ranges from 0 to 90. The status bar at the bottom of the window displays 'Wavelength: 1.5406 Å', 'Angle: 0.000°', 'Intensity: 0.000 cts', and 'd-Spacing: 0.000 Å'.

PHASE=Corundum // Lewis Schwarzenbach Flack
Reference=amcsd_0009325 //
Formula=Al2O3 //
SpacegroupNo=167 Setting=1 HermannMauguin=R-32/c Lattice=Trigonal UniqueAxis=c //
PARAM=A=0.476020_0.471260^0.480780 PARAM=C=1.299330_1.286337^1.312323 //
RP=4 k1=0 k2=0 PARAM=B1=0_0^0.01 GEWICHT=SPHARO //
GOAL:Corundum=GEWICHT*ifthenelse(ifdef(d),exp(my*d^3/4),1) //
GOAL=GrainSize(1,1,1) //
E=AL Wyckoff=c x=0.00000000 y=0.00000000 z=0.35216000 TDS=0.00224588
E=O Wyckoff=e x=0.30624000 y=0.00000000 z=0.25000000 TDS=0.00273278

You could decide to refine or fix selected parameters

- Typically we will refine lattice parameters, crystallite size (B1), scale (Gewicht), specimen displacement (EPS1). Background is automatically refined
- Parameters like thermal (TDS) and site occupancy are best left fixed
- Preferred orientation is refined judiciously and it is always best to obtain data with minimal preferred orientation.

A good rule is less is better – do no harm!

Initialize Profex, Insert Scan

The screenshot shows the Profex software interface with the 'Insert Graph File' dialog box open. The dialog is set to the folder '86_HNO3_Example'. The file list contains the following items:

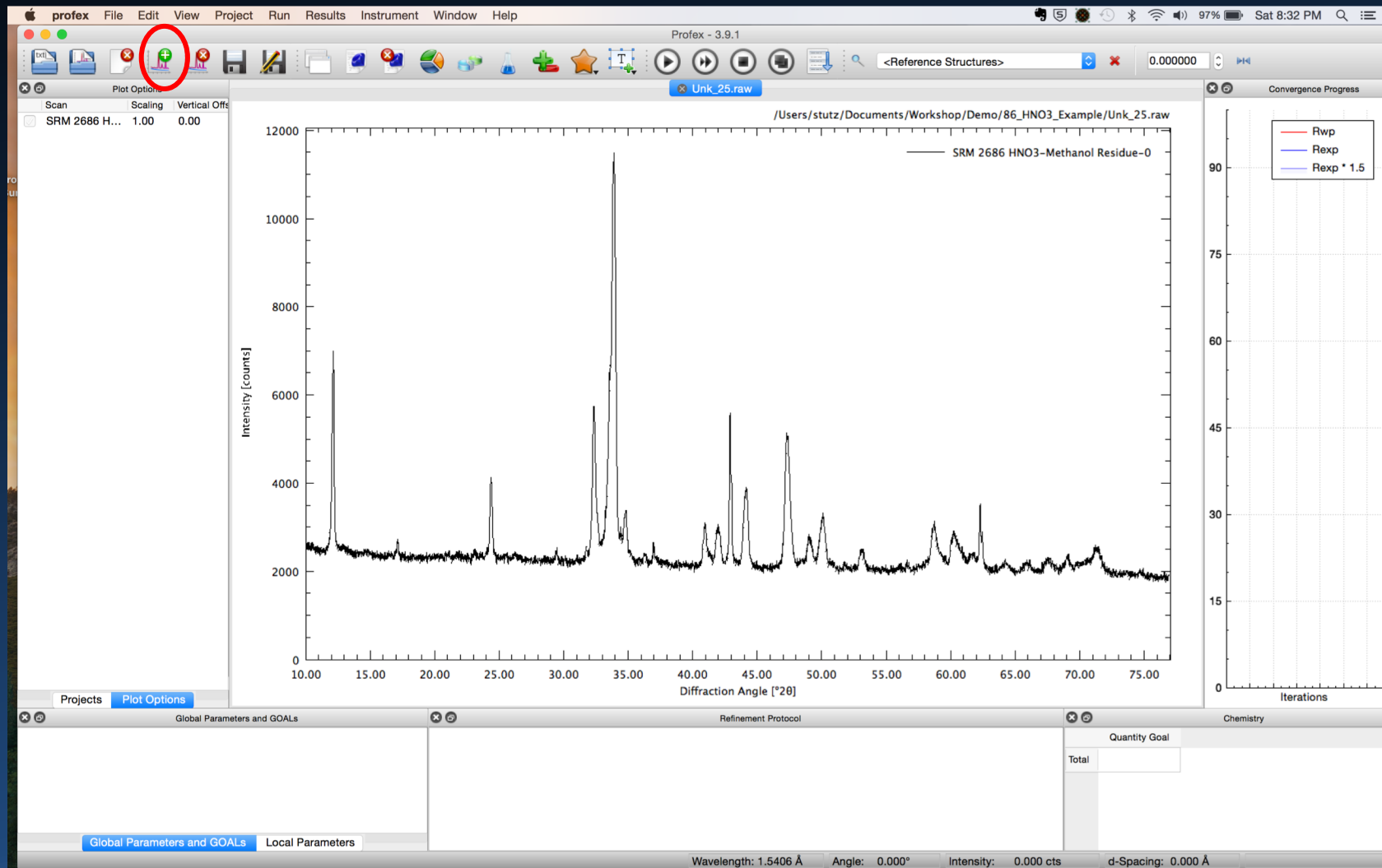
Name	Date Modified	Size	Kind
Unk_25.jpg	May 9, 2016, 11:12 AM	102 KB	JPEG image
Unk_25.raw	May 5, 2016, 11:29 AM	17 KB	Panaso...image
Unk_25.txt	May 9, 2016, 11:12 AM	342 bytes	text

The file type is set to 'Bruker RAW scan (*.raw *.RAW)'. The 'Open' button is highlighted.

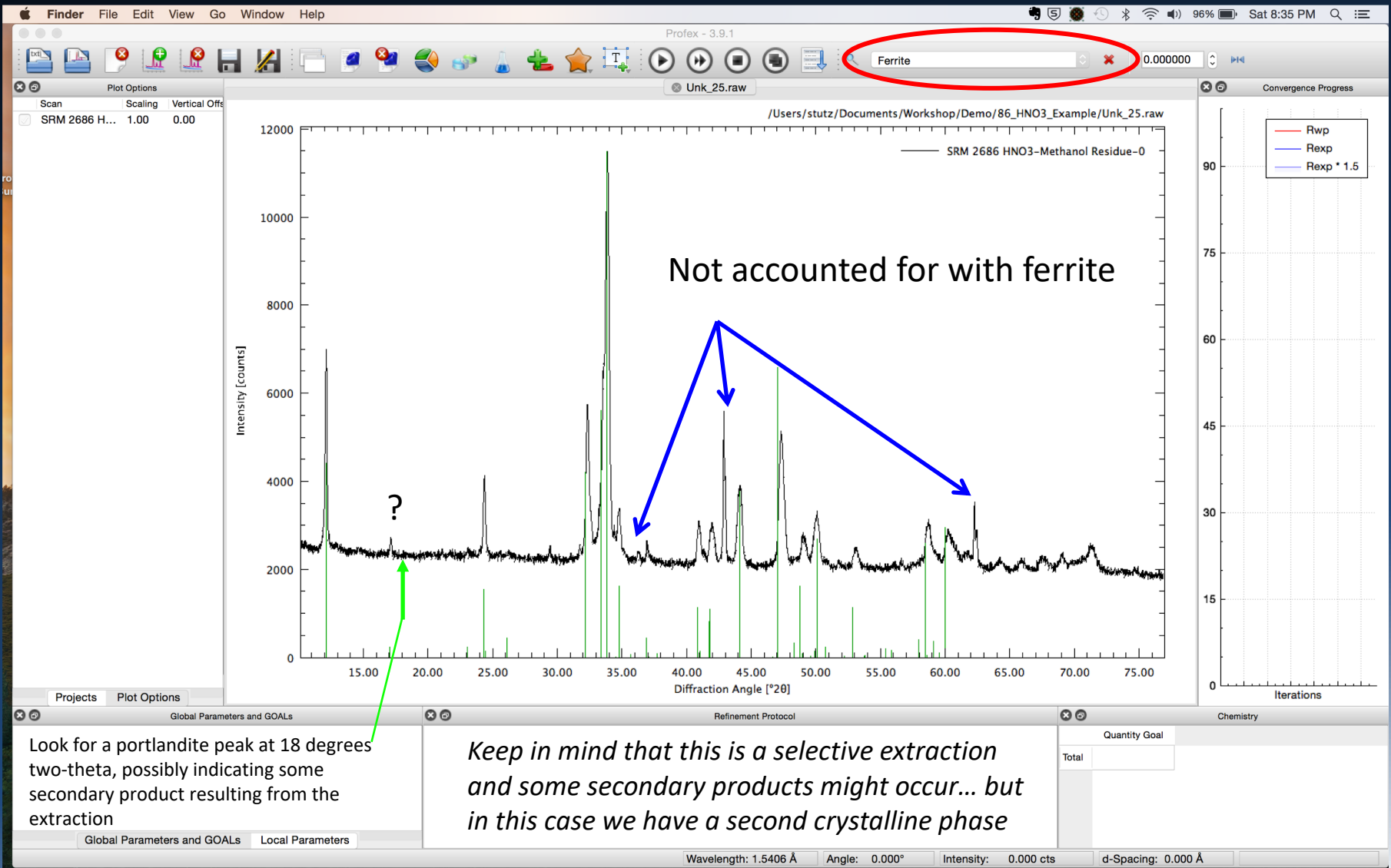
The main interface shows the 'Plot Options' tab selected in the 'Projects' section. The status bar at the bottom displays the following parameters:

- Wavelength: 1.5406 Å
- Angle: 0.000°
- Intensity: 0.000 cts
- d-Spacing: 0.000 Å

Initialize Profex, Insert Scan



Phase d&I Search for Phase Identification



Look for a portlandite peak at 18 degrees two-theta, possibly indicating some secondary product resulting from the extraction

Keep in mind that this is a selective extraction and some secondary products might occur... but in this case we have a second crystalline phase

Add Phase

The screenshot displays the Profex software interface. The main window shows a plot of Intensity [counts] versus 2-theta [degrees]. The plot has a y-axis from 0 to 12000 and an x-axis from 15.00 to 30.00. A red circle highlights the 'Add Phases' button in the top toolbar. A dialog box titled 'Add / Remove Phases' is open, showing a list of phases. The 'Ferrite.str' phase is selected, and a red circle highlights the 'Add Phases' button and the selected phase. The dialog box also contains a 'Select one' label and a 'Generate default control file for instrument configuration:' checkbox.

Profex - 3.9.1
Add / Remove Phases

Generate default control file for instrument configuration: D8-06mm.geq

Add Phases Remove Phases

File Name	Phase	Comment
<input type="checkbox"/> Ferrite_C4AF.str	Ferrite	
<input type="checkbox"/> Ferrite_Colville.str	Brownmillerite	
<input checked="" type="checkbox"/> Ferrite.str	Ferrite	
<input type="checkbox"/> Gypsum_1.str	Gypsum	De La Torre
<input type="checkbox"/> Gypsum_2.str	Gypsum	De La Torre
<input type="checkbox"/> Gypsum_Atoji.str	Gypsum	Atoji and Rundle
<input type="checkbox"/> Gypsum_BGMN.str	Gypsum	
<input type="checkbox"/> Gypsum_Cole.str	Gypsum	Cole
<input type="checkbox"/> Gypsum_Comodi.str	Gypsum	Comodi
<input type="checkbox"/> Gypsum_DeLaTorre.str	Gypsum	De la Torre
<input type="checkbox"/> Gypsum_Pedersen.str	Gypsum	Pedersen and Semmingsen
<input type="checkbox"/> Gypsum.str	Gypsum	
<input type="checkbox"/> Langbeinite_Ca.str	Langbeinite	Ca variant of Mereiter K
<input type="checkbox"/> Langbeinite_Mg.str	Langbeinite	Mereiter K
<input type="checkbox"/> Larnite-Jost.str	Larnite	
<input type="checkbox"/> Larnite.str	Larnite	
<input type="checkbox"/> Lime.str	CaO	04-007-9734
<input type="checkbox"/> Metathenardite.str	Metathenardite	
<input type="checkbox"/> Periclase.str	MgO	04-010-4039
<input type="checkbox"/> Portlandite.str	Portlandite	04-010-3117
<input type="checkbox"/> Quartz-p3121.str	SiO2p3121	04-008-4821
<input type="checkbox"/> Quartz-p3221.str	SiO2p3221	04-012-0490
<input type="checkbox"/> Syngenite.str	Syngenite	Corazza 1967
<input type="checkbox"/> Thenardite.str	Thenardite	
▼ /Applications/Profex-BGMN/BGMN-Te...		
<input type="checkbox"/> Akermanite.str	Akermanite	
<input type="checkbox"/> CarbonatedCaHemicarboalumin...	Carbonatedcalciumhemicarboalumin...	
<input type="checkbox"/> Gehlenite.str	Gehlenite	
<input type="checkbox"/> Hannebachite.str	Hannebachite	
<input type="checkbox"/> Hematite_Blake.str	Hematite	
<input type="checkbox"/> Hematite.str	Hematite	
<input type="checkbox"/> Hercynite.str	Hercynite	
<input type="checkbox"/> Magnetite.str	Magnetite	
<input type="checkbox"/> Mayenite.str	Mayenite	
<input type="checkbox"/> Mellilite.str	Mellilite	

Overwrite existing files

Expand/Collapse Cancel OK

Wavelength: 1.5406 Å Angle: 0.000° Intensity: 0.000 cts d-Spacing: 0.000 Å

Display Structure

Initiate refinement

The screenshot shows the profex software interface. The main window displays the refinement protocol for Ferrite, including parameters like PHASE, Formula, Spacegroup, and various refinement goals. A red circle highlights the 'Run' button in the toolbar, and a green arrow points to it. The 'Convergence Progress' plot on the right shows the Rwp, Rexp, and Rexp * 1.5 values over iterations. The bottom panel shows the 'Global Parameters and GOALS' section, which includes atom positions and vibrational factors.

```
PHASE=Ferrite //
Formula=Ca2_Fe_Al2_O5 //
SpacegroupNo=46 Setting=2 HermannMauguin=Ibm2 Lattice=Orthorhombic //
PARAM=A=0.5557 0.551^0.563 PARAM=B=1.4543 1.43^1.465 PARAM=C=0.53616 0.533^0.542 //
RP=4 k1=0 k2=0 PARAM=B1=0_0^0.01 GEWICHT=SPHARO //
GOAL=GrainSize(1,1,1) //
GOAL:Ferrite=GEWICHT*ifthenelse(ifdef(d),exp(my*d^3/4),1) //
E=CA+2 Wyckoff=c x=0.02730000 y=0.10870000 z=0.49200000 TDS=0.00971169
E=FE+3(0.6400) Wyckoff=a x=0.00000000 y=0.00000000 z=0.00000000 TDS=0.00971169
E=AL+3(0.8300) Wyckoff=b x=0.92830000 y=0.25000000 z=0.95330000 TDS=0.00971169
E=O-2 Wyckoff=c x=0.25230000 y=0.98610000 z=0.24910000 TDS=0.00971169
E=O-2 Wyckoff=c x=0.06800000 y=0.14390000 z=0.02460000 TDS=0.00971169
E=O-2 Wyckoff=b x=0.86070000 y=0.25000000 z=0.61930000 TDS=0.00971169
E=AL+3(0.3600) Wyckoff=a x=0.00000000 y=0.00000000 z=0.00000000 TDS=0.00971169
E=FE+3(0.1700) Wyckoff=b x=0.92830000 y=0.25000000 z=0.95330000 TDS=0.00971169
```

For the most part, refined parameters are pre-set and indicated by **PARAM**

Some parameters are automatic: Background, Scale (gewicht)

Other parameters

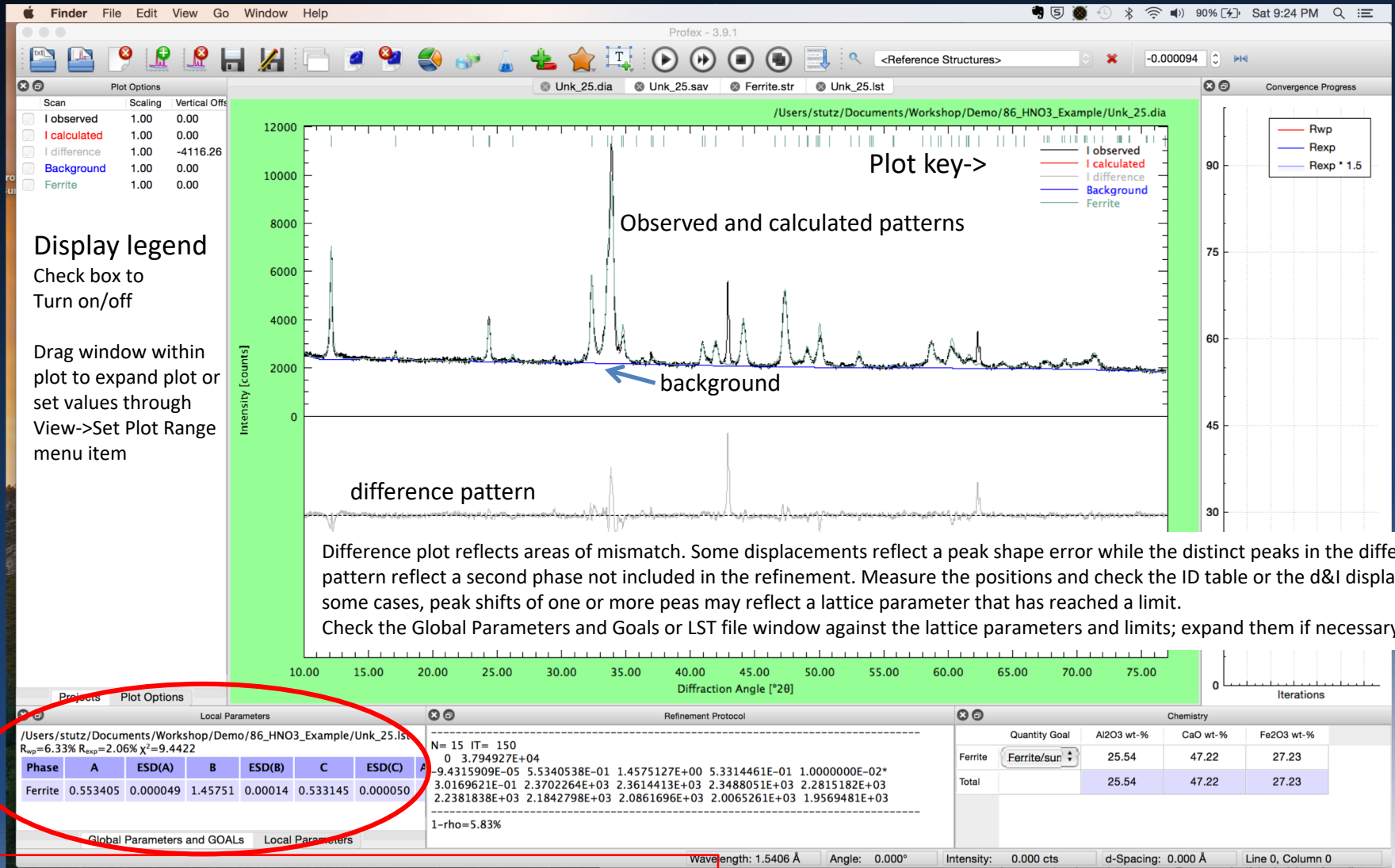
- Lattice parameters a, b, and c
- B1 (Lorentzian line shape related to crystallite size broadening)
- Goals: Computed values, crystallite size, adjustments to scale
- Preferred orientation: SPHARn, where n=0 (none), 2, 4, 6 *Ideally set to 0!*

Generally you will not need to initiate or deselect any refined parameters aside from preferred orientation, and only if warranted by peak intensity mismatch and potential for orientation based upon crystal habit or cleavage properties – alite, perhaps ferrite and belite and, for cements, any of the calcium sulfates and calcite

Atom positions (x,y,z) and vibrational (thermal) factors (TDS) are not refined partly because the data range is too limited. Site occupancy might be refined, but the initial values for ferrite are based upon earlier refinements, providing typical industrial values.

Wavelength: 1.5406 Å Angle: 0.000° Intensity: 0.000 cts d-Spacing: 0.000 Å Line 0, Column 0

Examine Results: Plot, Parameters, LST



Display legend

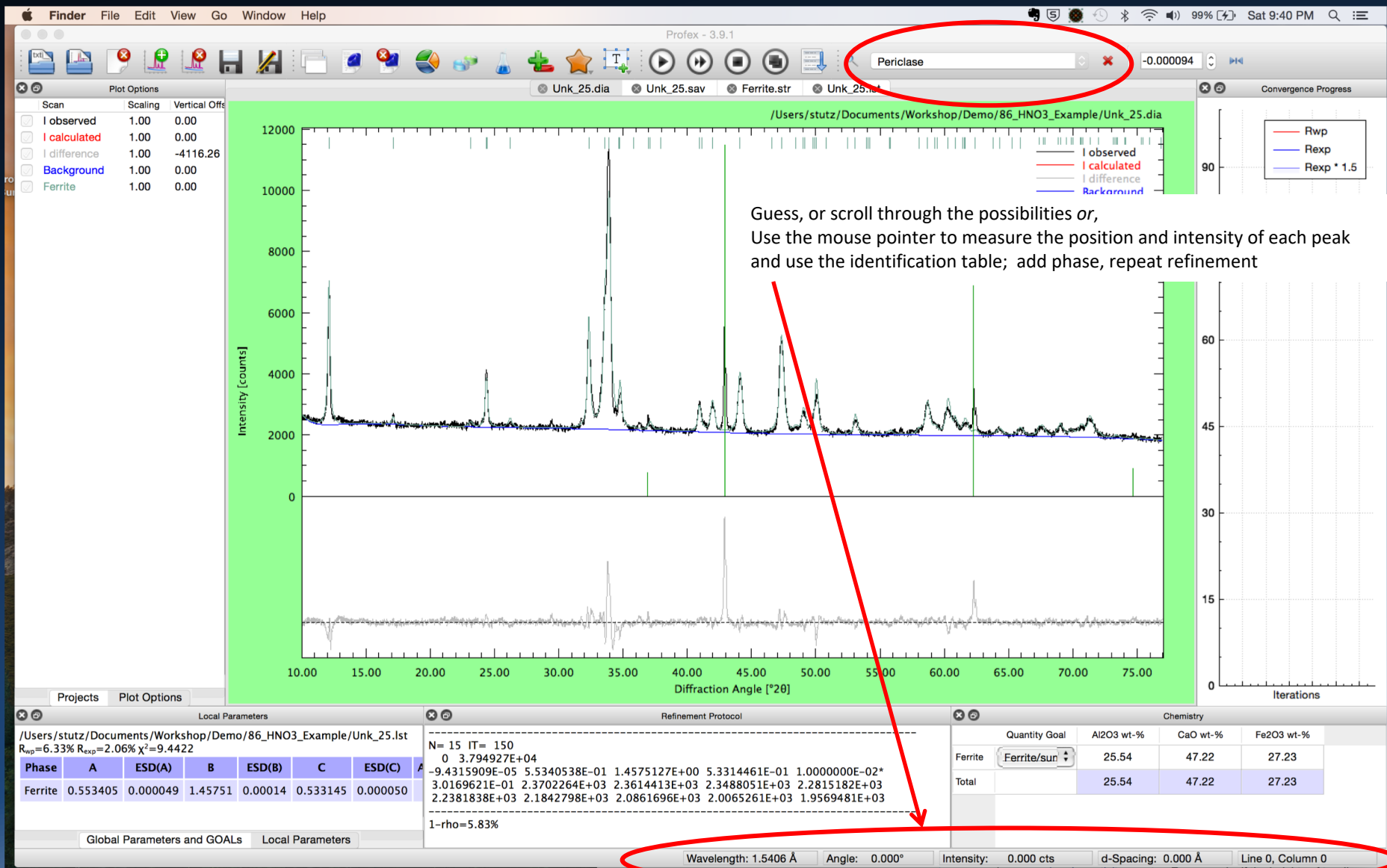
Check box to Turn on/off

Drag window within plot to expand plot or set values through View->Set Plot Range menu item

Difference plot reflects areas of mismatch. Some displacements reflect a peak shape error while the distinct peaks in the difference pattern reflect a second phase not included in the refinement. Measure the positions and check the ID table or the d&l display. In some cases, peak shifts of one or more peaks may reflect a lattice parameter that has reached a limit. Check the Global Parameters and Goals or LST file window against the lattice parameters and limits; expand them if necessary

Compare refined values to parameter limits, adjust limits if justified

Search for Missing Phase



Ferrite and Periclase Refinement

profex File Edit View Project Run Results Instrument Window Help Profex - 3.9.1

Unk_25.dia Unk_25.sav Ferrite.str Unk_25.lst

Plot Options

Scan	Scaling	Vertical Offset
<input checked="" type="checkbox"/> I observed	1.00	0.00
<input checked="" type="checkbox"/> I calculated	1.00	0.00
<input checked="" type="checkbox"/> I difference	1.00	-2305.42
<input checked="" type="checkbox"/> Background	1.00	0.00
<input checked="" type="checkbox"/> Ferrite	1.00	0.00
<input checked="" type="checkbox"/> MgO	1.00	0.00

Click on an item to highlight it on the plot

This is useful to look at individual phase contributions and to assess which phase may be mismatched with the raw data

Convergence Progress

Iterations	Rwp	Rexp	Rexp * 1.5
0	~4.13%	~2.05%	~6.19%
10	~4.13%	~2.05%	~6.19%
20	~4.13%	~2.05%	~6.19%
30	~4.13%	~2.05%	~6.19%
40	~4.13%	~2.05%	~6.19%
50	~4.13%	~2.05%	~6.19%
60	~4.13%	~2.05%	~6.19%
70	~4.13%	~2.05%	~6.19%
80	~4.13%	~2.05%	~6.19%
90	~4.13%	~2.05%	~6.19%

Looks much better; low angle mismatch is common, slight intensity mismatch may be related to sampling preferred orientation, or chemical substitution
We could exclude the low angle region by adding the line WMIN=15 to the .SAV tab

Global Parameters and GOALS

Refinement Protocol

Chemistry

	Quantity Goal	MgO wt-%	Al ₂ O ₃ wt-%	CaO wt-%	Fe ₂ O ₃ wt-%
Ferrite	Ferrite/sun	0.00	23.18	42.86	24.71
MgO	MgO/sum	9.25	0.00	0.00	0.00
Total		9.25	23.18	42.86	24.71

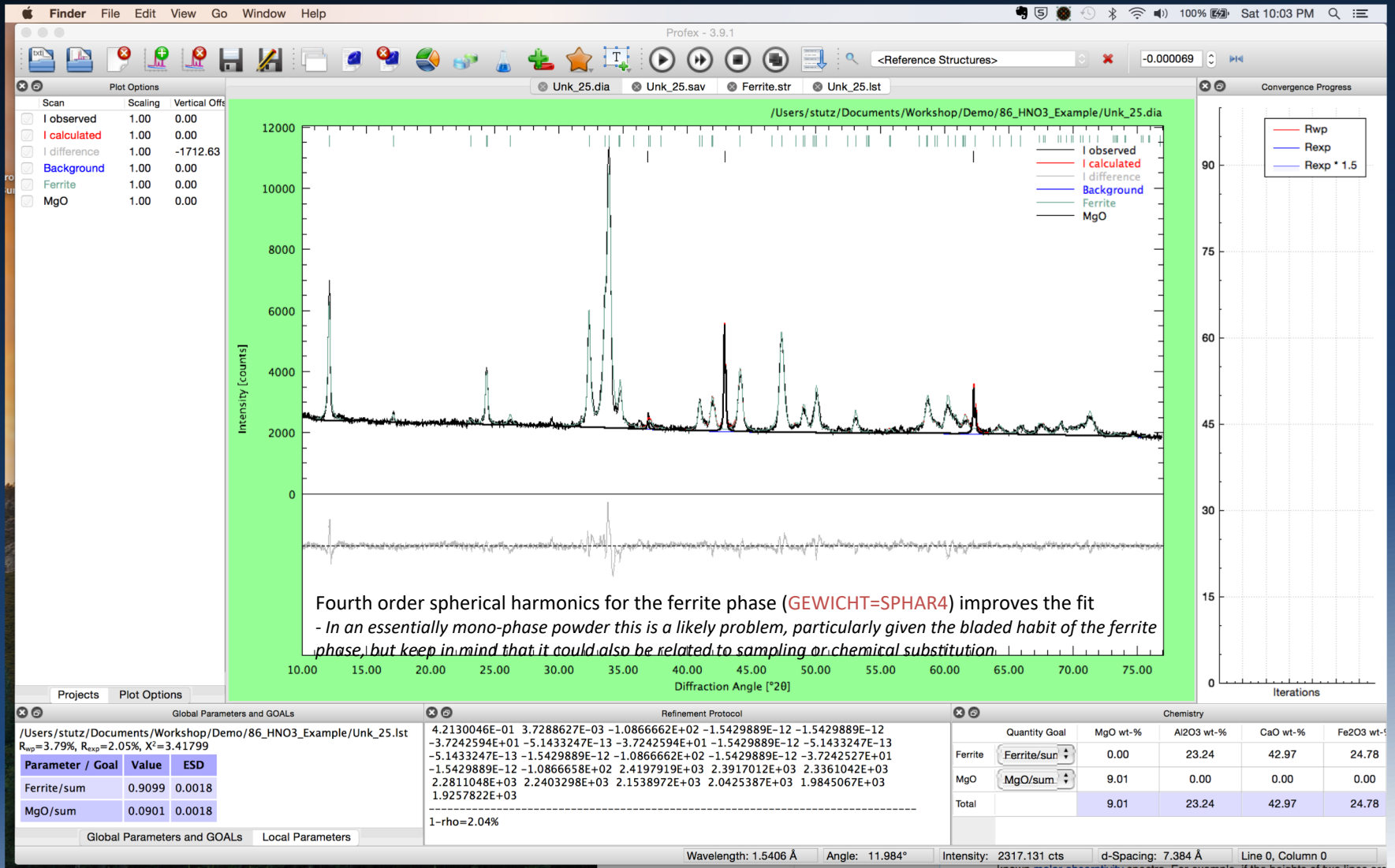
Relative phase proportions!

Global Parameters and GOALS Local Parameters

Wavelength: 1.5406 Å Angle: 0.000° Intensity: 0.000 cts d-Spacing: 0.000 Å Line 0, Column 0

Preferred Orientation

Since ferrite can exhibit a tabular habit it is possible it could be oriented, skewing the representative orientation ideal and so, the relative peak intensities. Change the zero to 2 and later 4 if necessary after the variable SPHAR and repeat the refinement to see if it improves. Profex runs the refinement and introduces the orientation correction at the last stages, but only if the phase fraction is above a minimum to make it practical.



Check Parameters

Profex - 3.9.1

<Reference Structures> -0.000100

Unk_25.dia Unk_25.sav Unk_25.lst Ferrite.str Periclase.str

Plot Options

Scan	Scaling	Vertical Offset	Horizo
<input checked="" type="checkbox"/> I observed	1.00	0.00	0.000
<input checked="" type="checkbox"/> I calculated	1.00	0.00	0.000
<input checked="" type="checkbox"/> I difference	1.00	-1749.42	0.000
<input checked="" type="checkbox"/> Background	1.00	0.00	0.000
<input type="checkbox"/> Ferrite	1.00	0.00	0.000
<input type="checkbox"/> MgO	1.00	0.00	0.000

Rietveld refinement to file(s) Unk_25.xy
 BGMN version 4.2.22, 4026 measured points, 80 peaks, 46 parameters
 Start: Tue Jul 19 09:09:23 2016; End: Tue Jul 19 09:09:25 2016
 24 iteration steps

Rp=2.93% Rpb=22.25% R=4.73% Rwp=3.78% Rexp=2.05%
 Durbin-Watson d=0.61
 1-rho=2.04%

Global parameters and GOALS

Ferrite/sum=0.9090+-0.0019
 MgO/sum=0.0910+-0.0019
 EPS2=-0.000100+-0.000015

Local parameters and GOALS for phase Ferrite

SpacegroupNo=46
 HermannMauguin=Ibm2
 XrayDensity=3.667
 Rphase=5.65%
 UNIT=NM
 A=0.553276+-0.000031
 B=1.457555+-0.000088
 C=0.533351+-0.000032
 B1=0.009941+-0.000087
 GrainSize(1,1,1)=42.69+-0.37
 GEWICHT=SPHAR4, MeanValue(GEWICHT)=0.312406

Atomic positions for phase Ferrite

#	x	y	z	E
8	0.0273	0.1087	0.4920	E=(CA+2(1.0000))
4	0.0000	0.0000	0.0000	E=(FE+3(0.6400))
4	0.9283	0.2500	0.9533	E=(AL+3(0.8300))
8	0.2523	0.9861	0.2491	E=(O-2(1.0000))
8	0.0680	0.1439	0.0246	E=(O-2(1.0000))
4	0.8607	0.2500	0.6193	E=(O-2(1.0000))
4	0.0000	0.0000	0.0000	E=(AL+3(0.3600))
4	0.9283	0.2500	0.9533	E=(FE+3(0.1700))

Local parameters and GOALS for phase MgO

SpacegroupNo=225
 HermannMauguin=F4/m-32/m
 XrayDensity=3.580
 Rphase=2.60%
 UNIT=NM
 A=0.421317+-0.000015
 B1=0.00358+-0.00013
 GrainSize(1,1,1)=118.6+-4.2
 GEWICHT=SPHAR4, MeanValue(GEWICHT)=0.0312892

Atomic positions for phase MgO

#	x	y	z	E
4	0.0000	0.0000	0.0000	E=(MG+2(1.0000))
4	0.5000	0.5000	0.5000	E=(O-2(1.0000))

Convergence Progress

21 iterations

Global Parameters and GOALS

/Users/stutz/Documents/ID_Exercise/U25/Unk_25.lst
 Rwp=3.78%, Rexp=2.05%, X²=3.39998

Parameter / Goal	Value	ESD
Ferrite/sum	0.909	0.0019
MgO/sum	0.091	0.0019

Local Parameters

/Users/stutz/Documents/ID_Exercise/U25/Unk_25.lst
 Rwp=3.78% Rexp=2.05% X²=3.39998

Phase	A	ESD(A)	B	ESD(B)	C	ESD(C)	ALPHA	ESD(ALPHA)	BETA	ESD(BETA)	GAMMA	ESD(GAMMA)
Ferrite	0.553276	0.000031	1.457555	0.000088	0.533351	0.000032						
MgO	0.421317	0.000015										

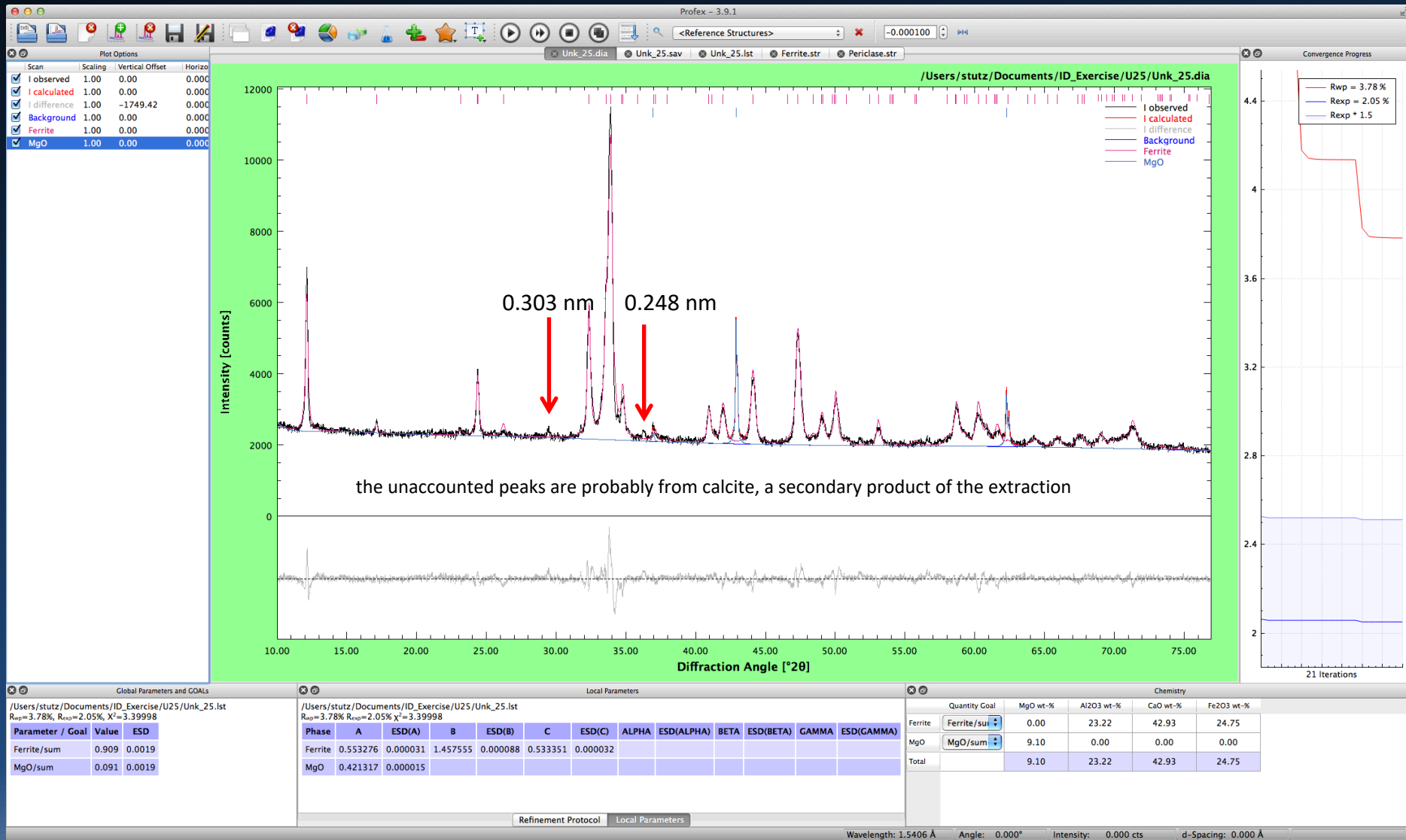
Chemistry

	Quantity	Goal	MgO wt-%	Al2O3 wt-%	CaO wt-%	Fe2O3 wt-%
Ferrite	Ferrite/sum		0.00	23.22	42.93	24.75
MgO	MgO/sum		9.10	0.00	0.00	0.00
Total			9.10	23.22	42.93	24.75

Refinement Protocol Local Parameters

Wavelength: 1.5406 Å Angle: 0.000° Intensity: 0.000 cts d-Spacing: 0.000 Å Line 0, Column 0

Look for additional phases



d-Spacing	Two-Theta	Phase	d-Spacing	Two-Theta	Phase
7.627	11.593	gypsum (100)	3.038	29.375	M1 C3S (50)
7.249	12.200	C4AF (45)	3.036	29.400	calcite (100)
5.997	14.759	bassanite (80)	3.036	29.395	mono C3S (40)
5.970	14.827	triclinic C3S (12)	3.034	29.415	m1 C3S (50)
5.953	14.869	triclinic C3S (12)	3.025	29.504	triclinic C3S (65)
5.927	14.935	triclinic C3S (12)	3.025	29.504	mono C3S (75)
5.927	14.935	mono. C3S (12)	3.011	29.645	γC2S (80)
5.610	15.784	γC2S (19)	3.002	29.736	bassanite (80)
5.107	17.350	C3Ao (10)	3.000	29.756	arcanite (77)
4.917	18.026	aphthitalite (10)	2.985	29.909	triclinic C3S (25)
4.659	19.033	thenardite (71)	2.974	30.022	triclinic C3S (18)
4.640	19.112	α' C2S (30)	2.972	30.043	M1 C3S (20)
4.316	20.561	γC2S (45)	2.968	30.084	mono C3S (12)
4.284	20.717	gypsum (100)	2.968	30.084	M1 C3S (20)
4.253	20.869	langbeinite (30)	2.965	30.115	triclinic C3S (20)
4.235	20.959	C3Ac (6)	2.961	30.157	mono C3S (25)
4.222	21.024	langbeinite (25)	2.940	30.378	aphthitalite (75)
4.188	21.197	langbeinite (16)	2.902	30.785	arcanite (100)
4.175	21.264	arcanite (28)	2.894	30.872	γC2S (25)
4.158	21.352	arcanite (23)	2.886	30.960	arcanite (53)
4.091	21.706	aphthitalite (30)	2.880	31.026	langbeinite (18)
4.079	21.770	C3Ac (12)	2.876	31.070	βC2S (21)
4.059	21.879	γ C2S (20)	2.872	31.115	gypsum (45)
3.900	22.783	αC2S (20)	2.870	31.137	α' C2S (30)
3.886	22.866	triclinic C3S (10)	2.850	31.361	anhydrite (29)
3.855	23.052	calcite (9)	2.843	31.440	calcite (2)
3.838	23.156	thenardite (17)	2.838	31.497	aphthitalite (100)
3.817	23.285	γC2S (509)	2.813	31.784	βC2S (22)
3.810	23.328	α' C2S (30)	2.813	31.784	bassanite (100)
3.799	23.397	gypsum (17)	2.810	31.819	αC2S (80)
3.764	23.617	γC2S (119)	2.790	32.053	βC2S (97)
3.744	23.745	arcanite (18)	2.788	32.077	triclinic C3S (100)
3.670	24.231	aphthitalite (20)	2.788	32.077	gypsum (10)
3.653	24.346	C4AF (16)	2.786	32.101	langbeinite (45)
3.497	25.450	anhydrite (100)	2.784	32.124	C4AF (25)
3.468	25.666	bassanite (40)	2.784	32.124	thenardite (100)
3.462	25.711	langbeinite (12)	2.782	32.148	βC2S (100)
3.424	26.002	C3Ao (11)	2.776	32.220	free lime (36)
3.385	26.307	arcanite (13)	2.775	32.231	M1 C3S (100)
3.379	26.354	γC2S (25)	2.775	32.231	langbeinite (50)
3.370	26.426	α' C2S (30)	2.773	32.255	mono C3S (85)
3.313	26.889	langbeinite (95)	2.767	32.327	triclinic C3S (70)
3.271	27.241	langbeinite (80)	2.754	32.484	triclinic C3S (65)
3.263	27.309	langbeinite (80)	2.750	32.533	γC2S (70)
3.225	27.637	langbeinite (100)	2.750	32.533	langbeinite (45)
3.180	28.036	thenardite (52)	2.747	32.569	mono C3S (45)
3.153	28.281	langbeinite (18)	2.747	32.569	M1 C3S (40)
3.114	28.643	langbeinite (18)	2.745	32.593	βC2S (83)
3.077	28.995	thenardite (55)	2.743	32.618	M1 C3S (60)
3.065	29.111	gypsum (75)	2.743	32.618	langbeinite (45)
3.056	29.198	triclinic C3S (60)	2.740	32.655	α' C2S (100)
3.045	29.306	bassanite (10)	2.737	32.691	mono C3S (75)

d-Spacing	Two-Theta	Phase	d-Spacing	Two-Theta	Phase
2.736	32.704	triclinic C3S (60)	2.268	39.709	bassanite (10)
2.717	32.939	βC2S (30)	2.230	40.415	α' C2S (30)
2.714	32.976	C3Ao (65)	2.220	40.605	αC2S (40)
2.714	32.976	bassanite (10)	2.218	40.643	gypsum (15)
2.710	33.026	αC2S (100)	2.209	40.816	anhydrite (20)
2.698	33.178	C3Ac (100)	2.205	40.893	C3Ao (20)
2.692	33.254	C3Ao (100)	2.205	40.893	arcanite (14)
2.684	33.356	gypsum (35)	2.203	40.932	C3Ac (10)
2.680	33.407	α' C2S (75)	2.196	41.068	langbeinite (12)
2.673	33.497	C4AF (35)	2.195	41.088	triclinic C3S (75)
2.647	33.836	thenardite (52)	2.189	41.206	βC2S (51)
2.644	33.875	C4AF (100)	2.184	41.304	M1 C3S (40)
2.618	34.222	triclinic C3S (60)	2.181	41.364	mono C3S (60)
2.612	34.303	triclinic C3S (90)	2.180	41.383	α' C2S (30)
2.610	34.330	βC2S (42)	2.179	41.403	triclinic C3S (17)
2.607	34.371	M1 C3S (70)	2.179	41.403	M1 C3S (40)
2.605	34.398	M1 C3S (80)	2.171	41.563	triclinic C3S (11)
2.603	34.425	mono C3S (100)	2.169	41.603	M1 C3S (10)
2.590	34.604	γC2S (14)	2.166	41.663	M1 C3S (10)
2.576	34.798	C4AF(17)	2.164	41.704	βC2S (13)
2.517	35.640	arcanite (13)	2.164	41.704	mono C3S (15)
2.514	35.684	γC2S (25)	2.163	41.724	triclinic C3S (11)
2.499	35.906	arcanite (15)	2.162	41.744	M1 C3S (10)
2.495	35.968	calcite (15)	2.136	42.276	bassanite (20)
2.494	35.980	gypsum (11)	2.109	42.844	langbeinite (18)
2.458	36.526	triclinic C3S (12)	2.105	42.930	periclase (100)
2.458	36.526	aphthitalite (10)	2.094	43.157	calcite (15)
2.455	36.572	γC2S (17)	2.093	43.188	langbeinite (20)
2.448	36.680	βC2S (12)	2.088	43.297	arcanite (25)
2.442	36.774	aphthitalite (16)	2.085	43.362	gypsum (25)
2.430	36.962	periclase (10)	2.082	43.428	arcanite (25)
2.422	37.088	arcanite (25)	2.073	43.626	gypsum (15)
2.409	37.296	βC2S (13)	2.051	44.118	C4AF(35)
2.405	37.360	free lime (100)	2.050	44.141	βC2S (14)
2.402	37.408	βC2S (18)	2.041	44.346	aphthitalite (45)
2.385	37.685	arcanite (13)	2.036	44.461	langbeinite (14)
2.374	37.866	arcanite (17)	2.026	44.692	βC2S (15)
2.360	38.100	α' C2S (30)	2.024	44.738	γC2S (13)
2.339	38.455	triclinic C3S (15)	2.020	44.832	α' C2S (30)
2.329	38.627	triclinic C3S (20)	2.019	44.855	βC2S (15)
2.329	38.627	thenardite (25)	2.017	44.902	langbeinite (20)
2.329	38.627	aphthitalite (14)	2.009	45.091	langbeinite (14)
2.328	38.644	anhydrite (20)	1.994	45.449	triclinic C3S (10)
2.325	38.696	γC2S (10)	1.982	45.740	M1 C3S (10)
2.323	38.725	M1 C3S (45)	1.981	45.764	βC2S (20)
2.319	38.800	M1 C3S (20)	1.973	45.960	mono C3S (10)
2.315	38.870	triclinic C3S (25)	1.940	46.788	αC2S (60)
2.315	38.870	mono C3S (20)	1.937	46.865	M1 C3S (10)
2.285	39.408	calcite (20)	1.933	46.968	M1 C3S (10)
2.280	39.491	βC2S (22)	1.930	47.045	α' C2S (30)
2.280	39.491	triclinic C3S (110)	1.930	47.045	mono C3S (13)
2.270	39.672	α' C2S (10)	1.928	47.097	C4AF(35)