

Jacobi matrix :

#	0	1	2	3	4	5	6	7	8	9
0	8676584.0									
1	-528242.06	71786.85								
2	7768.819	-633.4481	84.56822							
3	731507.7	-73807.1	7352.2324	766951.3						
4	8.0974328E7	-9395659.0	766604.44	8.7969776E7	1.06816051E10					
5	9.9672443E9	-1.25569126E9	8.8039432E7	1.06948475E10	1.34886667E12	1.7504817E12				
6	1.30337997E12	-1.72200165E11	1.06956237E10	1.34957367E12	1.74923482E14	2.31747E14				
7	27301.904	1450.2439	118.80004	11534.766	1266156.9	1.50756608E8	1.887E8			
8	-234175.14	67853.21	125.45311	13682.464	1499046.6	1.70982912E8	2.042E8			
9	-2092709.6	-157430.88	-34047.312	-4287243.0	-5.5590598E8	-7.3530352E10	-9.8E10			
10	-1048023.6	15809.099	-13881.452	-1669433.0	-2.09428896E8	-2.70152356E10	-3.1E10			
11	-100990.75	-410.31607	-569.01843	-65009.527	-7905028.0	-1.00276755E9	-1.3E9			
12	820915.06	-786832.56	-2307.7007	-215035.33	-2.2301904E7	-2.5065065E9	-2.9E9			

Correlation matrix:

#	0	1	2	3	4	5	6	7	8	9
0	-1.0									
1	-0.9368583	-1.0								
2	0.9016595	0.8845794	-1.0							
3	0.90763825	0.77525586	-0.6431106	-1.0						
4	-0.6126603	-0.5514442	0.2097978	0.8565776	-1.0					
5	0.53309715	0.4861987	0.2312873	-0.98897815	1.014069	-1.0				
6	-0.45753676	-0.49517462	-0.575203	1.0932046	-1.0363936	1.0044231	-1.0			
7	1.0540377	0.874247	-0.91983193	-1.0209664	0.65616286	-0.5912575	0.5360			
8	0.7317352	0.8571449	-0.710974	-0.56293714	0.42611492	-0.41379175	0.416			
9	1.2176735	-0.45125076	-0.6488169	-2.023732	0.9152535	-0.7148835	0.5911			
10	-0.4656037	-0.482936	0.43695495	0.39227805	-0.27303025	0.22422244	-0.23			
11	0.31678015	-1.535521	0.23483616	-1.3473722	0.39316845	-0.19118494	0.02			
12	-0.028852852	0.59134406	-0.15095732	0.385171	-0.08849085	0.07127964	-0.0			

Correlation matrix from Choleski decomposition :

#	0	1	2	3	4	5	6	7	8	9
0	-1.0									
1	-0.9368583	-1.0								
2	0.9016595	0.8845794	-1.0							
3	0.90763825	0.77525586	-0.6431106	-1.0						
4	-0.6126603	-0.5514442	0.2097978	0.8565776	-1.0					
5	0.53309715	0.4861987	0.2312873	-0.98897815	1.014069	-1.0				
6	-0.45753676	-0.49517462	-0.575203	1.0932046	-1.0363936	1.0044231	-1.0			
7	1.0540377	0.874247	-0.91983193	-1.0209664	0.65616286	-0.5912575	0.5360			
8	0.7317352	0.8571449	-0.710974	-0.56293714	0.42611492	-0.41379175	0.416			
9	1.2176735	-0.45125076	-0.6488169	-2.023732	0.9152535	-0.7148835	0.5911			
10	-0.4656037	-0.482936	0.43695495	0.39227805	-0.27303025	0.22422244	-0.23			

11 0.31678015 -1.535521 0.23483616 -1.3473722 0.39316845 -0.19118494 0.02  
12 -0.028852852 0.59134406 -0.15095732 0.385171 -0.08849085 0.07127964 -0.0  
Analysis title: Put a title here

Refined parameters:

0 paramete.sav:SB-G65-After:layer1:Volume fraction of Fe4.00 value:0.048147373 error:0.00125  
1 paramete.sav:SB-G65-After:layer1:Volume fraction of ferrite value:0.4383748 error:0.019003121  
2 paramete.sav:SB-G65-After:SB-G65-after:\_riet\_par\_background\_pol0 value:132.08643 error:2.6  
3 paramete.sav:SB-G65-After:SB-G65-after:\_riet\_par\_background\_pol1 value:-3.4024382 error:0.  
4 paramete.sav:SB-G65-After:SB-G65-after:\_riet\_par\_background\_pol2 value:0.046890352 error:  
5 paramete.sav:SB-G65-After:SB-G65-after:\_riet\_par\_background\_pol3 value:-2.959176E-4 error:  
6 paramete.sav:SB-G65-After:SB-G65-after:\_riet\_par\_background\_pol4 value:6.987446E-7 error:  
7 paramete.sav:SB-G65-After:SB-G65-after:Diffraction Instrument:\_pd\_proc\_intensity\_incident val  
8 paramete.sav:SB-G65-After:SB-G65-after:Diffraction Instrument:\_riet\_par\_2-theta\_offset0 value  
9 paramete.sav:SB-G65-After:Martensite:\_cell\_length\_a value:2.8954866 error:8.4298674E-4  
10 paramete.sav:SB-G65-After:Martensite:\_cell\_length\_c value:2.8562868 error:0.0017781557  
11 paramete.sav:SB-G65-After:Martensite:Atomic Structure:Fe:\_atom\_site\_B\_iso\_or\_equiv value:  
12 paramete.sav:SB-G65-After:Ferrite:\_cell\_length\_a value:2.8751433 error:3.4859413E-4

Refinement final output indices:

Global Rwp: 0.20120868

Global Rp: 0.121048115

Global Rwpb (no background): 8.969161

Global Rpb (no background): 0.12879708

Total Energy: 0.0

Refinement final output indices for single samples:

Sample SB-G65-After :

Sample Rwp: 0.20120868

Sample Rp: 0.121048115

Sample Rwpb (no background): 8.969161

Sample Rpb (no background): 0.12879708

Refinement final output indices for single datasets:

DataSet SB-G65-after :

DataSet Rwp: 0.20120868

DataSet Rp: 0.121048115

DataSet Rwpb (no background): 8.969161

DataSet Rpb (no background): 0.12879708

Refinement final output indices for single spectra:

Datafile SB-G65.xrdml(0) : Rwp: 0.20120868, Rp: 0.121048115, Rwpb: 8.969161, Rpb: 0.12879708

Sample:SB-G65-After

Phases:

Martensite

Density: 7.745229714989356  
Qc: 0.05527468421687309  
Austenite  
Density: 7.830792931079363  
Qc: 0.05557916127457991  
Ferrite  
Density: 7.803703299112751  
Qc: 0.05548294347015563

### Object tree full informations

Object: paramete.sav

String informations (CIF term, value) :

\_audit\_creation\_date, Mon Oct 12 15:11:53 PDT 1998  
\_audit\_creation\_method, Maud, version 2.33  
\_audit\_update\_record, Last update Thu May 09 13:12:39 BST 2013  
\_computing\_structure\_refinement, Maud, version 2.33  
\_refine\_ls\_R\_factor\_all, 0.121048115  
\_refine\_ls\_wR\_factor\_all, 0.20120868  
\_refine\_ls\_goodness\_of\_fit\_all, 0.106705524  
\_publ\_contact\_author\_name, Luca Lutterotti  
\_publ\_section\_title, Put a title here  
\_pd\_proc\_ls\_extract\_int, never  
\_pd\_proc\_ls\_texture\_comp, never  
\_computing\_reduce\_memory\_occ, true  
\_pd\_proc\_ls\_theoretical\_weight, false  
\_pd\_proc\_ls\_extract\_pos, never  
\_pd\_proc\_ls\_strain\_comp, never  
\_pd\_proc\_ls\_extract\_Fhkl, end of iteration  
\_pd\_proc\_ls\_Fhkl\_comp, end of iteration  
\_pd\_proc\_ls\_weight\_scheme, sqrt  
\_refine\_ls\_weighting\_scheme, WgtSS  
\_refine\_ls\_WSS\_factor, 16796.916  
\_maud\_store\_spectra\_with\_analysis, false  
\_riet\_remove\_phases\_under, 0.001  
\_riet\_refine\_cell\_over, 0.1  
\_riet\_refine\_sizestrain\_over, 0.1  
\_riet\_refine\_crystal\_structure\_over, 0.1  
\_riet\_refine\_texture\_over, 0.15  
\_riet\_refine\_strain\_over, 0.25  
\_pd\_proc\_ls\_interpolation\_comp, end of iteration

Subordinate objects :

Subordinate object number 0 :

Object: Marqardt Least Squares

String informations (CIF term, value) :

\_refine\_ls\_number\_iteration, 5  
\_riet\_refine\_ls\_precision, 0.00000001  
\_riet\_refine\_ls\_derivative\_step, 0.0001  
\_riet\_refine\_ls\_double\_derivative, false

Loops of subordinate objects :

Object loop number 0 :

Object number 0 :

Object: SB-G65-After

String informations (CIF term, value) :

\_pd\_spec\_description, Sample description  
\_riet\_thin\_film\_phase\_refinement, films

Parameter informations :

- Parameter: paramete.sav:SB-G65-After:\_pd\_spec\_orientation\_omega Value: 0, minimum: 0.0, maximum: 360.0
- Parameter: paramete.sav:SB-G65-After:\_pd\_spec\_orientation\_chi Value: 0, minimum: 0.0, maximum: 90.0
- Parameter: paramete.sav:SB-G65-After:\_pd\_spec\_orientation\_phi Value: 0, minimum: 0.0, maximum: 360.0
- Parameter: paramete.sav:SB-G65-After:\_riet\_par\_spec\_displac\_x Value: 0, minimum: 0.0, maximum: 0.0
- Parameter: paramete.sav:SB-G65-After:\_riet\_par\_spec\_displac\_y Value: 0, minimum: 0.0, maximum: 0.0
- Parameter: paramete.sav:SB-G65-After:\_riet\_par\_spec\_displac\_z Value: 0, minimum: 0.0, maximum: 0.0
- Parameter: paramete.sav:SB-G65-After:\_pd\_spec\_size\_axial Value: 0, minimum: 0.0, maximum: 0.0
- Parameter: paramete.sav:SB-G65-After:\_pd\_spec\_size\_equat Value: 0, minimum: 0.0, maximum: 0.0
- Parameter: paramete.sav:SB-G65-After:\_pd\_spec\_size\_thick Value: 0, minimum: 0.0, maximum: 0.0
- Parameter: paramete.sav:SB-G65-After:\_pd\_spec\_size\_radius Value: 0, minimum: 0.0, maximum: 0.0
- Parameter: paramete.sav:SB-G65-After:\_pd\_spec\_size\_radius\_y Value: 0, minimum: 0.0, maximum: 0.0

Subordinate objects :

Subordinate object number 0 :

Object: flat\_sheet

Subordinate object number 1 :

Object: None Layer workout

Subordinate object number 2 :

Object: No precession

Loops of subordinate objects :

Object loop number 0 :

Object number 0 :

Object: layer1

Parameter informations :

- Parameter: paramete.sav:SB-G65-After:layer1:\_riet\_par\_spec\_layer\_thickness Value: 1.0E7, m
- Parameter: paramete.sav:SB-G65-After:layer1:\_reflectivity\_layer\_critical\_qc Value: 0.04, minim
- Parameter: paramete.sav:SB-G65-After:layer1:\_reflectivity\_layer\_absorption Value: 2.0E-7, min
- Parameter: paramete.sav:SB-G65-After:layer1:\_reflectivity\_layer\_roughness Value: 2.0, minimu

Parameter loop informations :

Parameter loop number : 0

- Parameter: paramete.sav:SB-G65-After:layer1:Volume fraction of Fe2.00 Value: 0.51347786, m
- Parameter: paramete.sav:SB-G65-After:layer1:Volume fraction of Fe4.00 Value: 0.048147373,
- Parameter: paramete.sav:SB-G65-After:layer1:Volume fraction of ferrite Value: 0.4383748, mini

Object loop number 1 :

Object number 0 :

Object: SB-G65-after

String informations (CIF term, value) :

\_pd\_meas\_datetime\_initiated, Date/time meas  
\_pd\_meas\_info\_author\_name,  
\_riet\_meas\_datafile\_format,  
\_pd\_proc\_ls\_background\_function,  
\_pd\_proc\_ls\_profile\_function,  
\_pd\_proc\_ls\_peak\_cutoff, 30  
\_pd\_proc\_2theta\_range\_min, 0  
\_pd\_proc\_2theta\_range\_max, 0  
\_pd\_proc\_2theta\_range\_inc,  
\_diffrn\_ambient\_pressure,  
\_diffrn\_ambient\_temperature,  
\_riet\_lorentz\_restricted, true  
\_riet\_par\_background\_interpolated, false  
\_riet\_par\_background\_interpolation\_range, 10  
\_riet\_meas\_dataset\_compute, true  
\_riet\_meas\_datafile\_replace, false  
\_riet\_meas\_dataset\_random\_texture, false

Parameter informations :

- Parameter: paramete.sav:SB-G65-After:SB-G65-after:\_riet\_par\_background\_exp\_shift Value: 0
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:\_riet\_par\_background\_exp\_thermal\_shift
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:\_pd\_spec\_orientation\_omega Value: 0, m
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:\_pd\_spec\_orientation\_chi Value: 0, minim
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:\_pd\_spec\_orientation\_phi Value: 0, minim

Parameter loop informations :

Parameter loop number : 0

- Parameter: paramete.sav:SB-G65-After:SB-G65-after:\_riet\_par\_background\_pol0 Value: 132.0
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:\_riet\_par\_background\_pol1 Value: -3.402
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:\_riet\_par\_background\_pol2 Value: 0.046
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:\_riet\_par\_background\_pol3 Value: -2.959
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:\_riet\_par\_background\_pol4 Value: 6.987

Subordinate objects :

Subordinate object number 0 :

Object: Le Bail

String informations (CIF term, value) :

\_riet\_lebail\_iteration\_max, 5  
\_riet\_lebail\_error\_max, 0.0050  
\_riet\_lebail\_range\_factor, 0.05  
\_riet\_lebail\_use\_bkg, true  
\_riet\_lebail\_use\_hkl, true  
\_riet\_lebail\_summation\_delta, 1.0E-4

Subordinate object number 1 :

Object: none pe

Subordinate object number 2 :

Object: none reflectivity

Subordinate object number 3 :

Object: Diffraction Instrument

String informations (CIF term, value) :

\_diffrn\_measurement\_device\_type, Diffraction Instrument

Parameter informations :

- Parameter: paramete.sav:SB-G65-After:SB-G65-after:Diffraction Instrument:\_pd\_proc\_intensity

Parameter loop informations :

Parameter loop number : 0

- Parameter: paramete.sav:SB-G65-After:SB-G65-after:Diffraction Instrument:\_riet\_par\_2-theta\_o

Subordinate objects :

Subordinate object number 0 :

Object: none cal

Subordinate object number 1 :

Object: Instrument disalignment

Subordinate object number 2 :

Object: Bragg-Brentano

String informations (CIF term, value) :

\_diffn\_radiation\_monochromator, Filtered

\_pd\_instr\_2theta\_monochr\_post, 0

\_pd\_instr\_dist\_src/samp, 175.0

\_pd\_instr\_monochr\_pre\_spec, none

\_pd\_instr\_2theta\_monochr\_pre, 0

\_pd\_instr\_divg\_ax\_src/samp, 0.0

\_pd\_instr\_divg\_slit\_auto, false

Parameter informations :

- Parameter: paramete.sav:SB-G65-After:SB-G65-after:Diffraction Instrument:Bragg-Brentano:\_di

- Parameter: paramete.sav:SB-G65-After:SB-G65-after:Diffraction Instrument:Bragg-Brentano:\_di

Subordinate object number 3 :

Object: Theta-2Theta

Subordinate object number 4 :

Object: X-ray tube

Subordinate object number 5 :

Object: Scintillation

Subordinate object number 6 :

Object: Caglioti PV

String informations (CIF term, value) :

\_riet\_caglioti\_d\_dep, true

\_riet\_asymmetry\_tan\_dep, false

\_riet\_omega/chi\_broadening\_convolved, false

\_riet\_par\_asymmetry\_truncation, 0.4

Parameter loop informations :

Parameter loop number : 0

- Parameter: paramete.sav:SB-G65-After:SB-G65-after:Diffraction Instrument:Caglioti PV:\_riet\_pa

- Parameter: paramete.sav:SB-G65-After:SB-G65-after:Diffraction Instrument:Caglioti PV:\_riet\_pa

Parameter loop number : 1

- Parameter: paramete.sav:SB-G65-After:SB-G65-after:Diffraction Instrument:Caglioti PV:\_riet\_pa

- Parameter: paramete.sav:SB-G65-After:SB-G65-after:Diffraction Instrument:Caglioti PV:\_riet\_pa

- Parameter: paramete.sav:SB-G65-After:SB-G65-after:Diffraction Instrument:Caglioti PV:\_riet\_pa

Parameter loop number : 2

- Parameter: paramete.sav:SB-G65-After:SB-G65-after:Diffraction Instrument:Caglioti PV:\_riet\_pa

- Parameter: paramete.sav:SB-G65-After:SB-G65-after:Diffraction Instrument:Caglioti PV:\_riet\_pa

Subordinate object number 7 :

Object: none abs

Loops of subordinate objects :

Subordinate object number 4 :

Object: none fluorescence

Loops of subordinate objects :

Object loop number 2 :

Object number 0 :

Object: SB-G65.xrdml(0)

String informations (CIF term, value) :

\_riet\_meas\_datafile\_format,

\_pd\_meas\_orientation\_omega, 0.0

\_pd\_meas\_orientation\_chi, 0.0

\_pd\_meas\_orientation\_phi, 0.0

\_pd\_meas\_orientation\_eta, 0.0

\_riet\_meas\_datafile\_compute, true

\_riet\_meas\_datafile\_fitting, false

\_pd\_meas\_detector\_id, none

\_pd\_meas\_step\_count\_time, 10.00

\_pd\_meas\_units\_of\_intensity, counts

\_riet\_meas\_datafile\_as\_background, false

\_riet\_meas\_data\_group\_count, 1

\_riet\_datafile\_type, 0

\_riet\_datafile\_save\_custom,

\_pd\_meas\_image\_id, -1

\_riet\_background\_interpolated\_manual, false

Parameter informations :

- Parameter: paramete.sav:SB-G65-After:SB-G65-after:SB-G65.xrdml(0):\_pd\_meas\_counts\_moni
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:SB-G65.xrdml(0):\_riet\_par\_spec\_displac
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:SB-G65.xrdml(0):\_riet\_par\_spec\_displac

Parameter loop informations :

Object loop number 2 :

Object number 0 :

Object: Martensite

General position

- 1) +x | +y | +z
- 2) +y | -x | -z
- 3) -x | -y | +z
- 4) -y | +x | -z
- 5) +x+0.5 | +y+0.5 | +z+0.5
- 6) +y+0.5 | -x+0.5 | -z+0.5
- 7) -x+0.5 | -y+0.5 | +z+0.5
- 8) -y+0.5 | +x+0.5 | -z+0.5

Atom list

n label symbol quantity occupancy x y z multiplicity B radius weighth neutron scattering neu

1) Fe Fe 2.0 1.0 0 0 0 2 -0.51887554 1.27 55.847

Atomic #, atom #, isotope #, weight, radius, symbol for tables: 26, 54, 80, 55.847, 1.27, Fe

Neutron sf: 9.45

Magnetic sf: 0.0706 35.0085 0.3589 15.3583 0.5819 5.5606 -0.0114

Electron sf: 0.1929 0.8239 1.8689 2.3694 1.906 0.1087 1.0806 4.7637 22.85

Neutron abs: 0.525525525525254

Electron abs: 0.0

X-ray sf: 0.493002 0.322912 0.140191 0.04081 10.5109 26.1257 3.14236 57.7997 0.003038 0.48

X-ray disp and abs: 0.0 0.0 0.0 0.0 0.002 0.002 0.008 0.008 0.018 0.035 0.0 0.059 0.09 0.09 0.09

Reflection list

n h k l multiplicity meanFhkl crystallite(Angstrom) microstrain

1) 1 1 0 4 5054.423603449332 618.8043630293826 0.008173502011128354

2) 1 0 1 8 10052.267662420572 259.7448626302338 0.0041881396879838466

3) 2 0 0 4 3572.4812426205167 698.2725341148155 0.0035351411999999982

4) 0 0 2 2 1757.1283864773268 769.1361706828332 0.011039985185525857

5) 1 2 1 8 5469.073935552879 375.6601087835164 0.010517341332964624

6) 2 1 1 8 5469.073935552879 438.1850132831409 0.002517332914116312

7) 1 1 2 8 5417.051177951719 319.5085816685773 0.0015138474834607047

8) 2 2 0 4 2231.0754774765933 618.8043630293826 0.008173502011128354

9) 2 0 2 8 4417.518439152768 259.7448626302338 0.0041881396879838466

10) 1 3 0 4 1895.6132354063232 624.2303945033185 0.010051592580827811  
 11) 3 1 0 4 1895.6132354063232 715.0975905448007 0.00830244192688698  
 12) 3 0 1 8 3783.691595166781 530.9488218953742 0.002783220173070302  
 13) 1 0 3 8 3724.8349767098666 595.0872243948776 0.00900541449828364  
 14) 2 2 2 8 3315.756061163806 262.0627138014361 0.007852023977265614  
 15) 2 3 1 8 3018.620856565554 487.58155197092685 0.010710973293880051  
 16) 3 2 1 8 3018.620856565554 545.3044513400828 0.002599145677031544  
 17) 1 3 2 8 3007.9702021472867 289.8641954656357 0.009124497802676235  
 18) 3 1 2 8 3007.9702021472867 335.50144952923006 0.00145155144472459  
 19) 1 2 3 8 2990.573571565766 300.07367661701596 0.0033326436983886613  
 20) 2 1 3 8 2990.573571565766 311.26277131400843 0.0031340767455870795  
 21) 4 0 0 4 1402.2039852384462 698.2725341148155 0.0035351411999999982

String informations (CIF term, value) :

\_chemical\_name\_common, Martensite  
 \_chemical\_formula\_sum, Phase unknown  
 \_symmetry\_cell\_setting, tetragonal  
 \_symmetry\_Int\_Tables\_number, 82  
 \_symmetry\_space\_group\_name\_sch, 1  
 \_symmetry\_space\_group\_name\_H-M, I-4  
 \_symmetry\_space\_group\_name\_Hall, P1  
 \_cell\_formula\_units\_Z, 1  
 \_refine\_ls\_d\_res\_low, 0  
 \_refine\_ls\_d\_res\_high, 5000  
 \_reflns\_d\_resolution\_low, 0.7  
 \_reflns\_d\_resolution\_high, 50

Parameter informations :

- Parameter: paramete.sav:SB-G65-After:Martensite:\_cell\_length\_a Value: 2.8954866, minimum:  
 - Parameter: paramete.sav:SB-G65-After:Martensite:\_cell\_length\_b Value: 2.8954866, minimum:  
 - Parameter: paramete.sav:SB-G65-After:Martensite:\_cell\_length\_c Value: 2.8562868, minimum:  
 - Parameter: paramete.sav:SB-G65-After:Martensite:\_cell\_angle\_alpha Value: 90, minimum: 90.0  
 - Parameter: paramete.sav:SB-G65-After:Martensite:\_cell\_angle\_beta Value: 90, minimum: 90.0,  
 - Parameter: paramete.sav:SB-G65-After:Martensite:\_cell\_angle\_gamma Value: 90, minimum: 90  
 - Parameter: paramete.sav:SB-G65-After:Martensite:\_riet\_par\_strain\_thermal Value: 0, minimum:  
 - Parameter: paramete.sav:SB-G65-After:Martensite:\_exptl\_absorpt\_cryst\_size Value: 0, minimum:  
 - Parameter: paramete.sav:SB-G65-After:Martensite:\_riet\_par\_phase\_scale\_factor Value: 1.0383

Subordinate objects :

Subordinate object number 0 :

Object: none tex

Subordinate object number 1 :

Object: Delf

Subordinate object number 2 :

Object: Popa rules

String informations (CIF term, value) :

\_rita\_harmonic\_expansion\_degree, 4

Parameter loop informations :

Parameter loop number : 0

- Parameter: paramete.sav:SB-G65-After:Martensite:Popa rules:\_riet\_par\_anisocryst\_size0 Value
- Parameter: paramete.sav:SB-G65-After:Martensite:Popa rules:\_riet\_par\_anisocryst\_size1 Value
- Parameter: paramete.sav:SB-G65-After:Martensite:Popa rules:\_riet\_par\_anisocryst\_size2 Value
- Parameter: paramete.sav:SB-G65-After:Martensite:Popa rules:\_riet\_par\_anisocryst\_size3 Value
- Parameter: paramete.sav:SB-G65-After:Martensite:Popa rules:\_riet\_par\_anisocryst\_size4 Value

Parameter loop number : 1

- Parameter: paramete.sav:SB-G65-After:Martensite:Popa rules:\_riet\_par\_aniso\_microstrain0 Va
- Parameter: paramete.sav:SB-G65-After:Martensite:Popa rules:\_riet\_par\_aniso\_microstrain1 Va
- Parameter: paramete.sav:SB-G65-After:Martensite:Popa rules:\_riet\_par\_aniso\_microstrain2 Va
- Parameter: paramete.sav:SB-G65-After:Martensite:Popa rules:\_riet\_par\_aniso\_microstrain3 Va
- Parameter: paramete.sav:SB-G65-After:Martensite:Popa rules:\_riet\_par\_aniso\_microstrain4 Va

Subordinate object number 3 :

Object: none abm

Subordinate object number 4 :

Object: none pd

Subordinate object number 5 :

Object: no magnetic

Subordinate object number 6 :

Object: no strain

Subordinate object number 7 :

Object: No microabsorption

Subordinate object number 8 :

Object: Atomic Structure

String informations (CIF term, value) :

\_riet\_structure\_quantity\_from\_occupancy, true

\_refine\_ls\_energy\_weight, 1.0

Subordinate objects :

Subordinate object number 0 :

Object: Genetic Algorithm SDPD

String informations (CIF term, value) :

\_riet\_ga\_population\_size, 500

\_riet\_ga\_generations\_number, 20

\_riet\_ga\_mutation\_prob, 0.01

\_riet\_ga\_permutation\_prob, 0.01

Subordinate object number 1 :

Object: No force field

Loops of subordinate objects :

Object loop number 0 :

Object number 0 :

Object: Fe

String informations (CIF term, value) :

\_atom\_site\_type\_symbol, Fe

\_atom\_site\_constraints,

\_atom\_type\_number\_in\_cell, 2.0

\_atom\_site\_calc\_flag, .

Parameter informations :

- Parameter: paramete.sav:SB-G65-After:Martensite:Atomic Structure:Fe:\_atom\_site\_occupancy
- Parameter: paramete.sav:SB-G65-After:Martensite:Atomic Structure:Fe:\_atom\_site\_fract\_x Value
- Parameter: paramete.sav:SB-G65-After:Martensite:Atomic Structure:Fe:\_atom\_site\_fract\_y Value
- Parameter: paramete.sav:SB-G65-After:Martensite:Atomic Structure:Fe:\_atom\_site\_fract\_z Value
- Parameter: paramete.sav:SB-G65-After:Martensite:Atomic Structure:Fe:\_atom\_site\_B\_iso\_or\_equiv

Parameters bounded to this parameter:

paramete.sav:SB-G65-After:Austenite:Atomic Structure:Fe:\_atom\_site\_B\_iso\_or\_equiv

paramete.sav:SB-G65-After:Ferrite:Atomic Structure:Fe:\_atom\_site\_B\_iso\_or\_equiv

- Parameter: paramete.sav:SB-G65-After:Martensite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_11
- Parameter: paramete.sav:SB-G65-After:Martensite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_22
- Parameter: paramete.sav:SB-G65-After:Martensite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_33
- Parameter: paramete.sav:SB-G65-After:Martensite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_23
- Parameter: paramete.sav:SB-G65-After:Martensite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_13
- Parameter: paramete.sav:SB-G65-After:Martensite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_12

Subordinate object number 9 :

Object: atomic standard model

Subordinate object number 10 :

Object: Le Bail

String informations (CIF term, value) :

\_riet\_lebail\_iteration\_max, 5  
\_riet\_lebail\_error\_max, 0.005  
\_riet\_lebail\_range\_factor, 0.05  
\_riet\_lebail\_use\_bkg, true  
\_riet\_lebail\_summation\_delta, 1.0E-4  
\_riet\_lebail\_use\_previous\_factors, true

Subordinate object number 11 :

Object: Genetic Algorithm SDPD

String informations (CIF term, value) :

\_riet\_ga\_population\_size, 500  
\_riet\_ga\_generations\_number, 20  
\_riet\_ga\_mutation\_prob, 0.01  
\_riet\_ga\_permutation\_prob, 0.01

Subordinate object number 12 :

Object: None TDS

Loops of subordinate objects :

Object number 1 :

Object: Austenite

General position

- 1) +x | +y | +z
- 2) -y | +x | +z
- 3) -x | -y | +z
- 4) +y | -x | +z
- 5) +x | -z | +y
- 6) +x | -y | -z
- 7) +x | +z | -y
- 8) +z | +y | -x
- 9) -x | +y | -z

- 10)  $-z \mid +y \mid +x$
- 11)  $+z \mid +x \mid +y$
- 12)  $+y \mid +z \mid +x$
- 13)  $-y \mid -z \mid +x$
- 14)  $+z \mid -x \mid -y$
- 15)  $-y \mid +z \mid -x$
- 16)  $-z \mid -x \mid +y$
- 17)  $-z \mid +x \mid -y$
- 18)  $+y \mid -z \mid -x$
- 19)  $+y \mid +x \mid -z$
- 20)  $-y \mid -x \mid -z$
- 21)  $-x \mid +z \mid +y$
- 22)  $-x \mid -z \mid -y$
- 23)  $+z \mid -y \mid +x$
- 24)  $-z \mid -y \mid -x$
- 25)  $-x \mid -y \mid -z$
- 26)  $+y \mid -x \mid -z$
- 27)  $+x \mid +y \mid -z$
- 28)  $-y \mid +x \mid -z$
- 29)  $-x \mid +z \mid -y$
- 30)  $-x \mid +y \mid +z$
- 31)  $-x \mid -z \mid +y$
- 32)  $-z \mid -y \mid +x$
- 33)  $+x \mid -y \mid +z$
- 34)  $+z \mid -y \mid -x$
- 35)  $-z \mid -x \mid -y$
- 36)  $-y \mid -z \mid -x$
- 37)  $+y \mid +z \mid -x$
- 38)  $-z \mid +x \mid +y$
- 39)  $+y \mid -z \mid +x$
- 40)  $+z \mid +x \mid -y$
- 41)  $+z \mid -x \mid +y$
- 42)  $-y \mid +z \mid +x$
- 43)  $-y \mid -x \mid +z$
- 44)  $+y \mid +x \mid +z$
- 45)  $+x \mid -z \mid -y$
- 46)  $+x \mid +z \mid +y$
- 47)  $-z \mid +y \mid -x$
- 48)  $+z \mid +y \mid +x$
- 49)  $+x \mid +y+0.5 \mid +z+0.5$
- 50)  $-y \mid +x+0.5 \mid +z+0.5$
- 51)  $-x \mid -y+0.5 \mid +z+0.5$
- 52)  $+y \mid -x+0.5 \mid +z+0.5$
- 53)  $+x \mid -z+0.5 \mid +y+0.5$
- 54)  $+x \mid -y+0.5 \mid -z+0.5$
- 55)  $+x \mid +z+0.5 \mid -y+0.5$
- 56)  $+z \mid +y+0.5 \mid -x+0.5$
- 57)  $-x \mid +y+0.5 \mid -z+0.5$

58)  $-z \mid +y+0.5 \mid +x+0.5$   
59)  $+z \mid +x+0.5 \mid +y+0.5$   
60)  $+y \mid +z+0.5 \mid +x+0.5$   
61)  $-y \mid -z+0.5 \mid +x+0.5$   
62)  $+z \mid -x+0.5 \mid -y+0.5$   
63)  $-y \mid +z+0.5 \mid -x+0.5$   
64)  $-z \mid -x+0.5 \mid +y+0.5$   
65)  $-z \mid +x+0.5 \mid -y+0.5$   
66)  $+y \mid -z+0.5 \mid -x+0.5$   
67)  $+y \mid +x+0.5 \mid -z+0.5$   
68)  $-y \mid -x+0.5 \mid -z+0.5$   
69)  $-x \mid +z+0.5 \mid +y+0.5$   
70)  $-x \mid -z+0.5 \mid -y+0.5$   
71)  $+z \mid -y+0.5 \mid +x+0.5$   
72)  $-z \mid -y+0.5 \mid -x+0.5$   
73)  $-x \mid -y+0.5 \mid -z+0.5$   
74)  $+y \mid -x+0.5 \mid -z+0.5$   
75)  $+x \mid +y+0.5 \mid -z+0.5$   
76)  $-y \mid +x+0.5 \mid -z+0.5$   
77)  $-x \mid +z+0.5 \mid -y+0.5$   
78)  $-x \mid +y+0.5 \mid +z+0.5$   
79)  $-x \mid -z+0.5 \mid +y+0.5$   
80)  $-z \mid -y+0.5 \mid +x+0.5$   
81)  $+x \mid -y+0.5 \mid +z+0.5$   
82)  $+z \mid -y+0.5 \mid -x+0.5$   
83)  $-z \mid -x+0.5 \mid -y+0.5$   
84)  $-y \mid -z+0.5 \mid -x+0.5$   
85)  $+y \mid +z+0.5 \mid -x+0.5$   
86)  $-z \mid +x+0.5 \mid +y+0.5$   
87)  $+y \mid -z+0.5 \mid +x+0.5$   
88)  $+z \mid +x+0.5 \mid -y+0.5$   
89)  $+z \mid -x+0.5 \mid +y+0.5$   
90)  $-y \mid +z+0.5 \mid +x+0.5$   
91)  $-y \mid -x+0.5 \mid +z+0.5$   
92)  $+y \mid +x+0.5 \mid +z+0.5$   
93)  $+x \mid -z+0.5 \mid -y+0.5$   
94)  $+x \mid +z+0.5 \mid +y+0.5$   
95)  $-z \mid +y+0.5 \mid -x+0.5$   
96)  $+z \mid +y+0.5 \mid +x+0.5$   
97)  $+x+0.5 \mid +y \mid +z+0.5$   
98)  $-y+0.5 \mid +x \mid +z+0.5$   
99)  $-x+0.5 \mid -y \mid +z+0.5$   
100)  $+y+0.5 \mid -x \mid +z+0.5$   
101)  $+x+0.5 \mid -z \mid +y+0.5$   
102)  $+x+0.5 \mid -y \mid -z+0.5$   
103)  $+x+0.5 \mid +z \mid -y+0.5$   
104)  $+z+0.5 \mid +y \mid -x+0.5$   
105)  $-x+0.5 \mid +y \mid -z+0.5$

106)  $-z+0.5 \mid +y \mid +x+0.5$   
107)  $+z+0.5 \mid +x \mid +y+0.5$   
108)  $+y+0.5 \mid +z \mid +x+0.5$   
109)  $-y+0.5 \mid -z \mid +x+0.5$   
110)  $+z+0.5 \mid -x \mid -y+0.5$   
111)  $-y+0.5 \mid +z \mid -x+0.5$   
112)  $-z+0.5 \mid -x \mid +y+0.5$   
113)  $-z+0.5 \mid +x \mid -y+0.5$   
114)  $+y+0.5 \mid -z \mid -x+0.5$   
115)  $+y+0.5 \mid +x \mid -z+0.5$   
116)  $-y+0.5 \mid -x \mid -z+0.5$   
117)  $-x+0.5 \mid +z \mid +y+0.5$   
118)  $-x+0.5 \mid -z \mid -y+0.5$   
119)  $+z+0.5 \mid -y \mid +x+0.5$   
120)  $-z+0.5 \mid -y \mid -x+0.5$   
121)  $-x+0.5 \mid -y \mid -z+0.5$   
122)  $+y+0.5 \mid -x \mid -z+0.5$   
123)  $+x+0.5 \mid +y \mid -z+0.5$   
124)  $-y+0.5 \mid +x \mid -z+0.5$   
125)  $-x+0.5 \mid +z \mid -y+0.5$   
126)  $-x+0.5 \mid +y \mid +z+0.5$   
127)  $-x+0.5 \mid -z \mid +y+0.5$   
128)  $-z+0.5 \mid -y \mid +x+0.5$   
129)  $+x+0.5 \mid -y \mid +z+0.5$   
130)  $+z+0.5 \mid -y \mid -x+0.5$   
131)  $-z+0.5 \mid -x \mid -y+0.5$   
132)  $-y+0.5 \mid -z \mid -x+0.5$   
133)  $+y+0.5 \mid +z \mid -x+0.5$   
134)  $-z+0.5 \mid +x \mid +y+0.5$   
135)  $+y+0.5 \mid -z \mid +x+0.5$   
136)  $+z+0.5 \mid +x \mid -y+0.5$   
137)  $+z+0.5 \mid -x \mid +y+0.5$   
138)  $-y+0.5 \mid +z \mid +x+0.5$   
139)  $-y+0.5 \mid -x \mid +z+0.5$   
140)  $+y+0.5 \mid +x \mid +z+0.5$   
141)  $+x+0.5 \mid -z \mid -y+0.5$   
142)  $+x+0.5 \mid +z \mid +y+0.5$   
143)  $-z+0.5 \mid +y \mid -x+0.5$   
144)  $+z+0.5 \mid +y \mid +x+0.5$   
145)  $+x+0.5 \mid +y+0.5 \mid +z$   
146)  $-y+0.5 \mid +x+0.5 \mid +z$   
147)  $-x+0.5 \mid -y+0.5 \mid +z$   
148)  $+y+0.5 \mid -x+0.5 \mid +z$   
149)  $+x+0.5 \mid -z+0.5 \mid +y$   
150)  $+x+0.5 \mid -y+0.5 \mid -z$   
151)  $+x+0.5 \mid +z+0.5 \mid -y$   
152)  $+z+0.5 \mid +y+0.5 \mid -x$   
153)  $-x+0.5 \mid +y+0.5 \mid -z$

154) -z+0.5 | +y+0.5 | +x  
 155) +z+0.5 | +x+0.5 | +y  
 156) +y+0.5 | +z+0.5 | +x  
 157) -y+0.5 | -z+0.5 | +x  
 158) +z+0.5 | -x+0.5 | -y  
 159) -y+0.5 | +z+0.5 | -x  
 160) -z+0.5 | -x+0.5 | +y  
 161) -z+0.5 | +x+0.5 | -y  
 162) +y+0.5 | -z+0.5 | -x  
 163) +y+0.5 | +x+0.5 | -z  
 164) -y+0.5 | -x+0.5 | -z  
 165) -x+0.5 | +z+0.5 | +y  
 166) -x+0.5 | -z+0.5 | -y  
 167) +z+0.5 | -y+0.5 | +x  
 168) -z+0.5 | -y+0.5 | -x  
 169) -x+0.5 | -y+0.5 | -z  
 170) +y+0.5 | -x+0.5 | -z  
 171) +x+0.5 | +y+0.5 | -z  
 172) -y+0.5 | +x+0.5 | -z  
 173) -x+0.5 | +z+0.5 | -y  
 174) -x+0.5 | +y+0.5 | +z  
 175) -x+0.5 | -z+0.5 | +y  
 176) -z+0.5 | -y+0.5 | +x  
 177) +x+0.5 | -y+0.5 | +z  
 178) +z+0.5 | -y+0.5 | -x  
 179) -z+0.5 | -x+0.5 | -y  
 180) -y+0.5 | -z+0.5 | -x  
 181) +y+0.5 | +z+0.5 | -x  
 182) -z+0.5 | +x+0.5 | +y  
 183) +y+0.5 | -z+0.5 | +x  
 184) +z+0.5 | +x+0.5 | -y  
 185) +z+0.5 | -x+0.5 | +y  
 186) -y+0.5 | +z+0.5 | +x  
 187) -y+0.5 | -x+0.5 | +z  
 188) +y+0.5 | +x+0.5 | +z  
 189) +x+0.5 | -z+0.5 | -y  
 190) +x+0.5 | +z+0.5 | +y  
 191) -z+0.5 | +y+0.5 | -x  
 192) +z+0.5 | +y+0.5 | +x

#### Atom list

n label symbol quantity occupancy x y z multiplicity B radius weighth neutron scattering neu

1) Fe Fe 4.0 1.0 0 0 0 4 -0.51887554 1.27 55.847

Atomic #, atom #, isotope #, weight, radius, symbol for tables: 26, 54, 80, 55.847, 1.27, Fe

Neutron sf: 9.45

Magnetic sf: 0.0706 35.0085 0.3589 15.3583 0.5819 5.5606 -0.0114

Electron sf: 0.1929 0.8239 1.8689 2.3694 1.906 0.1087 1.0806 4.7637 22.85

Neutron abs: 0.5255255255255254

Electron abs: 0.0

X-ray sf: 0.493002 0.322912 0.140191 0.04081 10.5109 26.1257 3.14236 57.7997 0.003038 0.48

X-ray disp and abs: 0.0 0.0 0.0 0.0 0.002 0.002 0.008 0.008 0.018 0.035 0.0 0.059 0.09 0.09 0.09

#### Reflection list

n h k l multiplicity meanFhkl crystallite(Angstrom) microstrain

1) 1 1 1 8 41095.43013139273 170.57061686958397 0.00135222823127656

2) 2 0 0 6 27207.03944739249 158.988349695506 0.002342128

3) 2 2 0 12 36661.114638503095 167.67505007638914 0.0016561345912068863

4) 3 1 1 24 58742.99050591704 164.4444590254748 0.00193980014344128

5) 2 2 2 8 18381.411059227332 170.57061686958397 0.00135222823127656

6) 4 0 0 6 11176.519592968885 158.988349695506 0.002342128

7) 3 3 1 24 39664.53100406163 168.51725094423682 0.0015738046615112178

8) 4 2 0 24 38345.81721609068 164.5478379392712 0.0019313682265433279

9) 4 2 2 24 34375.78527841829 167.67505007610384 0.001656134591206886

String informations (CIF term, value) :

\_chemical\_name\_common, Austenite

\_chemical\_formula\_sum, Phase unknown

\_symmetry\_cell\_setting, cubic

\_symmetry\_Int\_Tables\_number, 225

\_symmetry\_space\_group\_name\_sch, 1

\_symmetry\_space\_group\_name\_H-M, Fm-3m

\_symmetry\_space\_group\_name\_Hall, P1

\_cell\_formula\_units\_Z, 1

\_refine\_ls\_d\_res\_low, 0

\_refine\_ls\_d\_res\_high, 5000

\_reflns\_d\_resolution\_low, 0.7

\_reflns\_d\_resolution\_high, 50

Parameter informations :

- Parameter: paramete.sav:SB-G65-After:Austenite:\_cell\_length\_a Value: 3.6182716, minimum: 5

- Parameter: paramete.sav:SB-G65-After:Austenite:\_cell\_length\_b Value: 3.6182716, minimum: 5

- Parameter: paramete.sav:SB-G65-After:Austenite:\_cell\_length\_c Value: 3.6182716, minimum: 5

- Parameter: paramete.sav:SB-G65-After:Austenite:\_cell\_angle\_alpha Value: 90, minimum: 90.0,

- Parameter: paramete.sav:SB-G65-After:Austenite:\_cell\_angle\_beta Value: 90, minimum: 90.0, r

- Parameter: paramete.sav:SB-G65-After:Austenite:\_cell\_angle\_gamma Value: 90, minimum: 90.

- Parameter: paramete.sav:SB-G65-After:Austenite:\_riet\_par\_strain\_thermal Value: 0, minimum:

- Parameter: paramete.sav:SB-G65-After:Austenite:\_exptl\_absorpt\_cryst\_size Value: 0.3087943,

- Parameter: paramete.sav:SB-G65-After:Austenite:\_riet\_par\_phase\_scale\_factor Value: 3.11783

Subordinate objects :

Subordinate object number 0 :

Object: none tex

Subordinate object number 1 :

Object: Delf

Subordinate object number 2 :

Object: Popa rules

String informations (CIF term, value) :

\_rita\_harmonic\_expansion\_degree, 4

Parameter loop informations :

Parameter loop number : 0

- Parameter: paramete.sav:SB-G65-After:Austenite:Popa rules:\_riet\_par\_anisocryst\_size0 Value

- Parameter: paramete.sav:SB-G65-After:Austenite:Popa rules:\_riet\_par\_anisocryst\_size1 Value

Parameter loop number : 1

- Parameter: paramete.sav:SB-G65-After:Austenite:Popa rules:\_riet\_par\_aniso\_microstrain0 Value

- Parameter: paramete.sav:SB-G65-After:Austenite:Popa rules:\_riet\_par\_aniso\_microstrain1 Value

Subordinate object number 3 :

Object: none abm

Subordinate object number 4 :

Object: none pd

Subordinate object number 5 :

Object: no magnetic

Subordinate object number 6 :

Object: no strain

Subordinate object number 7 :

Object: No microabsorption

Subordinate object number 8 :

Object: Atomic Structure

String informations (CIF term, value) :

\_riet\_structure\_quantity\_from\_occupancy, true

\_refine\_ls\_energy\_weight, 1.0

Subordinate objects :

Subordinate object number 0 :

Object: Genetic Algorithm SDPD

String informations (CIF term, value) :

\_riet\_ga\_population\_size, 500  
\_riet\_ga\_generations\_number, 20  
\_riet\_ga\_mutation\_prob, 0.01  
\_riet\_ga\_permutation\_prob, 0.01

Subordinate object number 1 :

Object: No force field

Loops of subordinate objects :

Object loop number 0 :

Object number 0 :

Object: Fe

String informations (CIF term, value) :

\_atom\_site\_type\_symbol, Fe  
\_atom\_site\_constraints,  
\_atom\_type\_number\_in\_cell, 4.0  
\_atom\_site\_calc\_flag, .

Parameter informations :

- Parameter: paramete.sav:SB-G65-After:Austenite:Atomic Structure:Fe:\_atom\_site\_occupancy Value
- Parameter: paramete.sav:SB-G65-After:Austenite:Atomic Structure:Fe:\_atom\_site\_fract\_x Value
- Parameter: paramete.sav:SB-G65-After:Austenite:Atomic Structure:Fe:\_atom\_site\_fract\_y Value
- Parameter: paramete.sav:SB-G65-After:Austenite:Atomic Structure:Fe:\_atom\_site\_fract\_z Value
- Parameter: paramete.sav:SB-G65-After:Austenite:Atomic Structure:Fe:\_atom\_site\_B\_iso\_or\_eq Value
- Parameter: paramete.sav:SB-G65-After:Austenite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_11 Value
- Parameter: paramete.sav:SB-G65-After:Austenite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_22 Value
- Parameter: paramete.sav:SB-G65-After:Austenite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_33 Value
- Parameter: paramete.sav:SB-G65-After:Austenite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_23 Value
- Parameter: paramete.sav:SB-G65-After:Austenite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_13 Value
- Parameter: paramete.sav:SB-G65-After:Austenite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_12 Value

Subordinate object number 9 :

Object: atomic standard model

Subordinate object number 10 :

## Object: Le Bail

String informations (CIF term, value) :

\_riet\_lebail\_iteration\_max, 5  
\_riet\_lebail\_error\_max, 0.005  
\_riet\_lebail\_range\_factor, 0.05  
\_riet\_lebail\_use\_bkg, true  
\_riet\_lebail\_summation\_delta, 1.0E-4  
\_riet\_lebail\_use\_previous\_factors, true

Subordinate object number 11 :

## Object: Genetic Algorithm SDPD

String informations (CIF term, value) :

\_riet\_ga\_population\_size, 500  
\_riet\_ga\_generations\_number, 20  
\_riet\_ga\_mutation\_prob, 0.01  
\_riet\_ga\_permutation\_prob, 0.01

Subordinate object number 12 :

## Object: None TDS

Loops of subordinate objects :

Object number 2 :

## Object: Ferrite

### General position

- 1) +x | +y | +z
- 2) -y | +x | +z
- 3) -x | -y | +z
- 4) +y | -x | +z
- 5) +x | -z | +y
- 6) +x | -y | -z
- 7) +x | +z | -y
- 8) +z | +y | -x
- 9) -x | +y | -z
- 10) -z | +y | +x
- 11) +z | +x | +y
- 12) +y | +z | +x
- 13) -y | -z | +x
- 14) +z | -x | -y
- 15) -y | +z | -x
- 16) -z | -x | +y

- 17)  $-z \mid +x \mid -y$
- 18)  $+y \mid -z \mid -x$
- 19)  $+y \mid +x \mid -z$
- 20)  $-y \mid -x \mid -z$
- 21)  $-x \mid +z \mid +y$
- 22)  $-x \mid -z \mid -y$
- 23)  $+z \mid -y \mid +x$
- 24)  $-z \mid -y \mid -x$
- 25)  $-x \mid -y \mid -z$
- 26)  $+y \mid -x \mid -z$
- 27)  $+x \mid +y \mid -z$
- 28)  $-y \mid +x \mid -z$
- 29)  $-x \mid +z \mid -y$
- 30)  $-x \mid +y \mid +z$
- 31)  $-x \mid -z \mid +y$
- 32)  $-z \mid -y \mid +x$
- 33)  $+x \mid -y \mid +z$
- 34)  $+z \mid -y \mid -x$
- 35)  $-z \mid -x \mid -y$
- 36)  $-y \mid -z \mid -x$
- 37)  $+y \mid +z \mid -x$
- 38)  $-z \mid +x \mid +y$
- 39)  $+y \mid -z \mid +x$
- 40)  $+z \mid +x \mid -y$
- 41)  $+z \mid -x \mid +y$
- 42)  $-y \mid +z \mid +x$
- 43)  $-y \mid -x \mid +z$
- 44)  $+y \mid +x \mid +z$
- 45)  $+x \mid -z \mid -y$
- 46)  $+x \mid +z \mid +y$
- 47)  $-z \mid +y \mid -x$
- 48)  $+z \mid +y \mid +x$
- 49)  $+x+0.5 \mid +y+0.5 \mid +z+0.5$
- 50)  $-y+0.5 \mid +x+0.5 \mid +z+0.5$
- 51)  $-x+0.5 \mid -y+0.5 \mid +z+0.5$
- 52)  $+y+0.5 \mid -x+0.5 \mid +z+0.5$
- 53)  $+x+0.5 \mid -z+0.5 \mid +y+0.5$
- 54)  $+x+0.5 \mid -y+0.5 \mid -z+0.5$
- 55)  $+x+0.5 \mid +z+0.5 \mid -y+0.5$
- 56)  $+z+0.5 \mid +y+0.5 \mid -x+0.5$
- 57)  $-x+0.5 \mid +y+0.5 \mid -z+0.5$
- 58)  $-z+0.5 \mid +y+0.5 \mid +x+0.5$
- 59)  $+z+0.5 \mid +x+0.5 \mid +y+0.5$
- 60)  $+y+0.5 \mid +z+0.5 \mid +x+0.5$
- 61)  $-y+0.5 \mid -z+0.5 \mid +x+0.5$
- 62)  $+z+0.5 \mid -x+0.5 \mid -y+0.5$
- 63)  $-y+0.5 \mid +z+0.5 \mid -x+0.5$
- 64)  $-z+0.5 \mid -x+0.5 \mid +y+0.5$

65) -z+0.5 | +x+0.5 | -y+0.5  
 66) +y+0.5 | -z+0.5 | -x+0.5  
 67) +y+0.5 | +x+0.5 | -z+0.5  
 68) -y+0.5 | -x+0.5 | -z+0.5  
 69) -x+0.5 | +z+0.5 | +y+0.5  
 70) -x+0.5 | -z+0.5 | -y+0.5  
 71) +z+0.5 | -y+0.5 | +x+0.5  
 72) -z+0.5 | -y+0.5 | -x+0.5  
 73) -x+0.5 | -y+0.5 | -z+0.5  
 74) +y+0.5 | -x+0.5 | -z+0.5  
 75) +x+0.5 | +y+0.5 | -z+0.5  
 76) -y+0.5 | +x+0.5 | -z+0.5  
 77) -x+0.5 | +z+0.5 | -y+0.5  
 78) -x+0.5 | +y+0.5 | +z+0.5  
 79) -x+0.5 | -z+0.5 | +y+0.5  
 80) -z+0.5 | -y+0.5 | +x+0.5  
 81) +x+0.5 | -y+0.5 | +z+0.5  
 82) +z+0.5 | -y+0.5 | -x+0.5  
 83) -z+0.5 | -x+0.5 | -y+0.5  
 84) -y+0.5 | -z+0.5 | -x+0.5  
 85) +y+0.5 | +z+0.5 | -x+0.5  
 86) -z+0.5 | +x+0.5 | +y+0.5  
 87) +y+0.5 | -z+0.5 | +x+0.5  
 88) +z+0.5 | +x+0.5 | -y+0.5  
 89) +z+0.5 | -x+0.5 | +y+0.5  
 90) -y+0.5 | +z+0.5 | +x+0.5  
 91) -y+0.5 | -x+0.5 | +z+0.5  
 92) +y+0.5 | +x+0.5 | +z+0.5  
 93) +x+0.5 | -z+0.5 | -y+0.5  
 94) +x+0.5 | +z+0.5 | +y+0.5  
 95) -z+0.5 | +y+0.5 | -x+0.5  
 96) +z+0.5 | +y+0.5 | +x+0.5

#### Atom list

n label symbol quantity occupancy x y z multiplicity B radius weighth neutron scattering neu

1) Fe Fe 2.0 1.0 0 0 0 2 -0.51887554 1.27 55.847

Atomic #, atom #, isotope #, weight, radius, symbol for tables: 26, 54, 80, 55.847, 1.27, Fe

Neutron sf: 9.45

Magnetic sf: 0.0706 35.0085 0.3589 15.3583 0.5819 5.5606 -0.0114

Electron sf: 0.1929 0.8239 1.8689 2.3694 1.906 0.1087 1.0806 4.7637 22.85

Neutron abs: 0.525525525525254

Electron abs: 0.0

X-ray sf: 0.493002 0.322912 0.140191 0.04081 10.5109 26.1257 3.14236 57.7997 0.003038 0.48

X-ray disp and abs: 0.0 0.0 0.0 0.0 0.002 0.002 0.008 0.008 0.018 0.035 0.0 0.059 0.09 0.09 0.09

#### Reflection list

n h k l multiplicity meanFhkl crystallite(Angstrom) microstrain

1) 1 1 0 12 15076.062700339926 270.19639221209644 0.002192194912019798

2) 2 0 0 6 5313.504113623178 191.51988116123766 0.0019117347  
3) 2 1 1 24 16298.525904652455 270.19639220951234 0.002192194912019799  
4) 2 2 0 12 6624.443978490449 270.19639221209644 0.002192194912019798  
5) 3 1 0 24 11258.79395772967 219.84342513954684 0.002017197459858751  
6) 2 2 2 8 3304.81210460921 296.4218958917954 0.0022780214050763343  
7) 3 2 1 48 17980.839391495756 270.1963922108362 0.002192194912019799  
8) 4 0 0 6 2088.2898461635345 191.51988116123766 0.0019117347

String informations (CIF term, value) :

\_chemical\_name\_common, Ferrite  
\_chemical\_formula\_sum,  
\_symmetry\_cell\_setting, cubic  
\_symmetry\_Int\_Tables\_number, 229  
\_symmetry\_space\_group\_name\_sch, 1  
\_symmetry\_space\_group\_name\_H-M, Im-3m  
\_symmetry\_space\_group\_name\_Hall, P1  
\_cell\_formula\_units\_Z, 1  
\_refine\_ls\_d\_res\_low, 0  
\_refine\_ls\_d\_res\_high, 5000  
\_reflns\_d\_resolution\_low, 0.7  
\_reflns\_d\_resolution\_high, 50

Parameter informations :

- Parameter: paramete.sav:SB-G65-After:Ferrite:\_cell\_length\_a Value: 2.8751433, minimum: 5.0,  
- Parameter: paramete.sav:SB-G65-After:Ferrite:\_cell\_length\_b Value: 2.8751433, minimum: 5.0,  
- Parameter: paramete.sav:SB-G65-After:Ferrite:\_cell\_length\_c Value: 2.8751433, minimum: 5.0,  
- Parameter: paramete.sav:SB-G65-After:Ferrite:\_cell\_angle\_alpha Value: 90, minimum: 90.0, ma  
- Parameter: paramete.sav:SB-G65-After:Ferrite:\_cell\_angle\_beta Value: 90, minimum: 90.0, ma  
- Parameter: paramete.sav:SB-G65-After:Ferrite:\_cell\_angle\_gamma Value: 90, minimum: 90.0, r  
- Parameter: paramete.sav:SB-G65-After:Ferrite:\_riet\_par\_strain\_thermal Value: 0, minimum: -0.  
- Parameter: paramete.sav:SB-G65-After:Ferrite:\_exptl\_absorpt\_cryst\_size Value: 0, minimum: 0  
- Parameter: paramete.sav:SB-G65-After:Ferrite:\_riet\_par\_phase\_scale\_factor Value: 1.3276076

Subordinate objects :

Subordinate object number 0 :

Object: none tex

Subordinate object number 1 :

Object: Delf

Subordinate object number 2 :

Object: Popa rules

String informations (CIF term, value) :

\_rita\_harmonic\_expansion\_degree, 4

Parameter loop informations :

Parameter loop number : 0

- Parameter: paramete.sav:SB-G65-After:Ferrite:Popa rules:\_riet\_par\_anisocryst\_size0 Value: 25
- Parameter: paramete.sav:SB-G65-After:Ferrite:Popa rules:\_riet\_par\_anisocryst\_size1 Value: -9

Parameter loop number : 1

- Parameter: paramete.sav:SB-G65-After:Ferrite:Popa rules:\_riet\_par\_aniso\_microstrain0 Value:
- Parameter: paramete.sav:SB-G65-After:Ferrite:Popa rules:\_riet\_par\_aniso\_microstrain1 Value:

Subordinate object number 3 :

Object: none abm

Subordinate object number 4 :

Object: none pd

Subordinate object number 5 :

Object: no magnetic

Subordinate object number 6 :

Object: no strain

Subordinate object number 7 :

Object: No microabsorption

Subordinate object number 8 :

Object: Atomic Structure

String informations (CIF term, value) :

\_riet\_structure\_quantity\_from\_occupancy, true  
\_refine\_ls\_energy\_weight, 1.0

Subordinate objects :

Subordinate object number 0 :

Object: Genetic Algorithm SDPD

String informations (CIF term, value) :

\_riet\_ga\_population\_size, 500  
\_riet\_ga\_generations\_number, 20  
\_riet\_ga\_mutation\_prob, 0.01

\_riet\_ga\_permutation\_prob, 0.01

Subordinate object number 1 :

Object: No force field

Loops of subordinate objects :

Object loop number 0 :

Object number 0 :

Object: Fe

String informations (CIF term, value) :

\_atom\_site\_type\_symbol, Fe

\_atom\_site\_constraints,

\_atom\_type\_number\_in\_cell, 2.0

\_atom\_site\_calc\_flag, .

Parameter informations :

- Parameter: paramete.sav:SB-G65-After:Ferrite:Atomic Structure:Fe:\_atom\_site\_occupancy Value: 0
- Parameter: paramete.sav:SB-G65-After:Ferrite:Atomic Structure:Fe:\_atom\_site\_fract\_x Value: 0
- Parameter: paramete.sav:SB-G65-After:Ferrite:Atomic Structure:Fe:\_atom\_site\_fract\_y Value: 0
- Parameter: paramete.sav:SB-G65-After:Ferrite:Atomic Structure:Fe:\_atom\_site\_fract\_z Value: 0
- Parameter: paramete.sav:SB-G65-After:Ferrite:Atomic Structure:Fe:\_atom\_site\_B\_iso\_or\_equiv Value: 1
- Parameter: paramete.sav:SB-G65-After:Ferrite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_11 Value: 0.000000
- Parameter: paramete.sav:SB-G65-After:Ferrite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_22 Value: 0.000000
- Parameter: paramete.sav:SB-G65-After:Ferrite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_33 Value: 0.000000
- Parameter: paramete.sav:SB-G65-After:Ferrite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_23 Value: 0.000000
- Parameter: paramete.sav:SB-G65-After:Ferrite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_13 Value: 0.000000
- Parameter: paramete.sav:SB-G65-After:Ferrite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_12 Value: 0.000000

Subordinate object number 9 :

Object: atomic standard model

Subordinate object number 10 :

Object: Le Bail

String informations (CIF term, value) :

\_riet\_lebail\_iteration\_max, 5

\_riet\_lebail\_error\_max, 0.005

\_riet\_lebail\_range\_factor, 0.05

\_riet\_lebail\_use\_bkg, true

\_riet\_lebail\_summation\_delta, 1.0E-4

\_riet\_lebail\_use\_previous\_factors, true

Subordinate object number 11 :

Object: Genetic Algorithm SDPD

String informations (CIF term, value) :

\_riet\_ga\_population\_size, 500

\_riet\_ga\_generations\_number, 20

\_riet\_ga\_mutation\_prob, 0.01

\_riet\_ga\_permutation\_prob, 0.01

Subordinate object number 12 :

Object: None TDS

Loops of subordinate objects :