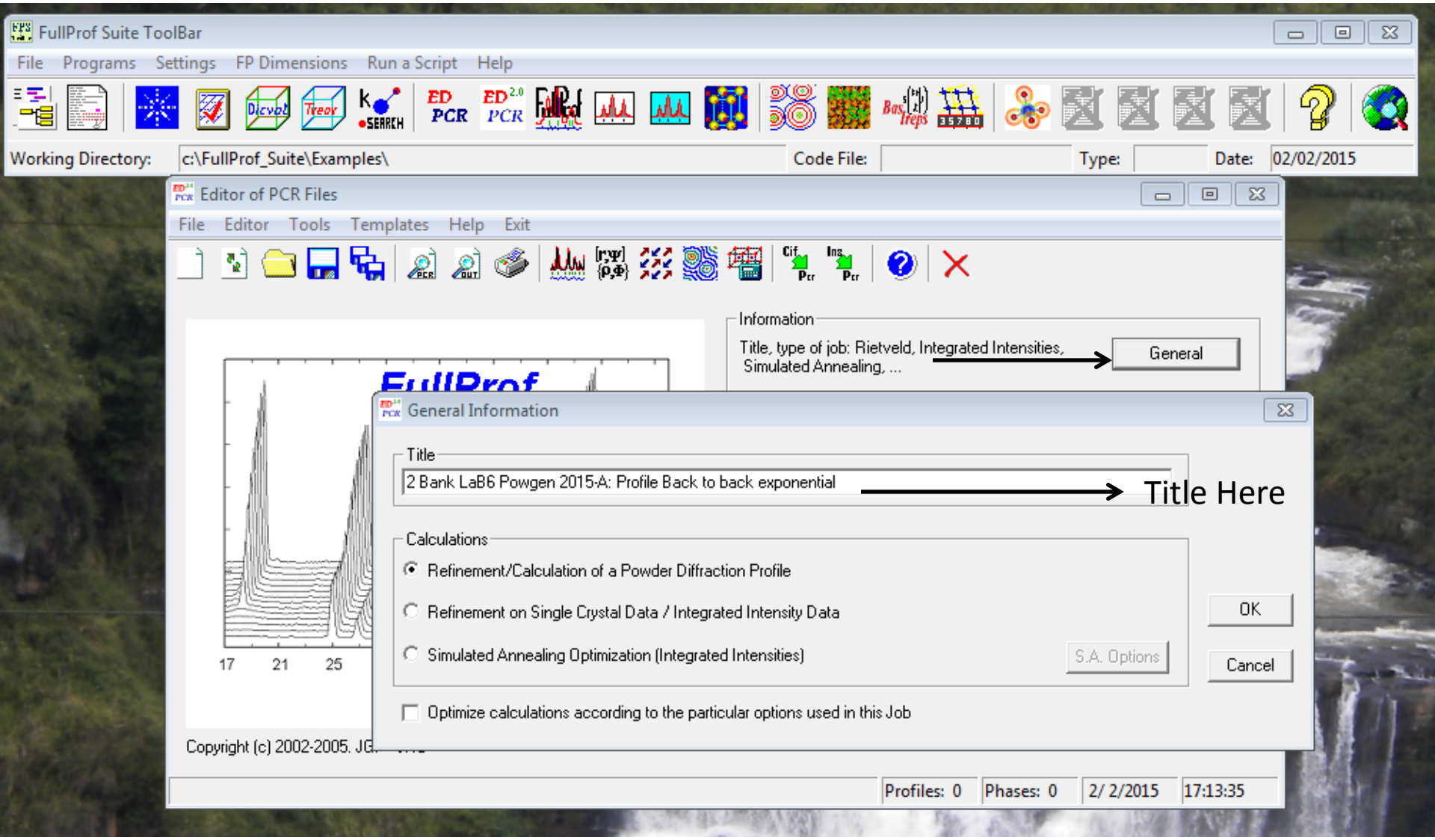
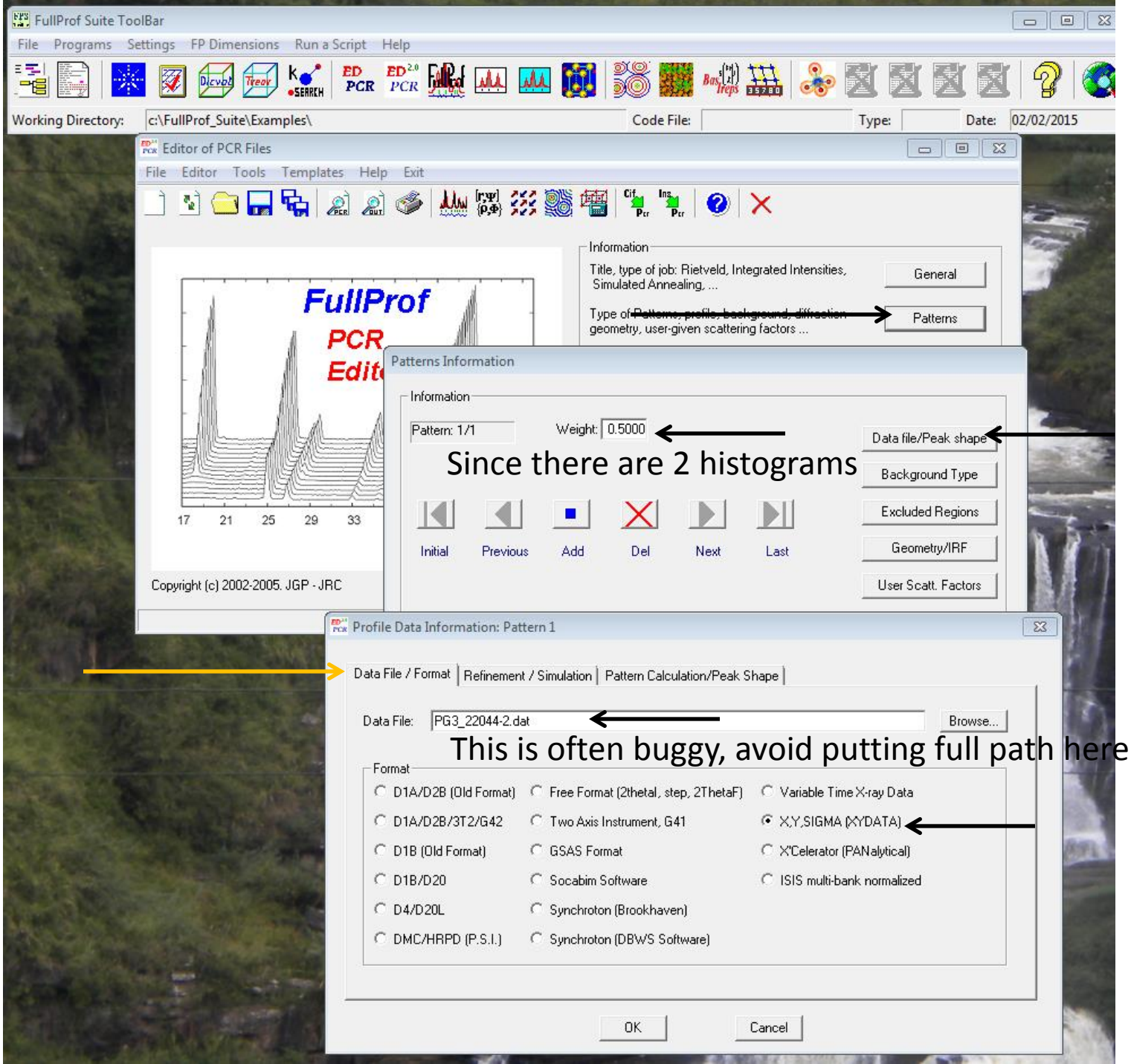
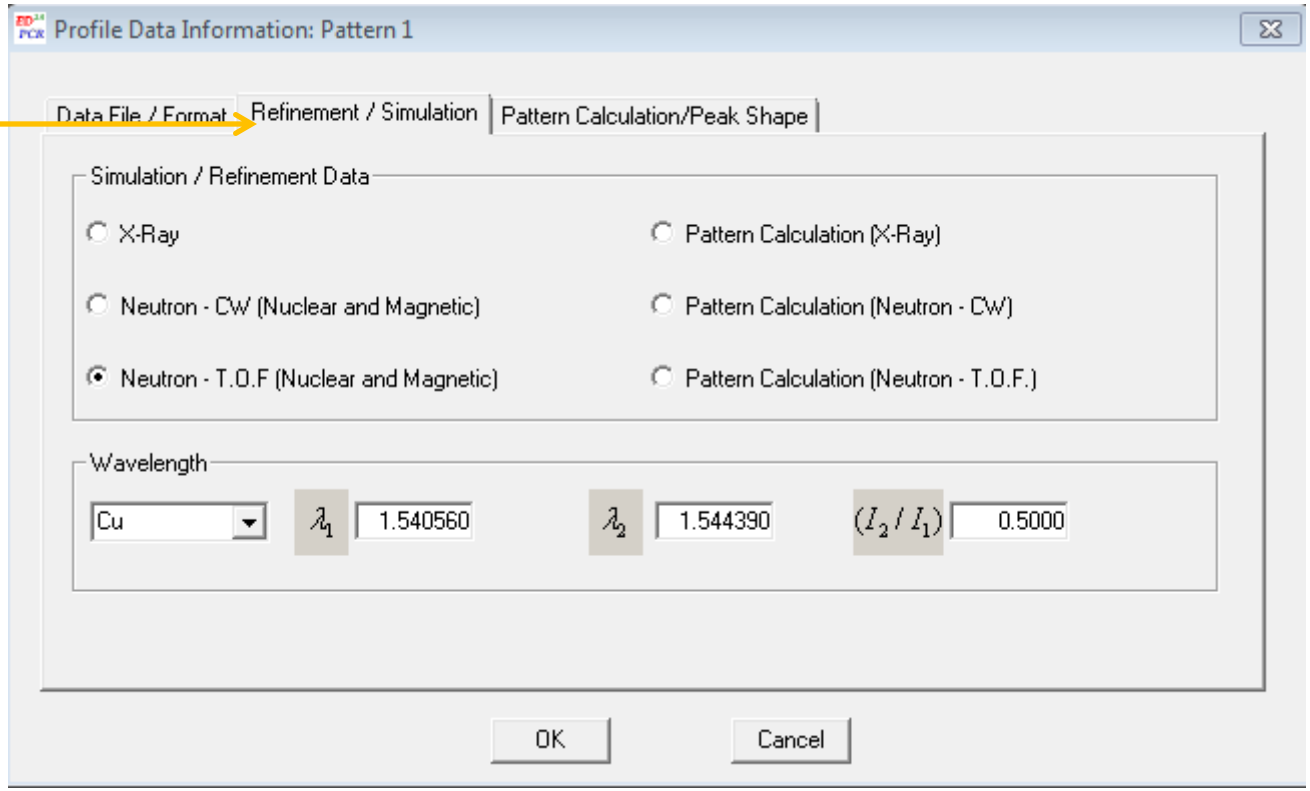
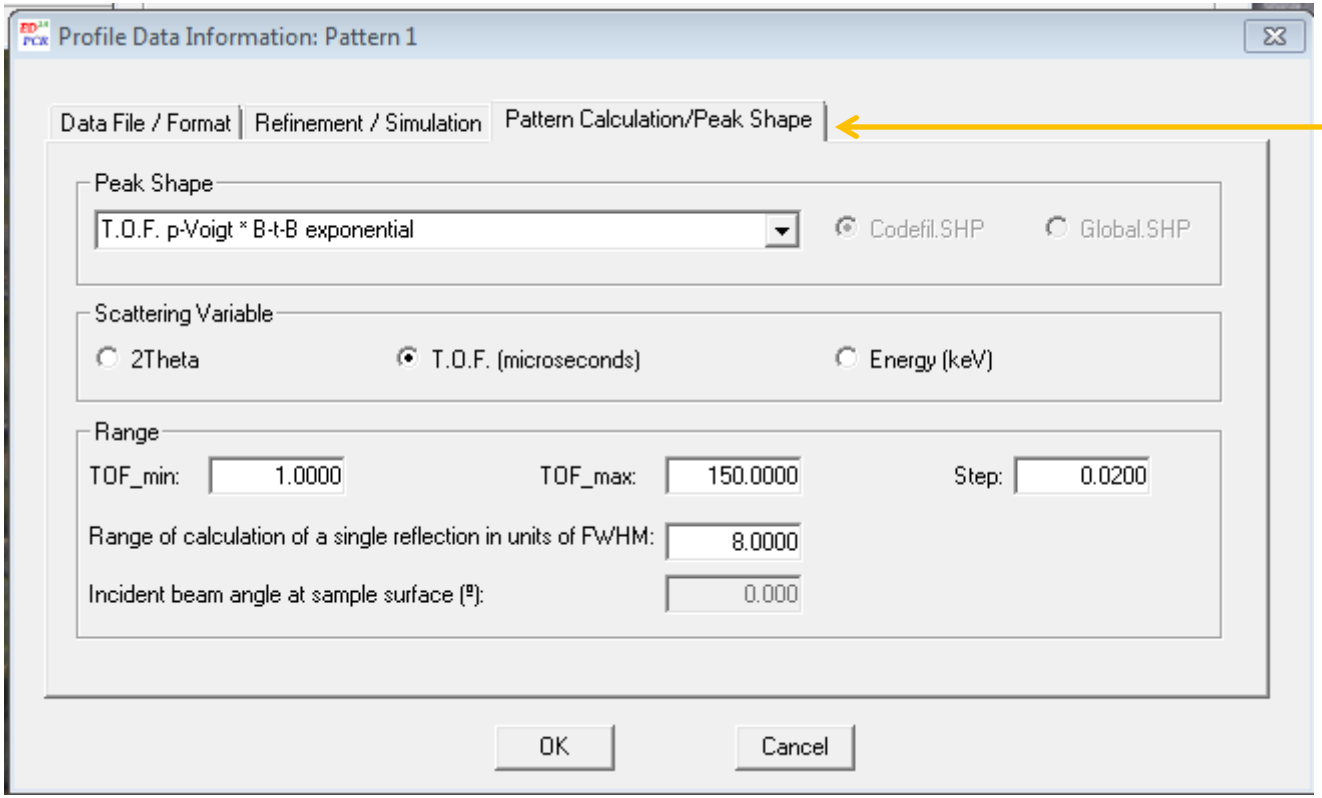
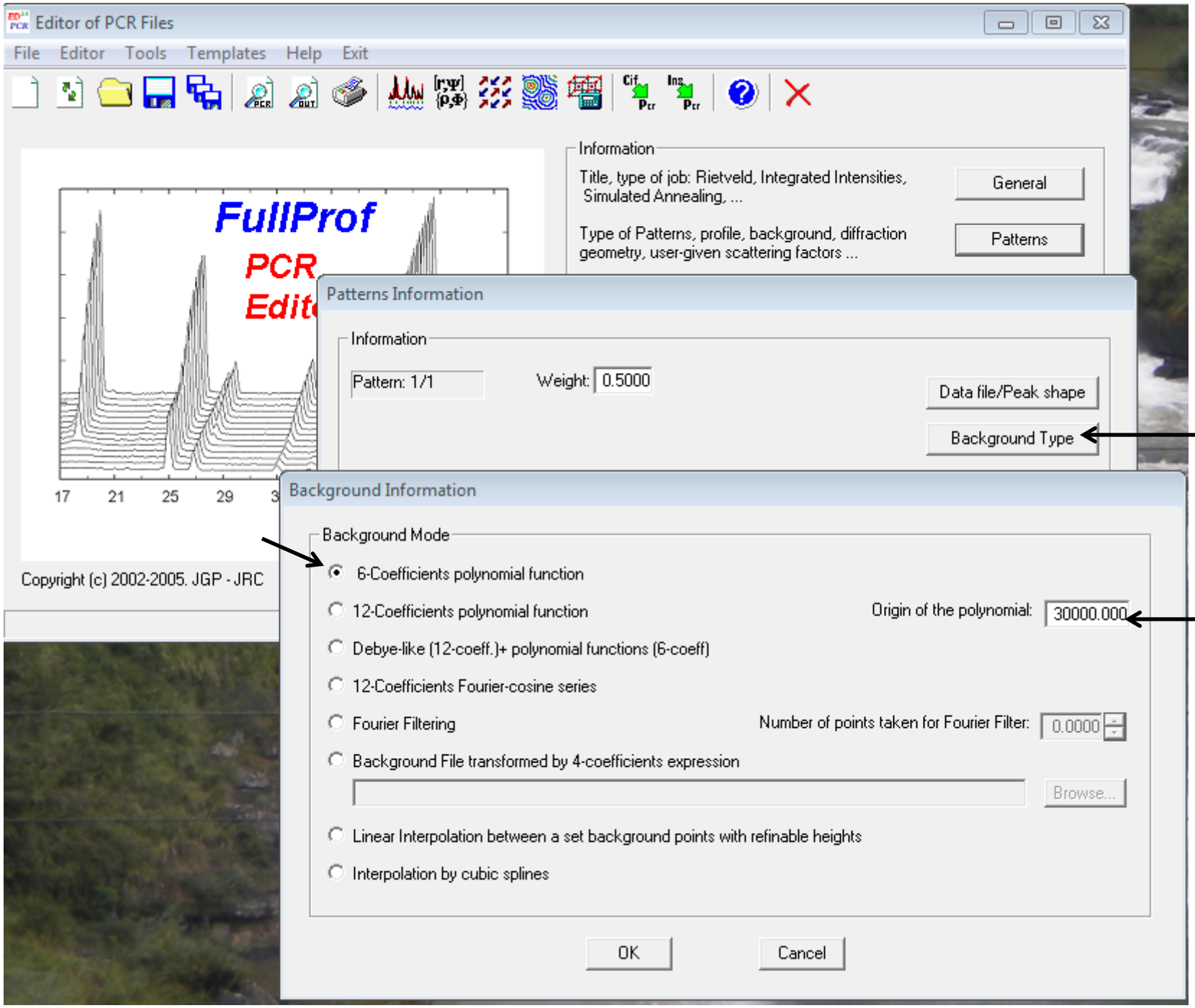
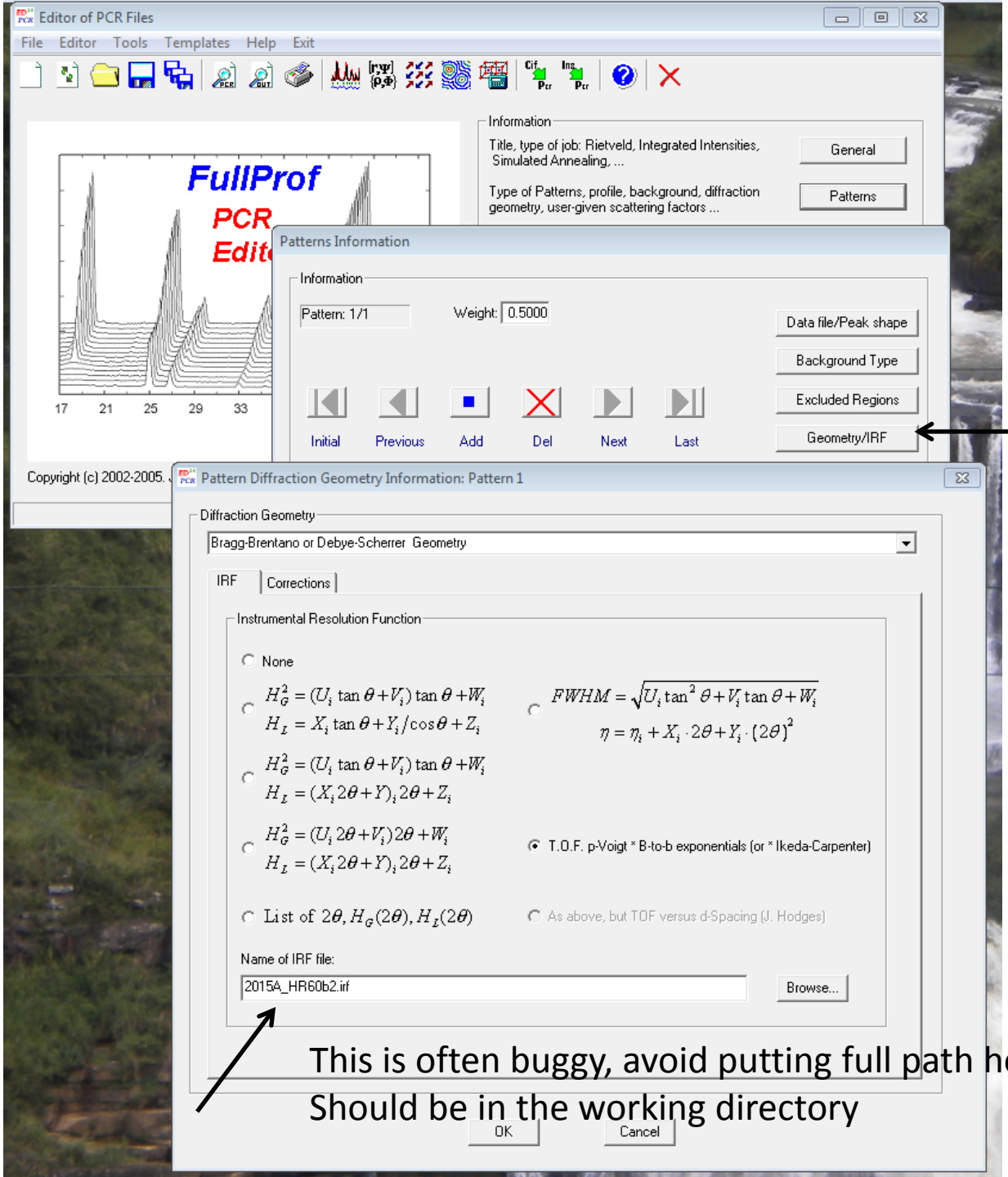

FullProf Suite ToolBar
File Programs Settings FP Dimensions Run a Script Help
Working Directory: c:\FullProf_Suite\Examples\
Code File:
Type:
Date: 02/02/2015
Editor of PCR Files
File Editor Tools Templates Help Exit
Information
Title, type of job: Rietveld, Integrated Intensities, Simulated Annealing, ...
General
FullProf
17 21 25
General Information
Title
2 Bank LaB6 Powgen 2015-A: Profile Back to back exponential
Title Here
Calculations
Refinement/Calculation of a Powder Diffraction Profile
Refinement on Single Crystal Data / Integrated Intensity Data
Simulated Annealing Optimization (Integrated Intensities)
S.A. Options
OK
Cancel
Optimize calculations according to the particular options used in this Job
Copyright (c) 2002-2005. JG
Profiles: 0
Phases: 0
2/ 2/2015
17:13:35


FullProf Suite ToolBar
File Programs Settings FP Dimensions Run a Script Help
Working Directory: c:\FullProf_Suite\Examples\
Code File:
Type:
Date: 02/02/2015
Editor of PCR Files
File Editor Tools Templates Help Exit
FullProf
PCR
Edit
17 21 25 29 33
Copyright (c) 2002-2005. JGP - JRC
Information
Title, type of job: Rietveld, Integrated Intensities, Simulated Annealing, ...
General
Type of Patterns, profile, background, diffraction geometry, user-given scattering factors ...
Patterns
Patterns Information
Information
Pattern: 1/1
Weight: 0.5000
Since there are 2 histograms
Data file/Peak shape
Background Type
Excluded Regions
Geometry/IRF
User Scatt. Factors
Initial
Previous
Add
Del
Next
Last
Profile Data Information: Pattern 1
Data File / Format
Refinement / Simulation
Pattern Calculation/Peak Shape
Data File: PG3_22044-2.dat
Browse...
This is often buggy, avoid putting full path here
Format
D1A/D2B (Old Format)
Free Format (2thetal, step, 2ThetaF)
Variable Time X-ray Data
D1A/D2B/3T2/G42
Two Axis Instrument, G41
X,Y,SIGMA (XYDATA)
D1B (Old Format)
GSAS Format
X'Celerator (PANalytical)
D1B/D20
Socabim Software
ISIS multi-bank normalized
D4/D20L
Synchroton (Brookhaven)
DMC/HRPD (P.S.I.)
Synchroton (DBWS Software)
OK
Cancel

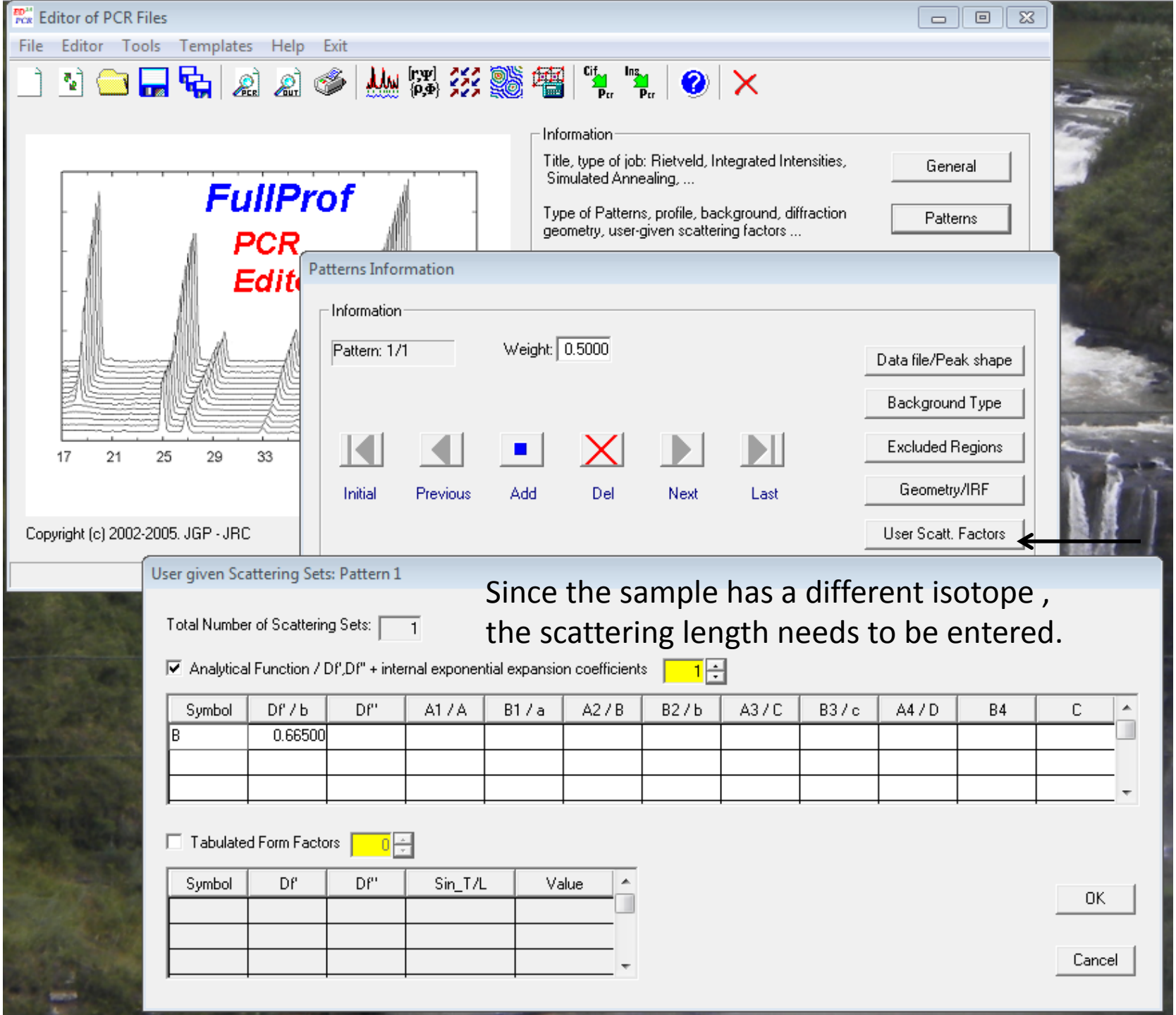

Profile Data Information: Pattern 1
Data File / Format
Refinement / Simulation
Pattern Calculation/Peak Shape
Simulation / Refinement Data
X-Ray
Pattern Calculation (X-Ray)
Neutron - CW (Nuclear and Magnetic)
Pattern Calculation (Neutron - CW)
Neutron - T.O.F (Nuclear and Magnetic)
Pattern Calculation (Neutron - T.O.F.)
Wavelength
Cu
λ1
1.540560
λ2
1.544390
(I2 / I1)
0.5000
OK
Cancel

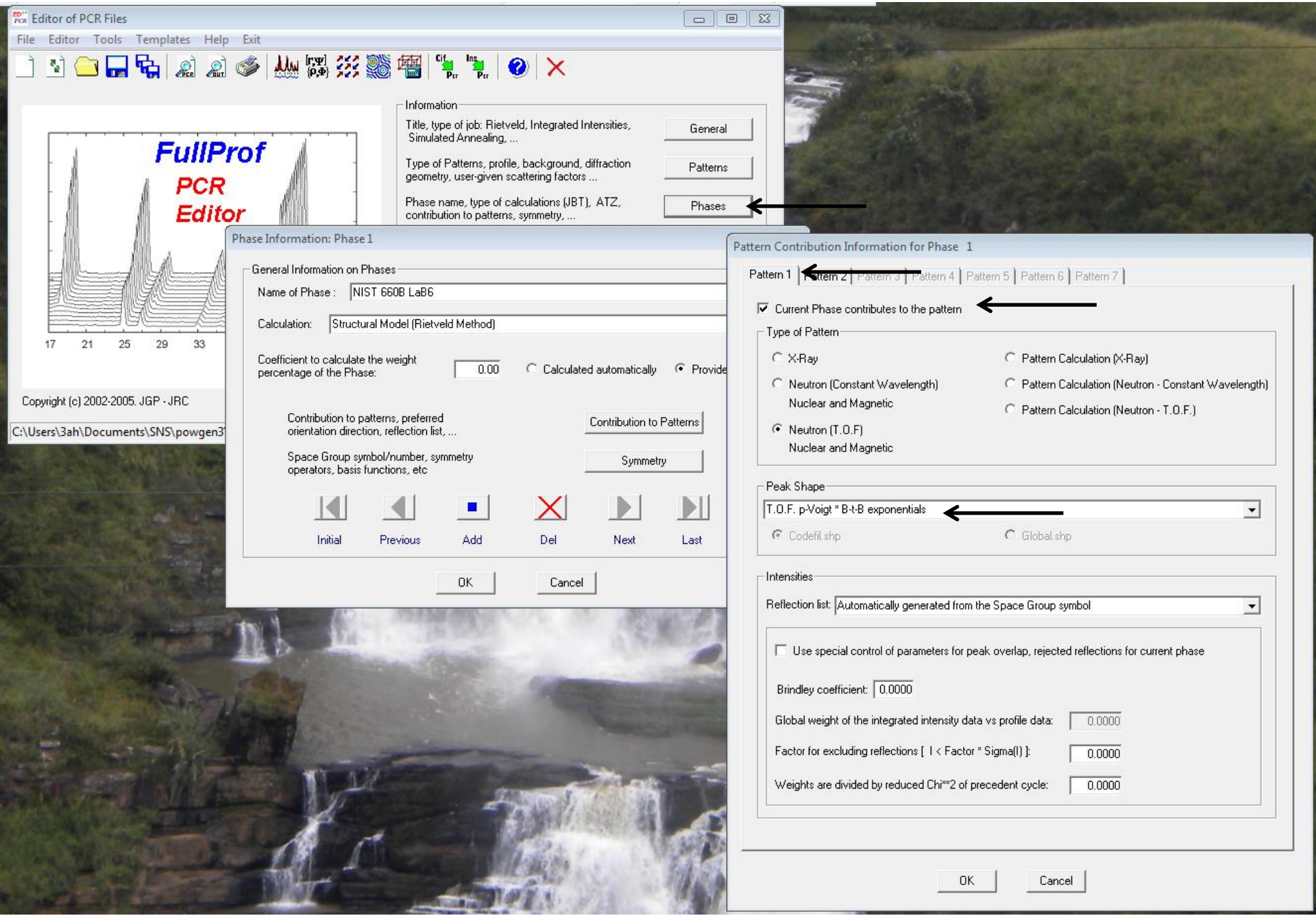

Profile Data Information: Pattern 1
Data File / Format
Refinement / Simulation
Pattern Calculation/Peak Shape
Peak Shape
T.O.F. p-Voigt * B-t-B exponential
Codefil.SHP
Global.SHP
Scattering Variable
2Theta
T.O.F. (microseconds)
Energy (keV)
Range
TOF_min:
1.0000
TOF_max:
150.0000
Step:
0.0200
Range of calculation of a single reflection in units of FWHM:
8.0000
Incident beam angle at sample surface (º):
0.000
OK
Cancel

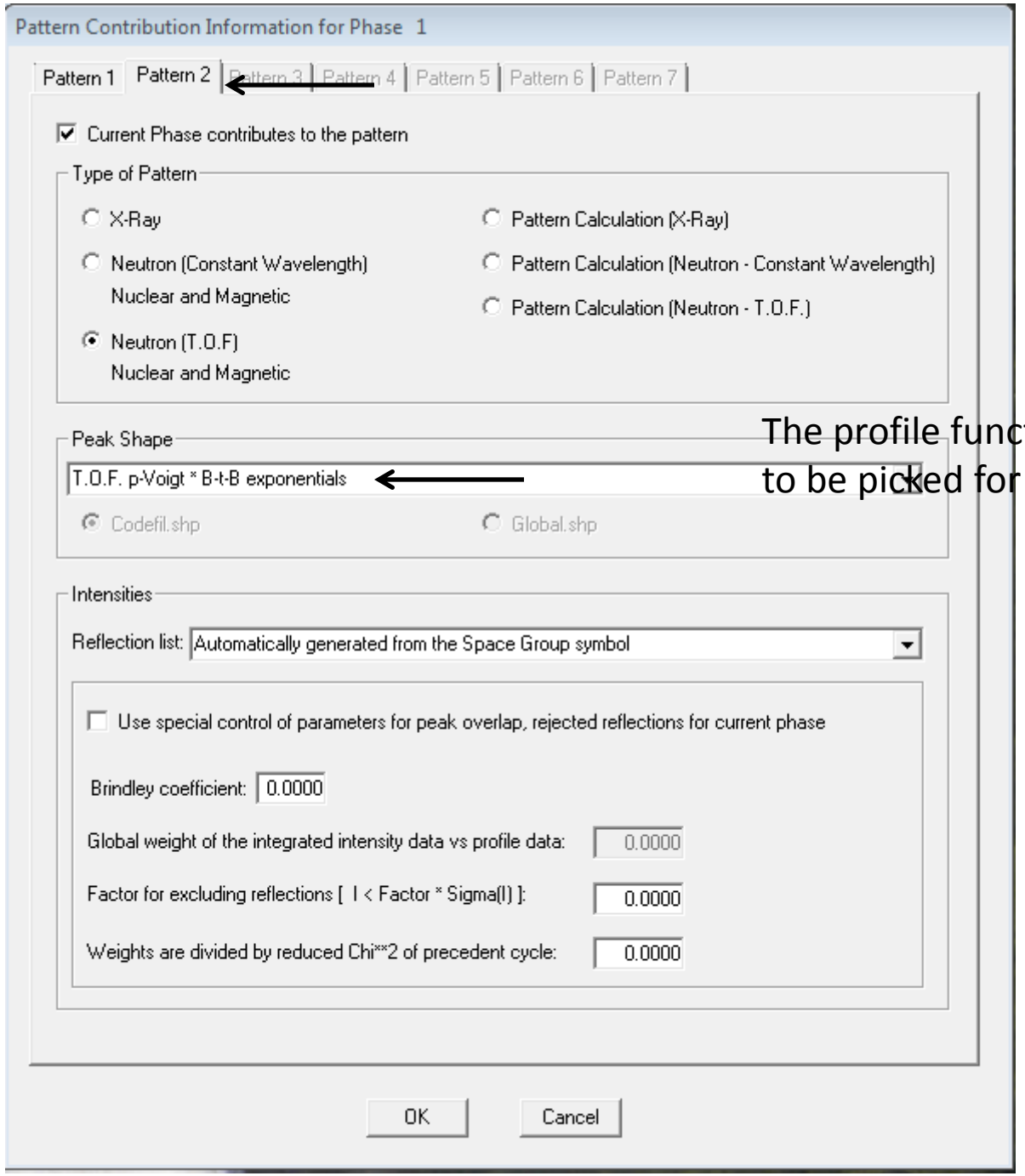

Editor of PCR Files
File Editor Tools Templates Help Exit
FullProf
PCR
Edit
17 21 25 29
Copyright (c) 2002-2005. JGP - JRC
Information
Title, type of job: Rietveld, Integrated Intensities, Simulated Annealing, ...
General
Type of Patterns, profile, background, diffraction geometry, user-given scattering factors ...
Patterns
Patterns Information
Information
Pattern: 1/1
Weight: 0.5000
Data file/Peak shape
Background Type
Background Information
Background Mode
6-Coefficients polynomial function
12-Coefficients polynomial function
Origin of the polynomial: 30000.000
Debye-like (12-coeff.)+ polynomial functions (6-coeff)
12-Coefficients Fourier-cosine series
Fourier Filtering
Number of points taken for Fourier Filter: 0.0000
Background File transformed by 4-coefficients expression
Browse...
Linear Interpolation between a set background points with refinable heights
Interpolation by cubic splines
OK
Cancel



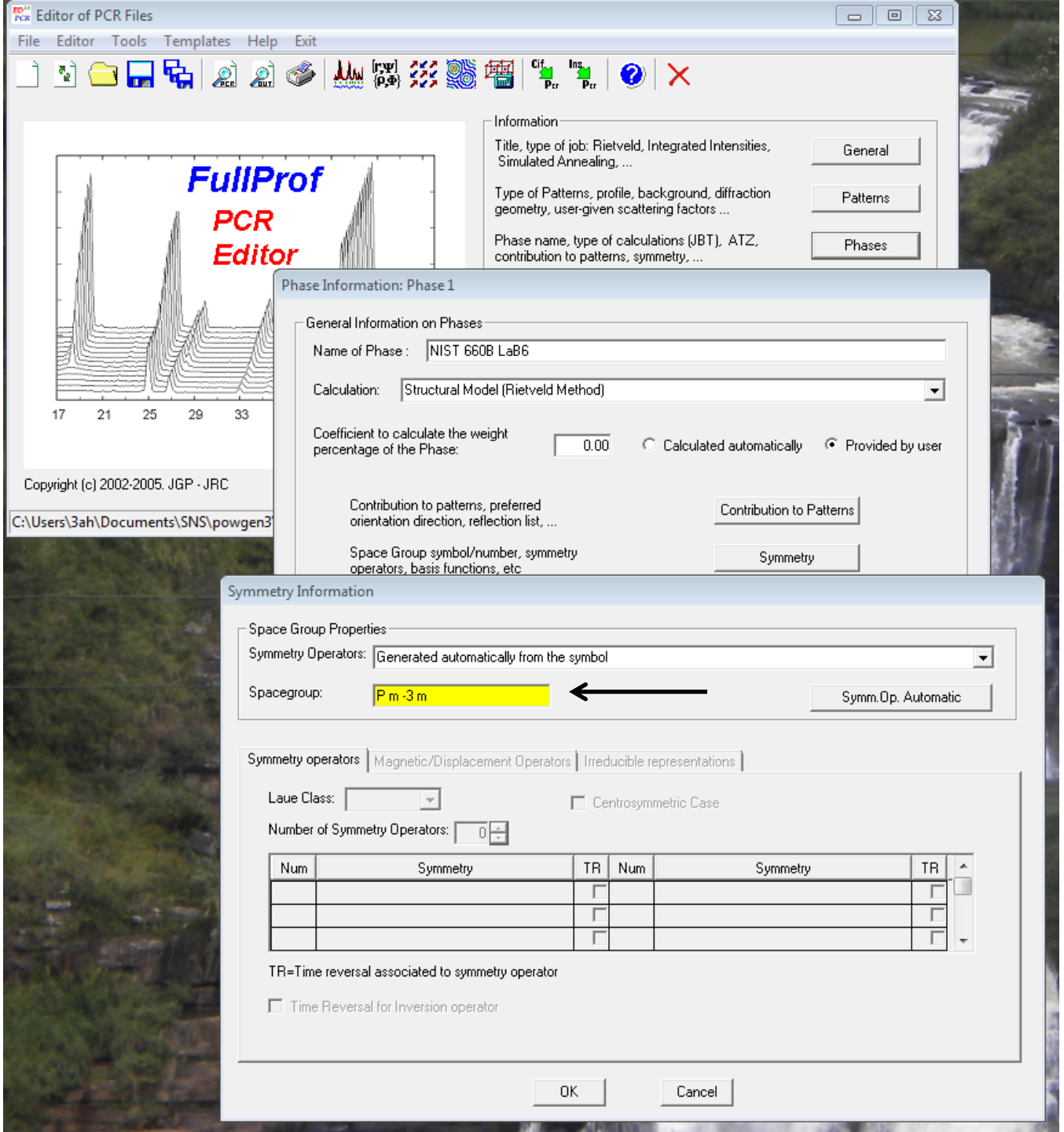
This is often buggy, avoid putting full path here. The irf file Should be in the working directory

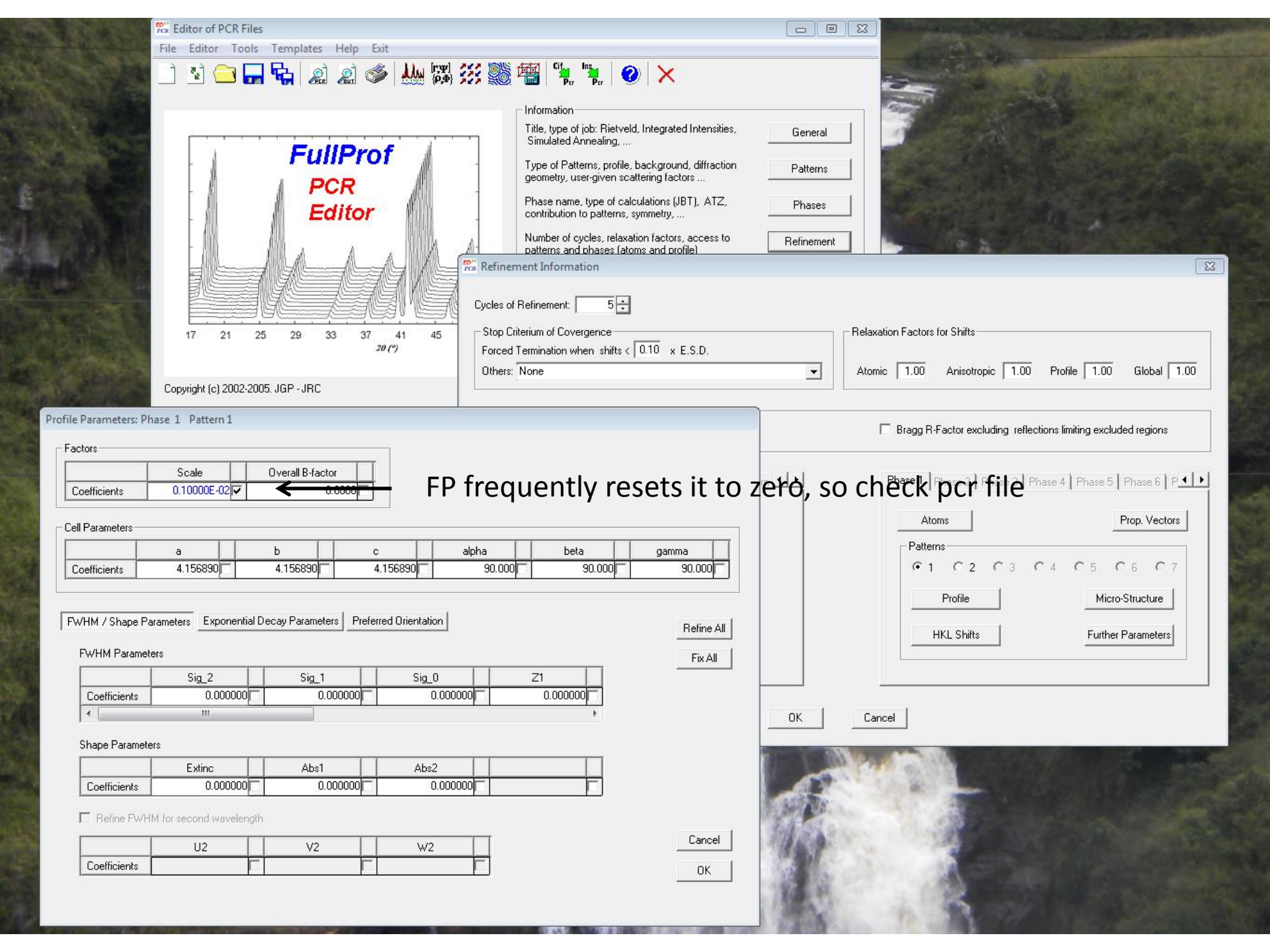

Editor of PCR Files
File Editor Tools Templates Help Exit
FullProf
PCR
17 21 25 29 33
Copyright (c) 2002-2005. JGP - JRC
Information
Title, type of job: Rietveld, Integrated Intensities, Simulated Annealing, ...
General
Type of Patterns, profile, background, diffraction geometry, user-given scattering factors ...
Patterns
Patterns Information
Information
Pattern: 1/1
Weight: 0.5000
Data file/Peak shape
Background Type
Excluded Regions
Geometry/IRF
User Scatt. Factors
Initial Previous Add Del Next Last
User given Scattering Sets: Pattern 1
Total Number of Scattering Sets: 1
Analytical Function / Df',Df'' + internal exponential expansion coefficients 1
Symbol Df' / b Df'' A1 / A B1 / a A2 / B B2 / b A3 / C B3 / c A4 / D B4 C
B 0.66500
Tabulated Form Factors 0
Symbol Df' Df'' Sin_T/L Value
OK
Cancel
Since the sample has a different isotope , the scattering length needs to be entered.

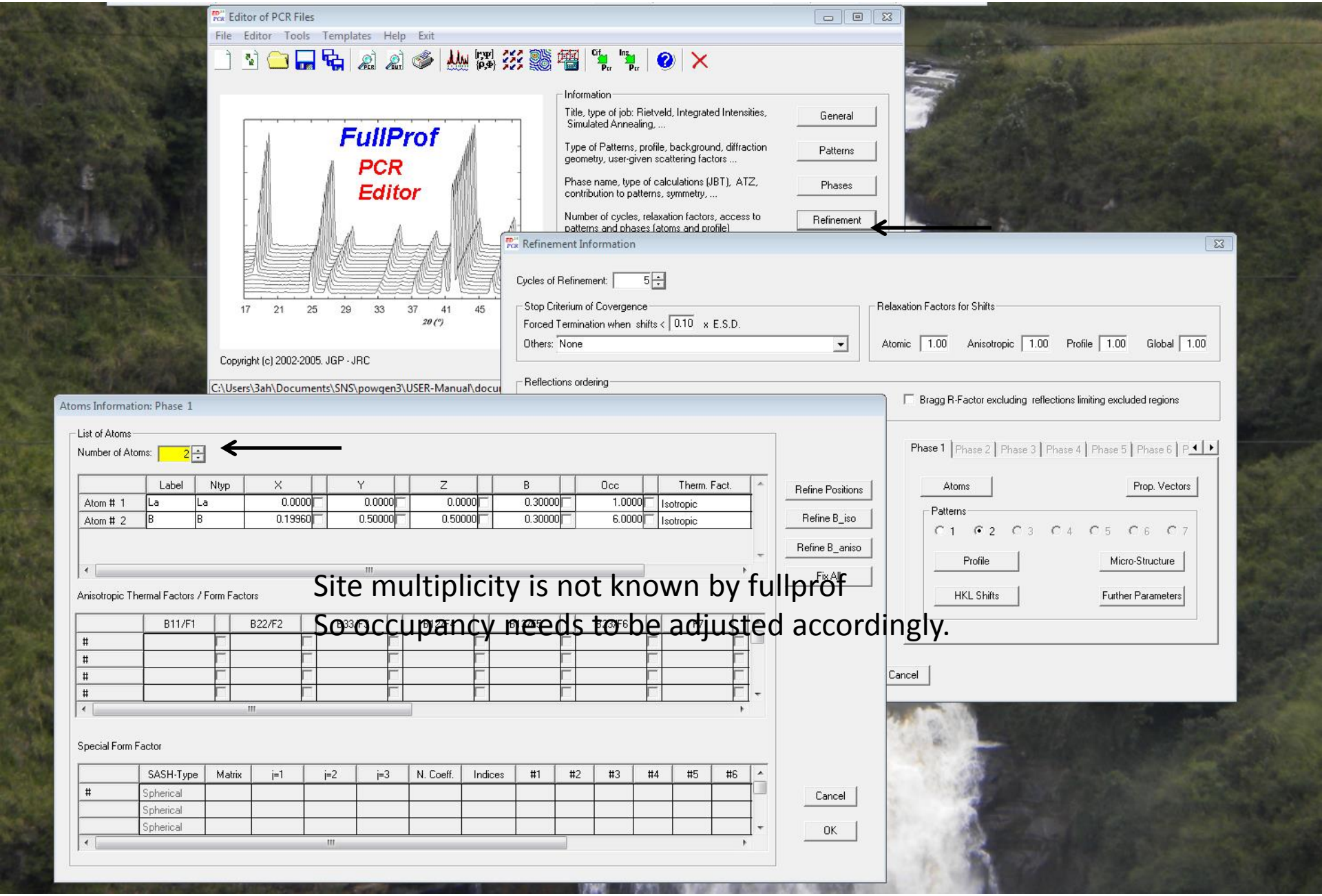

Editor of PCR Files
File Editor Tools Templates Help Exit
FullProf
PCR
Editor
17 21 25 29 33
Copyright (c) 2002-2005. JGP - JRC
C:\Users\3ah\Documents\SNS\powgen3
Information
Title, type of job: Rietveld, Integrated Intensities, Simulated Annealing, ...
General
Type of Patterns, profile, background, diffraction geometry, user-given scattering factors ...
Patterns
Phase name, type of calculations (JBT), ATZ, contribution to patterns, symmetry, ...
Phases
Phase Information: Phase 1
General Information on Phases
Name of Phase : NIST 660B LaB6
Calculation: Structural Model (Rietveld Method)
Coefficient to calculate the weight percentage of the Phase: 0.00
Calculated automatically
Provide
Contribution to patterns, preferred orientation direction, reflection list, ...
Contribution to Patterns
Space Group symbol/number, symmetry operators, basis functions, etc
Symmetry
Initial Previous Add Del Next Last
OK Cancel
Pattern Contribution Information for Phase 1
Pattern 1 Pattern 2 Pattern 3 Pattern 4 Pattern 5 Pattern 6 Pattern 7
Current Phase contributes to the pattern
Type of Pattern
X-Ray
Neutron (Constant Wavelength) Nuclear and Magnetic
Neutron (T.O.F) Nuclear and Magnetic
Pattern Calculation (X-Ray)
Pattern Calculation (Neutron - Constant Wavelength)
Pattern Calculation (Neutron - T.O.F.)
Peak Shape
T.O.F. p-Voigt * B-t-B exponentials
Codefil.shp
Global.shp
Intensities
Reflection list: Automatically generated from the Space Group symbol
Use special control of parameters for peak overlap, rejected reflections for current phase
Brindley coefficient: 0.0000
Global weight of the integrated intensity data vs profile data: 0.0000
Factor for excluding reflections [I < Factor * Sigma(I)]: 0.0000
Weights are divided by reduced Chi**2 of precedent cycle: 0.0000
OK Cancel



The profile function has to be picked for all histograms

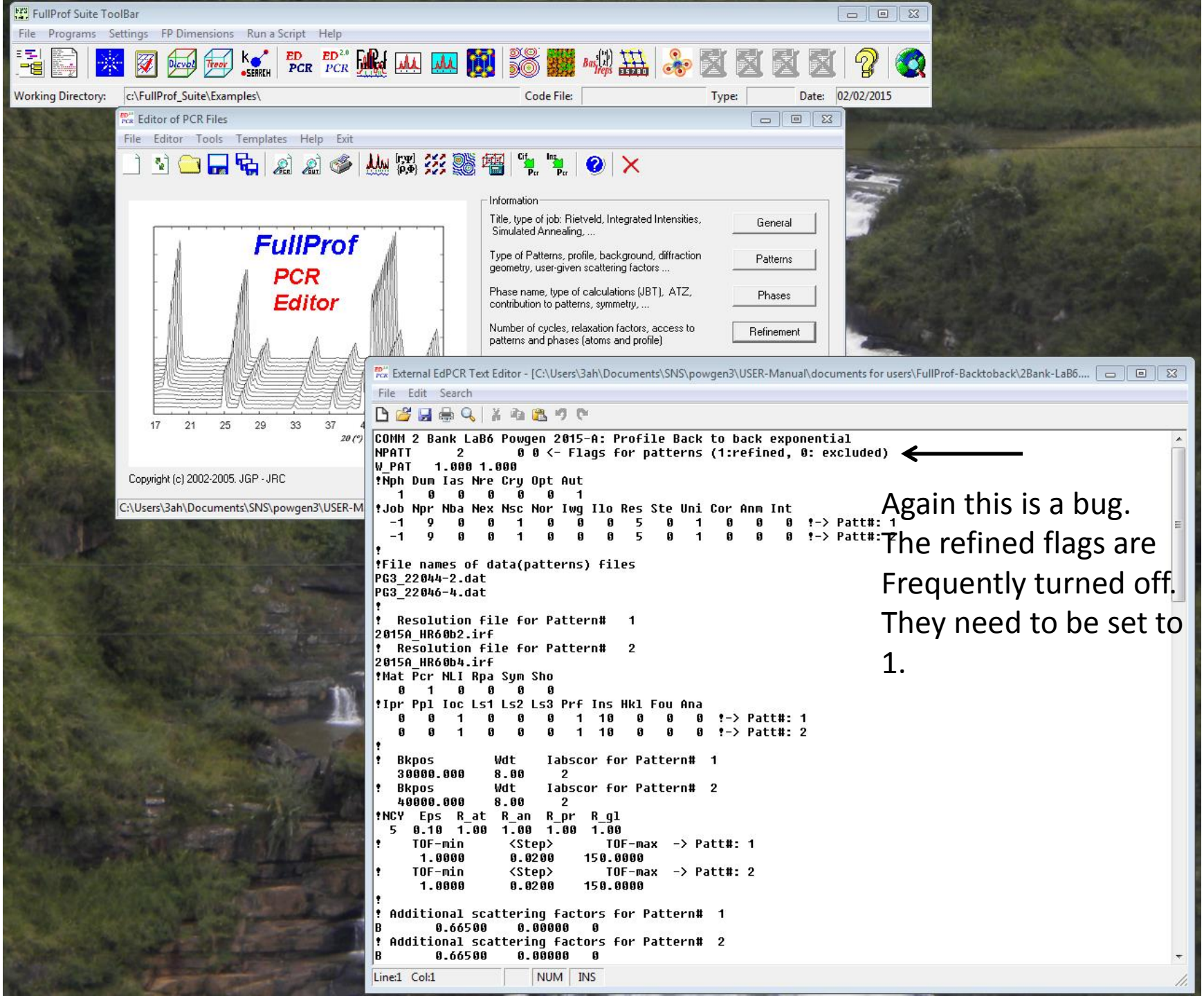

Editor of PCR Files
File Editor Tools Templates Help Exit
FullProf
PCR
Editor
17 21 25 29 33
Copyright (c) 2002-2005. JGP - JRC
C:\Users\3ah\Documents\SNS\powgen3
Information
Title, type of job: Rietveld, Integrated Intensities, Simulated Annealing, ...
General
Type of Patterns, profile, background, diffraction geometry, user-given scattering factors ...
Patterns
Phase name, type of calculations (JBT), ATZ, contribution to patterns, symmetry, ...
Phases
Phase Information: Phase 1
General Information on Phases
Name of Phase : NIST 660B LaB6
Calculation: Structural Model (Rietveld Method)
Coefficient to calculate the weight percentage of the Phase: 0.00
Calculated automatically
Provided by user
Contribution to patterns, preferred orientation direction, reflection list, ...
Contribution to Patterns
Space Group symbol/number, symmetry operators, basis functions, etc
Symmetry
Symmetry Information
Space Group Properties
Symmetry Operators: Generated automatically from the symbol
Spacegroup: P m -3 m
Symm.Op. Automatic
Symmetry operators
Magnetic/Displacement Operators
Irreducible representations
Laue Class:
Centrosymmetric Case
Number of Symmetry Operators: 0
Num Symmetry TR Num Symmetry TR
TR=Time reversal associated to symmetry operator
Time Reversal for Inversion operator
OK
Cancel

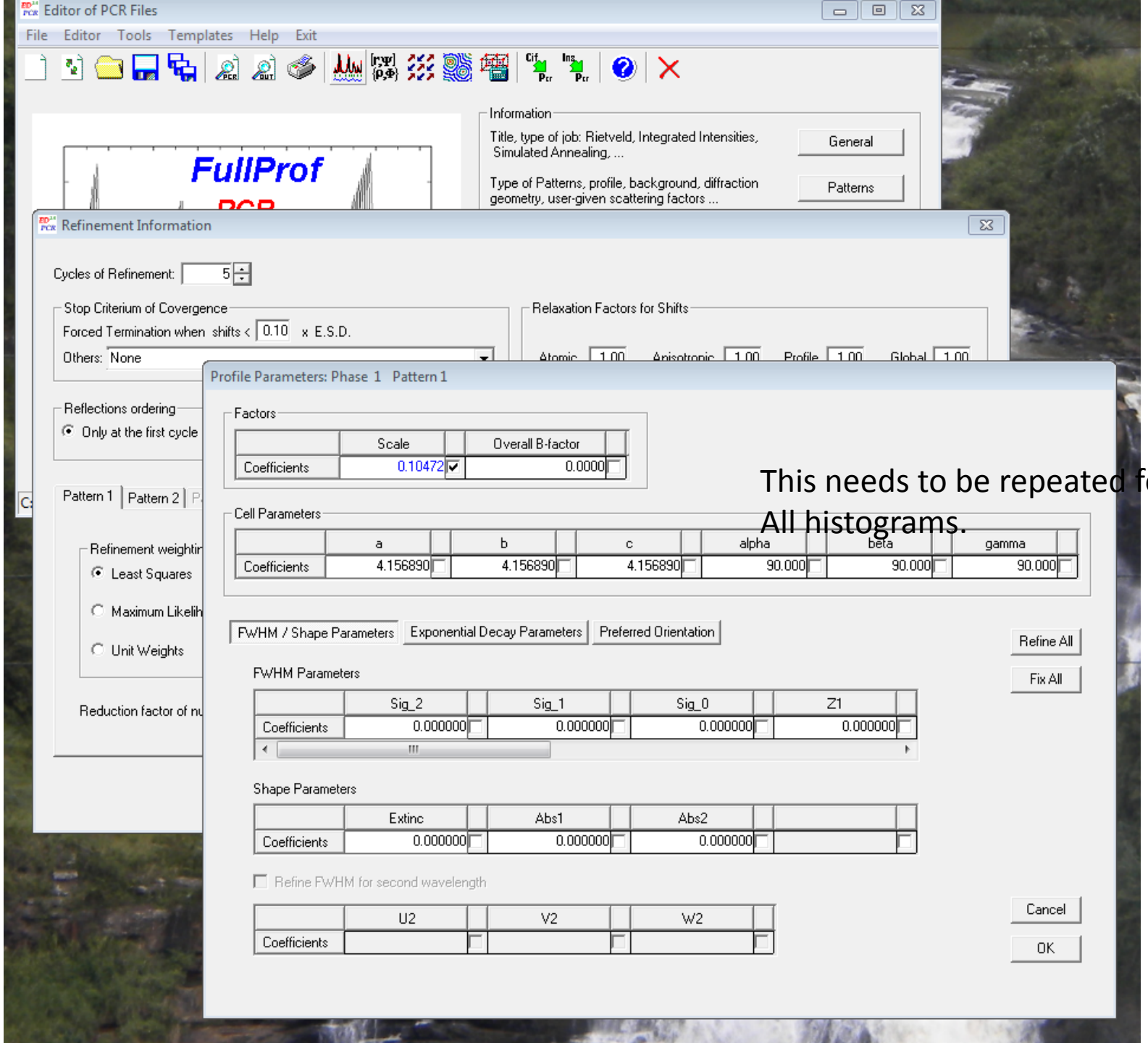

Editor of PCR Files
File Editor Tools Templates Help Exit
FullProf
PCR
Editor
17 21 25 29 33 37 41 45
2θ (°)
Information
Title, type of job: Rietveld, Integrated Intensities, Simulated Annealing, ...
General
Type of Patterns, profile, background, diffraction geometry, user-given scattering factors ...
Patterns
Phase name, type of calculations (JBT), ATZ, contribution to patterns, symmetry, ...
Phases
Number of cycles, relaxation factors, access to patterns and phases (atoms and profile)
Refinement
Copyright (c) 2002-2005. JGP - JRC
Refinement Information
Cycles of Refinement: 5
Stop Criterium of Covergence
Forced Termination when shifts < 0.10 x E.S.D.
Others: None
Relaxation Factors for Shifts
Atomic 1.00 Anisotropic 1.00 Profile 1.00 Global 1.00
Bragg R-Factor excluding reflections limiting excluded regions
Phase 1 Phase 2 Phase 3 Phase 4 Phase 5 Phase 6
Atoms
Prop. Vectors
Patterns
1 2 3 4 5 6 7
Profile
Micro-Structure
HKL Shifts
Further Parameters
OK
Cancel
Profile Parameters: Phase 1 Pattern 1
Factors
Scale
Overall B-factor
Coefficients 0.10000E-02
FP frequently resets it to zero, so check pcr file
Cell Parameters
a b c alpha beta gamma
Coefficients 4.156890 4.156890 4.156890 90.000 90.000 90.000
FWHM / Shape Parameters
Exponential Decay Parameters
Preferred Orientation
Refine All
Fix All
FWHM Parameters
Sig_2 Sig_1 Sig_0 Z1
Coefficients 0.000000 0.000000 0.000000 0.000000
Shape Parameters
Extinc Abs1 Abs2
Coefficients 0.000000 0.000000 0.000000
Refine FWHM for second wavelength
U2 V2 W2
Coefficients
Cancel
OK



Site multiplicity is not known by fullprof

So occupancy needs to be adjusted accordingly.


FullProf Suite ToolBar
File Programs Settings FP Dimensions Run a Script Help
Working Directory: c:\FullProf_Suite\Examples\
Code File:
Type:
Date: 02/02/2015
Editor of PCR Files
File Editor Tools Templates Help Exit
FullProf
PCR
Editor
Information
Title, type of job: Rietveld, Integrated Intensities, Simulated Annealing, ...
General
Type of Patterns, profile, background, diffraction geometry, user-given scattering factors ...
Patterns
Phase name, type of calculations (JBT), ATZ, contribution to patterns, symmetry, ...
Phases
Number of cycles, relaxation factors, access to patterns and phases (atoms and profile)
Refinement
Copyright (c) 2002-2005. JGP - JRC
C:\Users\3ah\Documents\SNS\powgen3\USER-M
External EdPCR Text Editor - [C:\Users\3ah\Documents\SNS\powgen3\USER-Manual\documents for users\FullProf-Backtoback\2Bank-LaB6....
File Edit Search
COMM 2 Bank LaB6 Powgen 2015-A: Profile Back to back exponential
NPATT 2 0 0 <- Flags for patterns (1:refined, 0: excluded)
W_PAT 1.000 1.000
!Nph Dum Ias Nre Cry Opt Aut
1 0 0 0 0 0 1
!Job Npr Nba Nex Nsc Nor Iwg Ilo Res Ste Uni Cor Anm Int
-1 9 0 0 1 0 0 0 5 0 1 0 0 0 !-> Patt#: 1
-1 9 0 0 1 0 0 0 5 0 1 0 0 0 !-> Patt#: 2
!
!File names of data(patterns) files
PG3_22044-2.dat
PG3_22046-4.dat
!
! Resolution file for Pattern# 1
2015A_HR60b2.irf
! Resolution file for Pattern# 2
2015A_HR60b4.irf
!Mat Pcr NLI Rpa Sym Sho
0 1 0 0 0 0
!Ipr Ppl Ioc Ls1 Ls2 Ls3 Prf Ins Hkl Fou Ana
0 0 1 0 0 0 1 10 0 0 0 !-> Patt#: 1
0 0 1 0 0 0 1 10 0 0 0 !-> Patt#: 2
!
! Bkpos Wdt Iabscor for Pattern# 1
30000.000 8.00 2
! Bkpos Wdt Iabscor for Pattern# 2
40000.000 8.00 2
!NCY Eps R_at R_an R_pr R_gl
5 0.10 1.00 1.00 1.00 1.00
! TOF-min <Step> TOF-max -> Patt#: 1
1.0000 0.0200 150.0000
! TOF-min <Step> TOF-max -> Patt#: 2
1.0000 0.0200 150.0000
!
! Additional scattering factors for Pattern# 1
B 0.66500 0.00000 0
! Additional scattering factors for Pattern# 2
B 0.66500 0.00000 0
Line:1 Col:1
NUM INS
Again this is a bug.
The refined flags are
Frequently turned off.
They need to be set to
1.

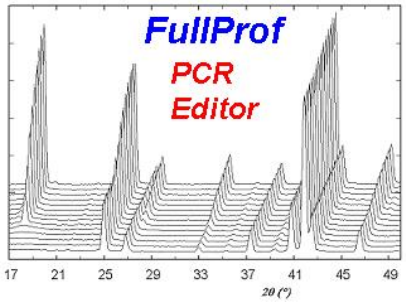

Editor of PCR Files
File Editor Tools Templates Help Exit
FullProf
Information
Title, type of job: Rietveld, Integrated Intensities, Simulated Annealing, ...
General
Type of Patterns, profile, background, diffraction geometry, user-given scattering factors ...
Patterns
Refinement Information
Cycles of Refinement: 5
Stop Criterium of Covergence
Forced Termination when shifts < 0.10 x E.S.D.
Others: None
Relaxation Factors for Shifts
Atomic 1.00 Anisotropic 1.00 Profile 1.00 Global 1.00
Reflections ordering
Only at the first cycle
Pattern 1 Pattern 2
Refinement weightir
Least Squares
Maximum Likelih
Unit Weights
Reduction factor of nu
Profile Parameters: Phase 1 Pattern 1
Factors
Scale
Overall B-factor
Coefficients 0.10472 0.0000
Cell Parameters
a b c alpha beta gamma
Coefficients 4.156890 4.156890 4.156890 90.000 90.000 90.000
FWHM / Shape Parameters
Exponential Decay Parameters
Preferred Orientation
Refine All
Fix All
FWHM Parameters
Sig_2 Sig_1 Sig_0 Z1
Coefficients 0.000000 0.000000 0.000000 0.000000
Shape Parameters
Extinc Abs1 Abs2
Coefficients 0.000000 0.000000 0.000000
Refine FWHM for second wavelength
U2 V2 W2
Coefficients
Cancel
OK
This needs to be repeated for
All histograms.

Run a Script Help

Code File: Type: Date: 02/02/2015

Editor of PCR Files

File Editor Tools Templates Help Exit



Information

Title, type of job: Rietveld, Integrated Intensities, Simulated Annealing, ... — General

Type of Patterns, profile, background, diffraction geometry, user-given scattering factors ... — Patterns

Phase name, type of calculations (JBT), ATZ, contribution to patterns, symmetry, ... — Phases

Number of cycles, relaxation factors, access to patterns and phases (atoms and profile) — Refinement

Constraints definitions, adding, deleting, modifying... — Constraints

Fixing range of parameters, distances, angles, magnetic moments and linear restraints — Box/Restraints

Output options for patterns and phases: Reflection lists, Fourier, distances, BVS... — Output

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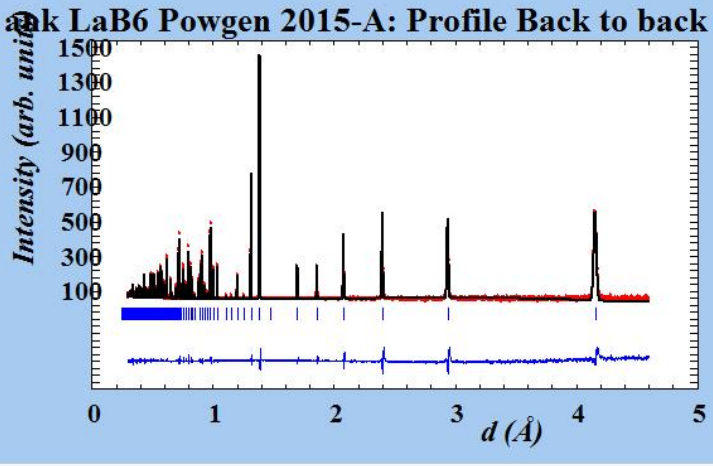
C:\Users\3ah\Documents\SNS\pow

WinPLOTR [CDIFX UMR6226 Rennes / ILL Grenoble]

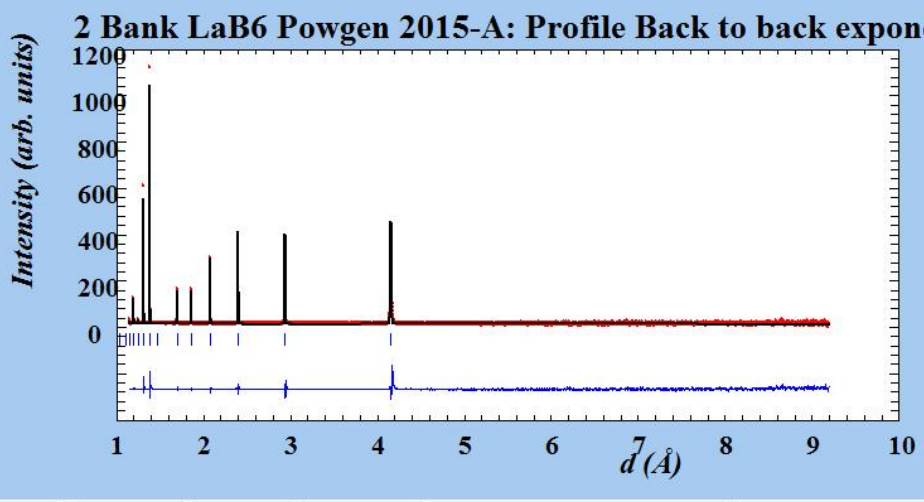
File Plot Options Points Selection X space Calculations Rietveld plot options Text External applications Tools Help



02-02-20 17:41 NUM X = Y =

WinPLOTR [CDIFX UMR6226 Rennes / ILL Grenoble]

File Plot Options Points Selection X space Calculations Rietveld plot options Text External applications Tools Help



02-02-2015 17:41 NUM X = Y =

In TOF there is often high density of reflections at high Q.
If you get an error that you have too many reflection, you might
Need to change some dimensions. The following numbers should
work. If you continue to get this error you might need to exclude parts of the
Low d data.