

Jacobi matrix :

#	0	1	2	3	4	5	6	7	8	9
0	2135664.8									
1	-240551.53	119169.836								
2	3092.4248	-1270.3441	84.64754							
3	274048.5	-144161.11	7359.9585	767844.56						
4	2.9161908E7	-1.7979004E7	767701.06	8.8105584E7	1.07021353E10					
5	3.5349353E9	-2.34965658E9	8.8116728E7	1.07054838E10	1.35071911E12	1.75192723E12				
6	4.62389871E11	-3.1525634E11	1.0698539E10	1.35009311E12	1.75056727E14	2.3179691E14	2.3179691E14			
7	16802.09	2833.5396	255.3346	26269.967	3025490.8	3.72330016E8	4.76951E8			
8	-94667.13	19518.14	940.66394	106245.664	1.3089831E7	1.68991373E9	2.24198688E9			
9	-5.2925284E7	2.9162102E7	-1334077.6	-1.41740528E8	-1.6942636E10	-2.14198688E11	-2.14198688E11			
10	-2.1043352E7	1.1172007E7	-583804.25	-5.8591176E7	-6.7198991E9	-8.2240288E11	-8.2240288E11			
11	-73044.69	15444.798	-1410.297	-157338.73	-1.9064148E7	-2.41929779E9	-3.11929779E9			

Correlation matrix:

#	0	1	2	3	4	5	6	7	8	9
0	1.0									
1	0.9379428	1.0								
2	0.4589572	-0.16389588	-1.0							
3	0.33858636	0.9126822	0.13914575	1.0						
4	0.8187173	-0.06386499	-1.0933962	0.08002708	-1.0					
5	0.057914324	0.51038116	1.1057235	0.19756736	0.11321757	1.0				
6	-0.62600124	-0.6302658	-0.7008377	-0.1711732	0.080449246	-1.0135853	1.0			
7	-1.2313623	-0.9405479	0.2983031	-0.7119054	0.09540001	-0.78108096	0.87408096	1.0		
8	-0.8200215	0.47490686	0.679758	0.7991848	0.41185138	-1.0967851	0.9771851	0.9771851	1.0	
9	-2.3883483	-1.0202318	0.7185207	-0.29742387	0.12621665	-0.91295666	0.9281666	0.9281666	0.9281666	1.0
10	2.0809135	0.98843324	-0.68783265	0.44928113	-0.22514263	0.9724573	-0.9724573	-0.9724573	-0.9724573	-0.9724573
11	-0.70068634	-1.4035591	-0.4376954	-1.243946	-0.553503	0.9695812	-0.7805812	-0.7805812	-0.7805812	-0.7805812

Correlation matrix from Choleski decomposition :

#	0	1	2	3	4	5	6	7	8	9
0	1.0									
1	0.9379428	1.0								
2	0.4589572	-0.16389588	-1.0							
3	0.33858636	0.9126822	0.13914575	1.0						
4	0.8187173	-0.06386499	-1.0933962	0.08002708	-1.0					
5	0.057914324	0.51038116	1.1057235	0.19756736	0.11321757	1.0				
6	-0.62600124	-0.6302658	-0.7008377	-0.1711732	0.080449246	-1.0135853	1.0			
7	-1.2313623	-0.9405479	0.2983031	-0.7119054	0.09540001	-0.78108096	0.87408096	1.0		
8	-0.8200215	0.47490686	0.679758	0.7991848	0.41185138	-1.0967851	0.9771851	0.9771851	1.0	
9	-2.3883483	-1.0202318	0.7185207	-0.29742387	0.12621665	-0.91295666	0.9281666	0.9281666	0.9281666	1.0
10	2.0809135	0.98843324	-0.68783265	0.44928113	-0.22514263	0.9724573	-0.9724573	-0.9724573	-0.9724573	-0.9724573
11	-0.70068634	-1.4035591	-0.4376954	-1.243946	-0.553503	0.9695812	-0.7805812	-0.7805812	-0.7805812	-0.7805812

Analysis title: Put a title here

Refined parameters:

0 SB-G65-after:SB-G65-After:layer1:\_pd\_phase\_atom\_%1 value:0.060538094 error:0.002035632  
1 SB-G65-after:SB-G65-After:layer1:\_pd\_phase\_atom\_%2 value:0.2980915 error:0.014526437  
2 SB-G65-after:SB-G65-After:SB-G65-after:\_riet\_par\_background\_pol0 value:133.58705 error:3.0  
3 SB-G65-after:SB-G65-After:SB-G65-after:\_riet\_par\_background\_pol1 value:-3.826253 error:0.2  
4 SB-G65-after:SB-G65-After:SB-G65-after:\_riet\_par\_background\_pol2 value:0.055763606 error:0  
5 SB-G65-after:SB-G65-After:SB-G65-after:\_riet\_par\_background\_pol3 value:-3.715651E-4 error:2  
6 SB-G65-after:SB-G65-After:SB-G65-after:\_riet\_par\_background\_pol4 value:8.722928E-7 error:2  
7 SB-G65-after:SB-G65-After:SB-G65-after:Diffraction Instrument:\_pd\_proc\_intensity\_incident val  
8 SB-G65-after:SB-G65-After:SB-G65-after:Diffraction Instrument:\_riet\_par\_2-theta\_offset0 value:  
9 SB-G65-after:SB-G65-After:Martensite:\_cell\_length\_a value:2.891999 error:5.940982E-4  
10 SB-G65-after:SB-G65-After:Martensite:\_cell\_length\_c value:2.8587143 error:0.0016789938  
11 SB-G65-after:SB-G65-After:Martensite:Atomic Structure:Fe:\_atom\_site\_B\_iso\_or\_equiv value:

Refinement final output indices:

Global Rwp: 0.19961345

Global Rp: 0.118839025

Global Rwpb (no background): 7.8397083

Global Rpb (no background): 0.12410355

Total Energy: 0.0

Refinement final output indices for single samples:

Sample SB-G65-After :

Sample Rwp: 0.19961345

Sample Rp: 0.118839025

Sample Rwpb (no background): 7.8397083

Sample Rpb (no background): 0.12410355

Refinement final output indices for single datasets:

DataSet SB-G65-after :

DataSet Rwp: 0.19961345

DataSet Rp: 0.118839025

DataSet Rwpb (no background): 7.8397083

DataSet Rpb (no background): 0.12410355

Refinement final output indices for single spectra:

Datafile SB-G65.xrdml(0) : Rwp: 0.19961345, Rp: 0.118839025, Rwpb: 7.8397083, Rpb: 0.12410355

Sample:SB-G65-After

Phases:

Martensite

Density: 7.7573288694543

Qc: 0.05531784084291778

Austenite

Density: 7.829752891451307

Qc: 0.05557547030419097  
Ferrite  
Density: 7.797424661633449  
Qc: 0.0554606189805659

## Object tree full informations

Object: SB-G65-after

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 15:18:51 BST 2013  
\_computing\_structure\_refinement, Maud, version 2.33  
\_refine\_ls\_R\_factor\_all, 0.118839025  
\_refine\_ls\_wR\_factor\_all, 0.19961345  
\_refine\_ls\_goodness\_of\_fit\_all, 0.10671681  
\_publ\_contact\_author\_name, Luca Lutterotti  
\_publ\_section\_title, Put a title here  
\_pd\_proc\_ls\_extract\_int, end of iteration  
\_pd\_proc\_ls\_texture\_comp, end of iteration  
\_computing\_reduce\_memory\_occ, true  
\_pd\_proc\_ls\_theoretical\_weight, false  
\_pd\_proc\_ls\_extract\_pos, end of iteration  
\_pd\_proc\_ls\_strain\_comp, end of iteration  
\_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, 16531.63  
\_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: Marquardt 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: SB-G65-after:SB-G65-After:\_pd\_spec\_orientation\_omega Value: 0, minimum: 0.0, maximum: 360.0, type: float
- Parameter: SB-G65-after:SB-G65-After:\_pd\_spec\_orientation\_chi Value: 0, minimum: 0.0, maximum: 90.0, type: float
- Parameter: SB-G65-after:SB-G65-After:\_pd\_spec\_orientation\_phi Value: 0, minimum: 0.0, maximum: 360.0, type: float
- Parameter: SB-G65-after:SB-G65-After:\_riet\_par\_spec\_displac\_x Value: 0, minimum: 0.0, maximum: 0.0, type: float
- Parameter: SB-G65-after:SB-G65-After:\_riet\_par\_spec\_displac\_y Value: 0, minimum: 0.0, maximum: 0.0, type: float
- Parameter: SB-G65-after:SB-G65-After:\_riet\_par\_spec\_displac\_z Value: 0, minimum: 0.0, maximum: 0.0, type: float
- Parameter: SB-G65-after:SB-G65-After:\_pd\_spec\_size\_axial Value: 0, minimum: 0.0, maximum: 0.0, type: float
- Parameter: SB-G65-after:SB-G65-After:\_pd\_spec\_size\_equat Value: 0, minimum: 0.0, maximum: 0.0, type: float
- Parameter: SB-G65-after:SB-G65-After:\_pd\_spec\_size\_thick Value: 0, minimum: 0.0, maximum: 0.0, type: float
- Parameter: SB-G65-after:SB-G65-After:\_pd\_spec\_size\_radius Value: 0, minimum: 0.0, maximum: 0.0, type: float
- Parameter: SB-G65-after:SB-G65-After:\_pd\_spec\_size\_radius\_y Value: 0, minimum: 0.0, maximum: 0.0, type: float

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: SB-G65-after:SB-G65-After:layer1:\_riet\_par\_spec\_layer\_thickness Value: 1.0E7, minimum
- Parameter: SB-G65-after:SB-G65-After:layer1:\_reflectivity\_layer\_critical\_qc Value: 0.04, minimum
- Parameter: SB-G65-after:SB-G65-After:layer1:\_reflectivity\_layer\_absorption Value: 2.0E-7, minimum
- Parameter: SB-G65-after:SB-G65-After:layer1:\_reflectivity\_layer\_roughness Value: 2.0, minimum

Parameter loop informations :

Parameter loop number : 0

- Parameter: SB-G65-after:SB-G65-After:layer1:\_pd\_phase\_atom\_%0 Value: 0.6413704, minimum
- Parameter: SB-G65-after:SB-G65-After:layer1:\_pd\_phase\_atom\_%1 Value: 0.060538094, minimum
- Parameter: SB-G65-after:SB-G65-After:layer1:\_pd\_phase\_atom\_%2 Value: 0.2980915, minimum

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: SB-G65-after:SB-G65-After:SB-G65-after:\_riet\_par\_background\_exp\_shift Value: 0, minimum
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:\_riet\_par\_background\_exp\_thermal\_shift Value: 0, minimum
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:\_pd\_spec\_orientation\_omega Value: 0, minimum
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:\_pd\_spec\_orientation\_chi Value: 0, minimum
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:\_pd\_spec\_orientation\_phi Value: 0, minimum

Parameter loop informations :

Parameter loop number : 0

- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:\_riet\_par\_background\_pol0 Value: 133.58
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:\_riet\_par\_background\_pol1 Value: -3.826

- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:\_riet\_par\_background\_pol2 Value: 0.0557
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:\_riet\_par\_background\_pol3 Value: -3.715
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:\_riet\_par\_background\_pol4 Value: 8.7229

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: SB-G65-after:SB-G65-After:SB-G65-after:Diffraction Instrument:\_pd\_proc\_intensity

Parameter loop informations :

Parameter loop number : 0

- Parameter: SB-G65-after: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) :

\_diffrn\_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: SB-G65-after:SB-G65-After:SB-G65-after:Diffraction Instrument:Bragg-Brentano:\_diffrn\_radiation\_monochromator, Filtered
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:Diffraction Instrument:Bragg-Brentano:\_pd\_instr\_2theta\_monochr\_post, 0

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\_convolutd, false  
\_riet\_par\_asymmetry\_truncation, 0.4

Parameter loop informations :

Parameter loop number : 0

- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:Diffraction Instrument:Caglioti PV:\_riet\_caglioti\_d\_dep, true
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:Diffraction Instrument:Caglioti PV:\_riet\_asymmetry\_tan\_dep, false

Parameter loop number : 1

- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:Diffraction Instrument:Caglioti PV:\_riet\_omega/chi\_broadening\_convolutd, false

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

Parameter loop number : 2

- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:Diffraction Instrument:Caglioti PV:\_riet\_pa
- Parameter: SB-G65-after: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: SB-G65-after:SB-G65-After:SB-G65-after:SB-G65.xrdml(0):\_pd\_meas\_counts\_moni
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:SB-G65.xrdml(0):\_riet\_par\_spec\_displac
- Parameter: SB-G65-after: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 -0.5603808 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 5074.580389254107 1249.127682077458 0.008399206813394733

2) 1 0 1 8 10101.495587192225 209.5008302930047 0.0047129082544769205

3) 2 0 0 4 3602.9067474750914 1092.1279698148635 0.005187216

4) 0 0 2 2 1776.897132799626 1319.9663126250769 0.01644604007021304

5) 1 2 1 8 5544.796626206823 750.8186754619819 0.012307017669380775

6) 2 1 1 8 5544.796626206823 523.2808230341068 0.0027648843205678618

7) 1 1 2 8 5500.937754620901 381.91435816491855 0.005295680531183022

8) 2 2 0 4 2271.7916979971246 1249.127682077458 0.008399206813394733

9) 2 0 2 8 4506.042127162397 209.5008302930047 0.0047129082544769205

10) 1 3 0 4 1939.8635200430524 1313.7566730543972 0.011118882884590583

11) 3 1 0 4 1939.8635200430524 983.5390594043979 0.010357469725597755

12) 3 0 1 8 3873.4179354356056 749.4127662092583 0.003379500096451694

13) 1 0 3 8 3823.968708145283 944.9833931990421 0.0136279032616273

14) 2 2 2 8 3414.430350948024 344.07569285714 0.00936189107782995  
 15) 2 3 1 8 3121.5458275327455 1058.5924490603743 0.0121119174068579  
 16) 3 2 1 8 3121.5458275327455 848.6973789803867 2.681414390286593E-4  
 17) 1 3 2 8 3112.7597771836963 447.1576296318871 0.010963625121646092  
 18) 3 1 2 8 3112.7597771836963 280.9117398085282 0.0019881135623188093  
 19) 1 2 3 8 3098.37366646925 362.3061103333883 0.002357583233290552  
 20) 2 1 3 8 3098.37366646925 321.4268259294117 0.00584322637755813  
 21) 4 0 0 4 1457.1905496038487 1092.1279698148635 0.005187216  
 22) 0 0 4 2 720.8343332056419 1319.9663126250769 0.01644604007021304

String informations (CIF term, value) :

\_chemical\_name\_common, Martensite  
 \_chemical\_formula\_sum, Phase unknown  
 \_symmetry\_cell\_setting, tetragonal  
 \_symmetry\_Int\_Tables\_number, triclinic  
 \_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: SB-G65-after:SB-G65-After:Martensite:\_cell\_length\_a Value: 2.891999, minimum: 5  
 - Parameter: SB-G65-after:SB-G65-After:Martensite:\_cell\_length\_b Value: 2.891999, minimum: 5  
 - Parameter: SB-G65-after:SB-G65-After:Martensite:\_cell\_length\_c Value: 2.8587143, minimum:  
 - Parameter: SB-G65-after:SB-G65-After:Martensite:\_cell\_angle\_alpha Value: 90, minimum: 90.0  
 - Parameter: SB-G65-after:SB-G65-After:Martensite:\_cell\_angle\_beta Value: 90, minimum: 90.0,  
 - Parameter: SB-G65-after:SB-G65-After:Martensite:\_cell\_angle\_gamma Value: 90, minimum: 90  
 - Parameter: SB-G65-after:SB-G65-After:Martensite:\_riet\_par\_strain\_thermal Value: 0, minimum:  
 - Parameter: SB-G65-after:SB-G65-After:Martensite:\_exptl\_absorpt\_cryst\_size Value: 0, minimun  
 - Parameter: SB-G65-after: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: SB-G65-after:SB-G65-After:Martensite:Popa rules:\_riet\_par\_anisocryst\_size0 Value
- Parameter: SB-G65-after:SB-G65-After:Martensite:Popa rules:\_riet\_par\_anisocryst\_size1 Value
- Parameter: SB-G65-after:SB-G65-After:Martensite:Popa rules:\_riet\_par\_anisocryst\_size2 Value
- Parameter: SB-G65-after:SB-G65-After:Martensite:Popa rules:\_riet\_par\_anisocryst\_size3 Value
- Parameter: SB-G65-after:SB-G65-After:Martensite:Popa rules:\_riet\_par\_anisocryst\_size4 Value

Parameter loop number : 1

- Parameter: SB-G65-after:SB-G65-After:Martensite:Popa rules:\_riet\_par\_aniso\_microstrain0 Val
- Parameter: SB-G65-after:SB-G65-After:Martensite:Popa rules:\_riet\_par\_aniso\_microstrain1 Val
- Parameter: SB-G65-after:SB-G65-After:Martensite:Popa rules:\_riet\_par\_aniso\_microstrain2 Val
- Parameter: SB-G65-after:SB-G65-After:Martensite:Popa rules:\_riet\_par\_aniso\_microstrain3 Val
- Parameter: SB-G65-after:SB-G65-After:Martensite:Popa rules:\_riet\_par\_aniso\_microstrain4 Val

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

Parameters bounded to this parameter:

SB-G65-after:SB-G65-After:Austenite:Atomic Structure:Fe:\_atom\_site\_B\_iso\_or\_equiv  
SB-G65-after:SB-G65-After:Ferrite:Atomic Structure:Fe:\_atom\_site\_B\_iso\_or\_equiv

- Parameter: SB-G65-after:SB-G65-After:Martensite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_11
- Parameter: SB-G65-after:SB-G65-After:Martensite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_22
- Parameter: SB-G65-after:SB-G65-After:Martensite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_33
- Parameter: SB-G65-after:SB-G65-After:Martensite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_23
- Parameter: SB-G65-after:SB-G65-After:Martensite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_13
- Parameter: SB-G65-after: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 | +y | +x
- 11) +z | +x | +y
- 12) +y | +z | +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)  $-z+0.5 \mid +y+0.5 \mid +x$   
155)  $+z+0.5 \mid +x+0.5 \mid +y$   
156)  $+y+0.5 \mid +z+0.5 \mid +x$

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 -0.5603808 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 41292.76020359551 156.13226340182888 0.0011898097855989414
- 2) 2 0 0 6 27381.224307530145 127.14182989696118 0.0020608109999999999
- 3) 2 2 0 12 37131.122747501024 148.88465502642458 0.0014572134328438306
- 4) 3 1 1 24 59779.98530327603 140.79848039106793 0.0017068074304245403
- 5) 2 2 2 8 18735.585377122185 156.13226340182888 0.0011898097855989414
- 6) 4 0 0 6 11464.310660353638 127.14182989696118 0.0020608109999999999
- 7) 3 3 1 24 40879.6289213008 150.9926851633674 0.0013847722918190614
- 8) 4 2 0 24 39583.1324559923 141.05723797981776 0.0016993882854869512
- 9) 4 2 2 24 35710.356728789666 148.88465502571046 0.0014572134328438306

String informations (CIF term, value) :

\_chemical\_name\_common, Austenite  
\_chemical\_formula\_sum, Phase unknown  
\_symmetry\_cell\_setting, cubic  
\_symmetry\_Int\_Tables\_number, triclinic  
\_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: SB-G65-after:SB-G65-After:Austenite:\_cell\_length\_a Value: 3.6184318, minimum: 5
- Parameter: SB-G65-after:SB-G65-After:Austenite:\_cell\_length\_b Value: 3.6184318, minimum: 5
- Parameter: SB-G65-after:SB-G65-After:Austenite:\_cell\_length\_c Value: 3.6184318, minimum: 5
- Parameter: SB-G65-after:SB-G65-After:Austenite:\_cell\_angle\_alpha Value: 90, minimum: 90.0,
- Parameter: SB-G65-after:SB-G65-After:Austenite:\_cell\_angle\_beta Value: 90, minimum: 90.0, n
- Parameter: SB-G65-after:SB-G65-After:Austenite:\_cell\_angle\_gamma Value: 90, minimum: 90.0,
- Parameter: SB-G65-after:SB-G65-After:Austenite:\_riet\_par\_strain\_thermal Value: 0, minimum: -
- Parameter: SB-G65-after:SB-G65-After:Austenite:\_exptl\_absorpt\_cryst\_size Value: 0.46801862
- Parameter: SB-G65-after:SB-G65-After:Austenite:\_riet\_par\_phase\_scale\_factor Value: 3.11414

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: SB-G65-after:SB-G65-After:Austenite:Popa rules:\_riet\_par\_anisocryst\_size0 Value:

- Parameter: SB-G65-after:SB-G65-After:Austenite:Popa rules:\_riet\_par\_anisocryst\_size1 Value:

Parameter loop number : 1

- Parameter: SB-G65-after:SB-G65-After:Austenite:Popa rules:\_riet\_par\_aniso\_microstrain0 Value:

- Parameter: SB-G65-after: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: SB-G65-after:SB-G65-After:Austenite:Atomic Structure:Fe:\_atom\_site\_occupancy Value
- Parameter: SB-G65-after:SB-G65-After:Austenite:Atomic Structure:Fe:\_atom\_site\_fract\_x Value
- Parameter: SB-G65-after:SB-G65-After:Austenite:Atomic Structure:Fe:\_atom\_site\_fract\_y Value
- Parameter: SB-G65-after:SB-G65-After:Austenite:Atomic Structure:Fe:\_atom\_site\_fract\_z Value
- Parameter: SB-G65-after:SB-G65-After:Austenite:Atomic Structure:Fe:\_atom\_site\_B\_iso\_or\_equiv Value
- Parameter: SB-G65-after:SB-G65-After:Austenite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_11 Value
- Parameter: SB-G65-after:SB-G65-After:Austenite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_22 Value
- Parameter: SB-G65-after:SB-G65-After:Austenite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_33 Value
- Parameter: SB-G65-after:SB-G65-After:Austenite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_23 Value
- Parameter: SB-G65-after:SB-G65-After:Austenite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_13 Value
- Parameter: SB-G65-after: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 | +x | -y
- 18) +y | -z | -x
- 19) +y | +x | -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)  $-z+0.5 \mid +x+0.5 \mid -y+0.5$
- 66)  $+y+0.5 \mid -z+0.5 \mid -x+0.5$
- 67)  $+y+0.5 \mid +x+0.5 \mid -z+0.5$

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 -0.5603808 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 15155.247376696523 351.10910702138517 0.002394770409058373

2) 2 0 0 6 5368.83787299941 234.2359219287546 0.0034314161

3) 2 1 1 24 16551.96843565484 351.1091070175466 0.002394770409058373

4) 2 2 0 12 6761.417616153496 351.10910702138517 0.002394770409058373

5) 3 1 0 24 11549.318483049155 276.31026856210167 0.003098439549388316  
6) 2 2 2 8 3407.0551688821206 390.0668353797713 0.0019291694929051046  
7) 3 2 1 48 18629.631449118693 351.10910701951315 0.002394770409058372  
8) 4 0 0 6 2174.418349588474 234.2359219287546 0.0034314161

String informations (CIF term, value) :

\_chemical\_name\_common, Ferrite  
\_chemical\_formula\_sum, Phase unknown  
\_symmetry\_cell\_setting, cubic  
\_symmetry\_Int\_Tables\_number, triclinic  
\_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: SB-G65-after:SB-G65-After:Ferrite:\_cell\_length\_a Value: 2.8759148, minimum: 5.0,  
- Parameter: SB-G65-after:SB-G65-After:Ferrite:\_cell\_length\_b Value: 2.8759148, minimum: 5.0,  
- Parameter: SB-G65-after:SB-G65-After:Ferrite:\_cell\_length\_c Value: 2.8759148, minimum: 5.0,  
- Parameter: SB-G65-after:SB-G65-After:Ferrite:\_cell\_angle\_alpha Value: 90, minimum: 90.0, ma  
- Parameter: SB-G65-after:SB-G65-After:Ferrite:\_cell\_angle\_beta Value: 90, minimum: 90.0, max  
- Parameter: SB-G65-after:SB-G65-After:Ferrite:\_cell\_angle\_gamma Value: 90, minimum: 90.0, n  
- Parameter: SB-G65-after:SB-G65-After:Ferrite:\_riet\_par\_strain\_thermal Value: 0, minimum: -0.1  
- Parameter: SB-G65-after:SB-G65-After:Ferrite:\_exptl\_absorpt\_cryst\_size Value: 0, minimum: 0.  
- Parameter: SB-G65-after:SB-G65-After:Ferrite:\_riet\_par\_phase\_scale\_factor Value: 2.0065796

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: SB-G65-after:SB-G65-After:Ferrite:Popa rules:\_riet\_par\_anisocryst\_size0 Value: 32
- Parameter: SB-G65-after:SB-G65-After:Ferrite:Popa rules:\_riet\_par\_anisocryst\_size1 Value: -1

Parameter loop number : 1

- Parameter: SB-G65-after:SB-G65-After:Ferrite:Popa rules:\_riet\_par\_aniso\_microstrain0 Value:
- Parameter: SB-G65-after: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: SB-G65-after:SB-G65-After:Ferrite:Atomic Structure:Fe:\_atom\_site\_occupancy Value: 0
- Parameter: SB-G65-after:SB-G65-After:Ferrite:Atomic Structure:Fe:\_atom\_site\_fract\_x Value: 0
- Parameter: SB-G65-after:SB-G65-After:Ferrite:Atomic Structure:Fe:\_atom\_site\_fract\_y Value: 0
- Parameter: SB-G65-after:SB-G65-After:Ferrite:Atomic Structure:Fe:\_atom\_site\_fract\_z Value: 0
- Parameter: SB-G65-after:SB-G65-After:Ferrite:Atomic Structure:Fe:\_atom\_site\_B\_iso\_or\_equiv Value: 0
- Parameter: SB-G65-after:SB-G65-After:Ferrite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_11 Value: 0
- Parameter: SB-G65-after:SB-G65-After:Ferrite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_22 Value: 0
- Parameter: SB-G65-after:SB-G65-After:Ferrite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_33 Value: 0
- Parameter: SB-G65-after:SB-G65-After:Ferrite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_23 Value: 0
- Parameter: SB-G65-after:SB-G65-After:Ferrite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_13 Value: 0
- Parameter: SB-G65-after:SB-G65-After:Ferrite:Atomic Structure:Fe:\_atom\_site\_aniso\_B\_12 Value: 0

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 :