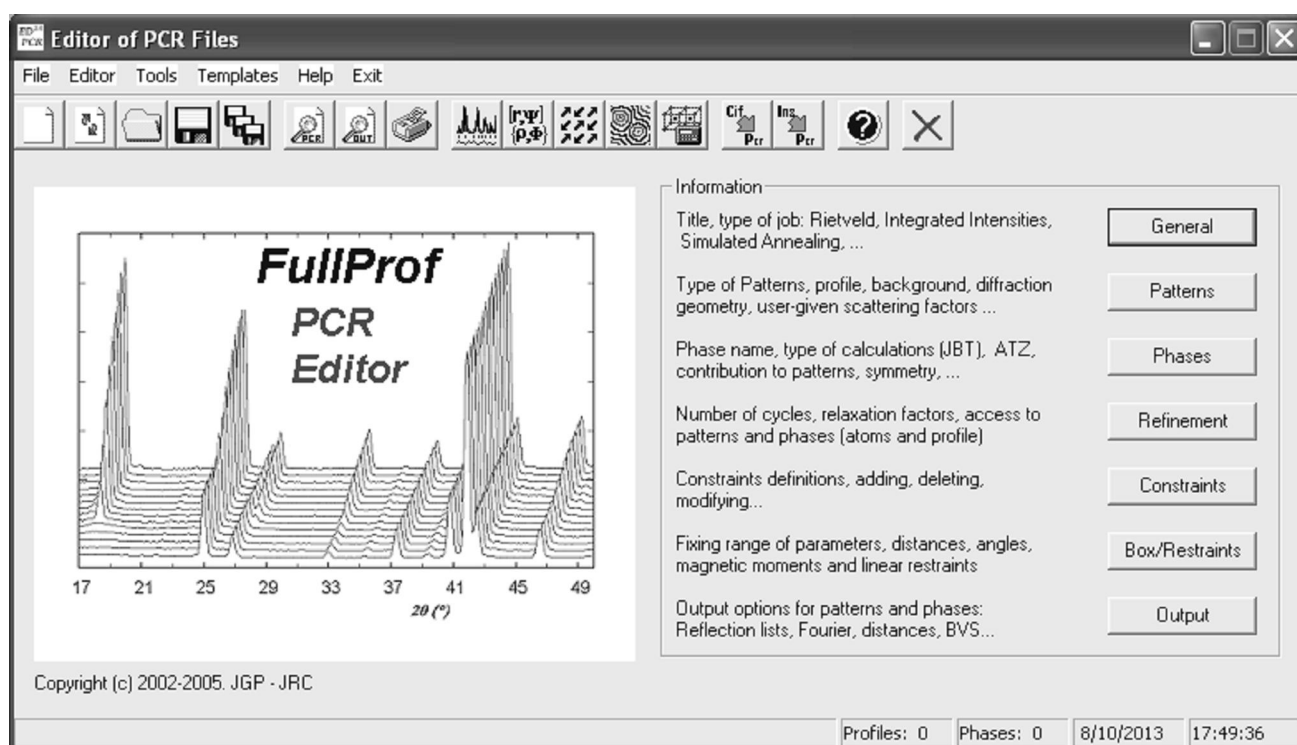
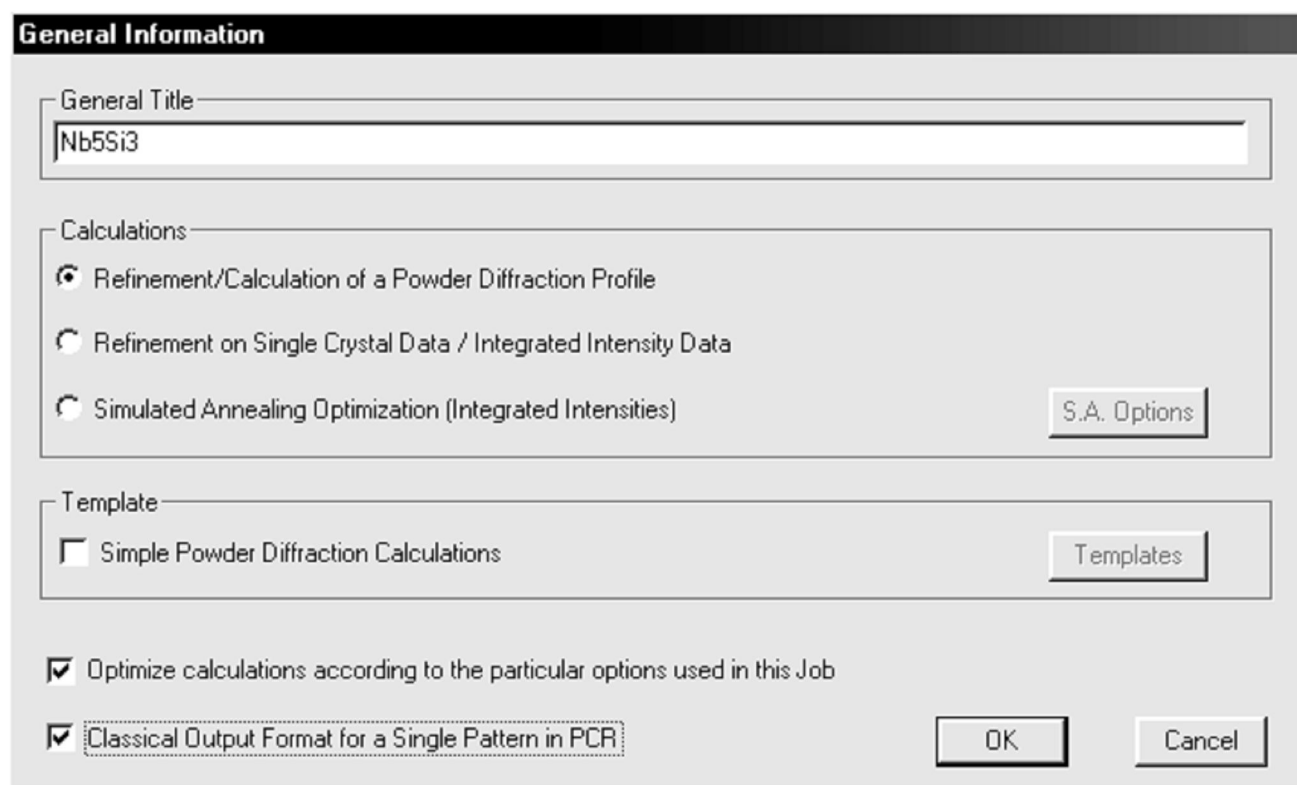


FullProf



Pasta: General



Pasta: Patterns

Patterns Information

General Information

Pattern: 1/1 Weight: 1.0000

Initial Previous Add Del Next Last

Data file/Peak shape

Background Type

Excluded Regions

Geometry/IRF

User Scatt. Factors

OK Cancel

Pasta: Patterns / Sub-pasta: Data file/Peak shape

Profile Data Information: Pattern 1

Name of Data File

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.)

Format of Data File

☐ D1A/D2B (Old Format) ☒ Free Format (2theta, step, 2thetaF) ☐ Variable Time X-ray

☐ D1A/D2B/3T2/G42 ☐ Two Axis Instrument, G41 ☐ X,Y,SIGMA (XYData)

☐ D1B (Old Format) ☐ GSAS Format ☐ X'Celerator (Philips)

☐ D1B/D20 ☐ Socabim Software

☐ D4/D20L ☐ Synchrotron (Brookhaven)

☐ DMC/HRPD (P.S.I.) ☐ Synchrotron (DBWS Software)

Scattering Variable

☒ 2Theta ☐ Energy (keV)

☐ T.O.F. (microseconds)

Wavelength

1: Ratio (I2/I1):

2:

Calculated Pattern

Theta_min: Theta_max: Step:

Range of calculation of a single reflection in units of FWHM: Incident beam angle at sample surface (°):

Peak Shape

☒ Codefil.shp ☐ Global.shp

Formato do arquivo de dados:

Free format: Nb5Si3.dat

1ª linha: âng. inicial passo angular âng. final

2ª linha até Nª linha: uma coluna contendo somente a intensidade.

Obs: = espaço

Pasta: Patterns / Sub-pasta: Background Type

Background Information

Background Mode

☒ 6-Coefficients polynomial function
☐ 12-Coefficients polynomial function
☐ Debye-like (12-coeff.)+ polynomial functions (6-coeff)
☐ 12-Coefficients Fourier-cosine series
☐ Fourier Filtering
☐ Background File transformed by 4-coefficients expression
☐ Linear Interpolation between a set background points with refinable heights
☐ Interpolation by cubic splines

Origin of the polynomial:

Number of points taken for Fourier Filter:

Number of Points:

Pasta: Patterns / Sub-pasta: Geometry / IRF

Diffraction Geometry

Bragg-Brentano or Debye-Scherrer Geometry

Instrumental Resolution Function (IRF) File

☒ None
☐ $H_G^2 = (U_i \tan \theta + V_i) \tan \theta + W_i$
☐ $H_L = X_i \tan \theta + Y_i / \cos \theta + Z_i$
☐ $H_G^2 = (U_i \tan \theta + V_i) \tan \theta + W_i$
☐ $H_L = (X_i 2\theta + Y_i) 2\theta + Z_i$
☐ List of $2\theta, H_G(2\theta), H_L(2\theta)$

Label

Name of IRF file:

External Correction of Integrated/Profile Intensities

☒ None
☐ Linear Interpolation
☐ Empirical Function

☒ Preferred orientation Function I
☐ Preferred orientation Function II (March)

Correction for illuminated area exceeding the Sample surface:

Fraction of mosaic-crystal (transmission):

Monochromator Polarization Correction ($\cos^2 2\theta_{\text{Mon}}$):

Absorption Correction Coefficient (μ_R):

Peaks below this 2Theta limit are corrected for asymmetry:

Absorption correction type for T.O.F.:

Pasta: Phases

Phase Information: Phase 1

General Information on Phases

Name of Phase :

Calculation:

Coefficient to calculate the weight percentage of the Phase: ☒ Calculated automatically ☐ Provided by user

Contribution to patterns, preferred orientation direction, reflection list, ...

Space Group symbol/number, symmetry operators, basis functions, etc

Pasta: Phases / Sub-pasta: Contribution to Patterns

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 ☐ Pattern Calculation (X-Ray)
☐ Neutron (Constant Wavelength) ☐ Pattern Calculation (Neutron - Constant Wavelength)
 Nuclear and Magnetic ☐ Pattern Calculation (Neutron - T.O.F.)
☐ Neutron (T.O.F.)
 Nuclear and Magnetic

Peak Shape

☒ Codefil.shp ☐ Global.shp

Intensities

Reflection list:

Brindley coefficient:

Global weight of the integrated intensity respect global profile:

Factor for excluding reflections [< Factor * Sigma(I)]:

Weights are divide by reduced Chi² of precedent cycle:

Pasta: Phases / Sub-pasta: Symmetry

Symmetry Information

Space Group Properties

Symmetry Operators: Generated automatically from the symbol

Spacegroup: I 4/m c m Symm.Op. Automatic

Symmetry operators | Magnetic/Displacement Operators | Irreducible representations |

Laue Class: 4/mmm ☒ Centrosymmetric Case

Number of Symmetry Operators: 32

Num	SYMMETRY	TR	Num	SYMMETRY	TR
1	X,Y,Z	☐	2	-Y,X,Z	☐
3	-X,Y,Z	☐	4	Y,X,Z	☐
5	-X,Y,Z+1/2	☐	6	Y,X,Z+1/2	☐

TR=Time reversal associated to symmetry operator

☐ Time Reversal for Inversion operator

OK Cancel

Pasta: Refinement

Refinement Information

Cycles of Refinement: 3

Stop Criterium of Coverage

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 ☐ Each cycle ☐ Bragg R-Factor excluding limits reflections

Pattern 1 | Pattern 2 | Pattern 3 | Pattern 4 | Pattern 5 | Pattern 6 | Pattern 7 |

Refinement weighting model

☒ Least Squares ☐ Maximum Likelihood ☐ Unit Weights

Background Instrumental Micro-Absorption

Reduction factor of number of data points: 0

Phase 1 | Phase 2 | Phase 3 | Phase 4 | Phase 5 | Phase 6 | Phase 7 |

Atoms Prop. Vectors

Patterns

☒ 1 ☐ 2 ☐ 3 ☐ 4 ☐ 5 ☐ 6 ☐ 7

Profile Micro-Structure HKL Shifts Further Parameters

OK Cancel

Pasta: Refinement / Sub-pasta: Background

Refinement Information

Cycles of Refinement:

Stop Criterion of Coverage
 Forced Termination when shifts < x E.S.D.
 Others:

Relaxation Factors for Shifts
 Atomic Anisotropic Profile Global

Reflections ordering
☒ Only at the first cycle ☐ Each cycle ☐ Bragg R-Factor excluding limits reflections

6 Coefficients Polynomial Background: Pattern 1

	d_0	d_1	d_2	d_3	d_4	d_5
Coefficients						

	d_6	d_7	d_8	d_9	d_10	d_11
Coefficients						

Background Polynomial

	a_0	a_1	a_2	a_3	a_4	a_5
Coefficients	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Buttons:

Pasta: Refinement / Sub-pasta: Profile

Profile Parameters: Phase 1 Pattern 1

Factors

	Scale	Overall Displacement
Coefficients	0.001	0.0000

Cell Parameters

	a	b	c	alpha	beta	gamma
Coefficients	6.570000	6.570000	11.884000	90.000	90.000	90.000

FWHM Parameters

	U	V	W	IG
Coefficients	0.000000	0.000000	0.010000	0.000000

Shape Parameters

	Eta_0	X
Coefficients	0.500000	0.000000

☐ Refine FWHM for second wavelength

	U2	V2	W2
Coefficients			

Buttons:

Pasta: Refinement / Sub-pasta: Atoms

Atoms Information: Phase 1

List of Atoms
Number of Atoms:

	Label	Ntyp	X	Y	Z	B	Occ	Therm. Fact.
Atom # 1	Nb1	NB	0.0000	0.0000	0.0000	1.0000	0.12500	Isotropic
Atom # 2	Nb2	NB	0.16600	0.66600	0.15000	1.0000	0.50000	Isotropic
Atom # 3	Si1	SI	0.0000	0.0000	0.25000	1.0000	0.12500	Isotropic
Atom # 4	Si2	SI	0.37500	0.87500	0.0000	1.0000	0.25000	Isotropic

Anisotropic Thermal Factors / Form Factors

	B11/F1	B22/F2	B33/F3	B12/F4	B13/F5	B23/F6	F7
#							
#							
#							
#							

Special Form Factor

	SASH-Type	Matrix	j=1	j=2	j=3	N. Coeff.	Indices	#1	#2	#3	#4	#5	#6
#	Spherical												
	Spherical												
	Spherical												

átomo	posição Wyckoff	x	y	z	B(Å ²)	Occ (ocupação) (*)
Nb 1	4(c)	0	0	0	1	4/32 = 0.125
Nb 2	16(l)	x	x+1/2	z	1	16/32 = 0.5
Si 1	4(a)	0	0	1/4	1	4/32 = 0.125
Si 2	8(h)	x	x+1/2	0	1	8/32 = 0.25

$$x(\text{Nb2})=0,166 \quad z(\text{Nb2})=0,15 \quad x(\text{Si2})=0,375$$

Grupo espacial: I 4/m c m: posição geral: 32(m)

(*) Obs: Para calcular a ocupação, dividir a posição Wyckoff pelo número de posição geral.

Pasta: Refinement / Sub-pasta: Instrumental

Instrumental Parameters Refinement: Pattern 1

2_Theta

	Zero	Displacement	Transparency	Wavelength
Coefficients	0.000000	0.000000	0.000000	0.000000