

Jacobi matrix :

#	0	1	2	3	4	5	6	7	8	9
	30	31	32	33						
0	1647945.9									
1	-98675.305	9555.37								
2	2344.2175	-354.79285	84.61098							
3	232389.73	-40128.14	7355.0566	767151.9						
4	2.677903E7	-4996283.5	766809.9	8.798268E7	1.06819348E10					
5	3.39072179E9	-6.5676493E8	8.8034176E7	1.06929295E10	1.34846887E12	1.74939622E13				
6	4.52637426E11	-8.9043747E10	1.0701866E10	1.35019666E12	1.74983578E14	2.3175133E15				
7	5765.963	-432.23538	97.13793	9472.145	1042092.1	1.24181136E8	1.5570113E9			
8	-89051.39	17764.922	16.888342	3101.2996	438107.88	6.051618E7	8.503118E8			
9	-207161.58	49744.19	-13134.928	-1714300.5	-2.2724096E8	-3.05375867E10	-4.155113E11			
10	-57450.258	16805.525	-4628.7905	-611971.06	-8.1879928E7	-1.10759997E10	-1.24181136E8			
11	-11.105561	0.84917736	-0.2613991	-18.909483	-1681.313	-173302.84	-1.952113E9			
12	0.21879539	-0.03808857	-0.026910013	-1.7342008	-138.08876	-12893.5625	-1.34846887E12			
13	0.60690796	-0.10231518	0.06042357	3.8157492	302.54352	29038.426	315211.3			
14	-0.7004527	0.11949393	-0.0066745426	-1.0202876	-151.68356	-22376.29	-32811.3			
15	1.6489085	-0.18999594	-0.012353116	-0.3108677	14.66813	4347.6323	69311.3			
16	-138683.64	24390.887	-168.79459	-14914.064	-903162.25	4.6621416E7	3.07113E9			
17	-79183.91	60046.0	-1063.9994	-149688.55	-2.1642182E7	-3.11937562E9	-4.4621416E7			
18	-465144.97	23986.46	300.87228	109514.29	2.0818488E7	3.47137562E9	5.57113E9			
19	-546265.6	86179.79	-7957.5483	-931548.94	-1.1669788E8	-1.51189688E10	-1.952113E9			
20	264353.12	-53725.254	6589.257	772980.5	9.4993648E7	1.21437225E10	1.60113E9			
21	-36721.273	4139.3125	-325.92365	-39821.383	-5117059.0	-6.7946752E8	-9.21113E9			
22	44092.29	8238.988	-221.43272	-42312.26	-6782647.5	-1.05832941E9	-1.646113E9			
23	48077.58	-2903.3528	92.966805	9174.007	1043660.94	1.30019592E8	1.708113E9			
24	105.026634	-4.707396	-0.05320421	-4.2335453	-404.94843	-44530.3	-53470.1			
25	-0.0021842269	0.10863573	-0.002403717	-0.057077043	12.787413	3276.8047	5.57113E9			
26	0.0	0.0	0.0	0.0	0.0	0.0	0.0			
27	0.0	0.0	0.0	0.0	0.0	0.0	0.0			
28	340020.8	-263966.66	-2558.2422	-245802.89	-2.6345302E7	-3.05201126E9	-3.71113E9			
29	-91.987595	18.320793	-0.6884257	-50.762894	-4277.5806	-403880.75	-4.155113E9			
30	5.360077	-1.4182633	-0.090615824	-7.7883935	-684.1714	-63348.832	-62101.3			
	0.022324573									
31	-13227.334	469707.16	-13668.5625	-1352686.6	-1.42265824E8	-1.56595261E10	-1.952113E9			
	231.07933	3.81627424E8								
32	501229.38	281049.28	-7259.7935	-738825.06	-8.079064E7	-9.324459E9	-1.12113E9			
	-462.57205	2.04036032E8	1.5727672E8							
33	3702.0164	-711.49115	-222.90092	-23129.5	-2554019.8	-2.94843424E8	-3.51113E9			
	-1.2791237	-261759.1	-145582.8	7436.2705						

Warning: error computing correlation matrix, no correlation matrix in output!

Correlation matrix:

#	0	1	2	3	4	5	6	7	8	9
	30	31	32	33						
0	0.0									
1	-76.86648	0.0								
2	1.8261079	-3.550712	0.0							
3	181.02788	-434.06693	661.6939	0.0						
4	20860.436	-56182.035	63865.316	53402.723	0.0					
5	2641318.0	-7513471.0	6822129.0	7418066.0	3117924.8	0.0				
6	3.52597312E8	-1.0256857E9	7.7426496E8	9.9998822E8	5.6592646E8	1.54964224E9				
7	4.491593	-1.4403528	10.115234	4.0770316	0.295639	2.8181362	-0.20633			
8	-69.369606	205.87497	105.539185	107.01042	78.86507	65.78633	33.2683			
9	-161.37556	618.3146	-1284.5682	-1723.4125	-1191.7844	-430.20853	24.392			
10	-44.75283	221.32146	-453.88824	-630.92615	-461.38947	-169.60063	44.616			
11	-0.008651054	0.003050211	-0.028331185	0.008293602	0.002927446	-0.010454704				
12	1.704381E-4	-4.1377256E-4	-0.0034622436	0.0010530907	-9.021238E-7	-0.001367717				
13	4.727716E-4	-0.0010924862	0.006719369	-0.0036195645	-3.5897613E-4	0.003644727				
14	-5.456414E-4	0.0012841994	-1.3495424E-4	-8.3564804E-4	-0.0011795507	-0.00104197				
15	0.0012844733	-0.0015112349	-0.0024213204	0.0012249654	-6.1787403E-4	-0.0022194				
16	-108.03234	266.38358	117.57878	129.15553	151.12363	217.40437	156.44			
17	-61.682995	915.7962	277.59903	229.02274	89.92194	109.24538	175.597			
18	-362.34048	-64.007225	88.729805	269.48022	373.7266	379.13626	285.08			
19	-425.53217	885.4266	-487.11853	-449.65164	-233.68806	95.84461	482.216			
20	205.92685	-627.5307	480.8971	441.27936	92.08547	92.85485	264.6610			
21	-28.605284	32.133385	-19.25877	-24.181576	-15.325753	-8.369924	-4.7293			
22	34.347187	180.14891	42.900574	3.8913307	-25.76912	-78.209015	-138.58			
23	37.451664	-0.40694723	2.791363	1.1268556	0.08635192	0.78610617	-0.05			
24	0.08181407	0.026185986	-0.013229289	0.0032723416	0.0023497678	-0.011141993				
25	-1.7014778E-6	0.0017967464	4.8018363E-4	0.0012328777	0.0013658202	2.1551314E				
26	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0		
27	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
28	264.8708	-4033.917	-2095.5608	-2001.4178	-1407.5828	-1126.7896	-524.80			
29	-0.07165686	0.2121684	0.023625474	0.11760392	0.10666352	0.028492106	0.0			

30	0.004175414	-0.018170552	-0.01964108	-0.010446535	0.0015924738	-0.009332636				
	0.0									
31	-10.303882	7764.822	1679.9166	2761.4463	3120.31	2204.2144	893.761			
	-2353.911	0.0								
32	390.44965	5150.909	1244.9645	1832.4072	1826.7775	1200.7361	501.762			
	-3773.09	3849.5278	0.0							
33	2.8838115	-8.1110325	-31.009716	-20.233503	-0.7043679	0.9363893	1.8425			
	-5.2883263	-7.7360945	-2.872988	0.0						

Correlation matrix from Choleski decomposition :

#	0	1	2	3	4	5	6	7	8	9
	30	31	32	33						
0	0.0									
1	-76.86648	0.0								
2	1.8261079	-3.550712	0.0							

3	181.02788	-434.06693	661.6939	0.0				
4	20860.436	-56182.035	63865.316	53402.723	0.0			
5	2641318.0	-7513471.0	6822129.0	7418066.0	3117924.8	0.0		
6	3.52597312E8	-1.0256857E9	7.7426496E8	9.9998822E8	5.6592646E8	1.54964224E8		
7	4.491593	-1.4403528	10.115234	4.0770316	0.295639	2.8181362	-0.20633	
8	-69.369606	205.87497	105.539185	107.01042	78.86507	65.78633	33.2683	
9	-161.37556	618.3146	-1284.5682	-1723.4125	-1191.7844	-430.20853	24.392	
10	-44.75283	221.32146	-453.88824	-630.92615	-461.38947	-169.60063	44.616	
11	-0.008651054	0.003050211	-0.028331185	0.008293602	0.002927446	-0.010454704		
12	1.704381E-4	-4.1377256E-4	-0.0034622436	0.0010530907	-9.021238E-7	-0.001367717		
13	4.727716E-4	-0.0010924862	0.006719369	-0.0036195645	-3.5897613E-4	0.003644727		
14	-5.456414E-4	0.0012841994	-1.3495424E-4	-8.3564804E-4	-0.0011795507	-0.00104197		
15	0.0012844733	-0.0015112349	-0.0024213204	0.0012249654	-6.1787403E-4	-0.0022194		
16	-108.03234	266.38358	117.57878	129.15553	151.12363	217.40437	156.44	
17	-61.682995	915.7962	277.59903	229.02274	89.92194	109.24538	175.597	
18	-362.34048	-64.007225	88.729805	269.48022	373.7266	379.13626	285.08	
19	-425.53217	885.4266	-487.11853	-449.65164	-233.68806	95.84461	482.216	
20	205.92685	-627.5307	480.8971	441.27936	92.08547	92.85485	264.6610	
21	-28.605284	32.133385	-19.25877	-24.181576	-15.325753	-8.369924	-4.7293	
22	34.347187	180.14891	42.900574	3.8913307	-25.76912	-78.209015	-138.58	
23	37.451664	-0.40694723	2.791363	1.1268556	0.08635192	0.78610617	-0.05	
24	0.08181407	0.026185986	-0.013229289	0.0032723416	0.0023497678	-0.011141993		
25	-1.7014778E-6	0.0017967464	4.8018363E-4	0.0012328777	0.0013658202	2.1551314E		
26	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
27	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
28	264.8708	-4033.917	-2095.5608	-2001.4178	-1407.5828	-1126.7896	-524.80	
29	-0.07165686	0.2121684	0.023625474	0.11760392	0.10666352	0.028492106	0.0	
30	0.004175414	-0.018170552	-0.01964108	-0.010446535	0.0015924738	-0.009332636	0.0	
31	-10.303882	7764.822	1679.9166	2761.4463	3120.31	2204.2144	893.761	
	-2353.911	0.0						
32	390.44965	5150.909	1244.9645	1832.4072	1826.7775	1200.7361	501.762	
	-3773.09	3849.5278	0.0					
33	2.8838115	-8.1110325	-31.009716	-20.233503	-0.7043679	0.9363893	1.8425	
	-5.2883263	-7.7360945	-2.872988	0.0				

Analysis title: Put a title here

Refined parameters:

0 paramete.sav:SB-G65-After:layer1:Volume fraction of Fe4.00 value:0.045788053 error:0.32283

1 paramete.sav:SB-G65-After:layer1:Volume fraction of ferrite value:0.7635263 error:0.14003392

2 paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol0 value:126.29527 error:2.8

3 paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol1 value:-3.024153 error:0.2

4 paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol2 value:0.0401779 error:0.0

5 paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol3 value:-2.4999186E-4 erro

6 paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol4 value:5.940357E-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:2.8928173 error:0.0023793494
10 paramete.sav:SB-G65-After:Martensite:_cell_length_c value:2.897531 error:0.00320598
11 paramete.sav:SB-G65-After:Martensite:Popa rules:_riet_par_anisocryst_size0 value:338.5291
12 paramete.sav:SB-G65-After:Martensite:Popa rules:_riet_par_anisocryst_size1 value:-165.5060
13 paramete.sav:SB-G65-After:Martensite:Popa rules:_riet_par_anisocryst_size2 value:499.22372
14 paramete.sav:SB-G65-After:Martensite:Popa rules:_riet_par_anisocryst_size3 value:43.124096
15 paramete.sav:SB-G65-After:Martensite:Popa rules:_riet_par_anisocryst_size4 value:78.03509
16 paramete.sav:SB-G65-After:Martensite:Popa rules:_riet_par_aniso_microstrain0 value:0.00312
17 paramete.sav:SB-G65-After:Martensite:Popa rules:_riet_par_aniso_microstrain1 value:0.01052
18 paramete.sav:SB-G65-After:Martensite:Popa rules:_riet_par_aniso_microstrain2 value:-0.0117
19 paramete.sav:SB-G65-After:Martensite:Popa rules:_riet_par_aniso_microstrain3 value:-0.0211
20 paramete.sav:SB-G65-After:Martensite:Popa rules:_riet_par_aniso_microstrain4 value:0.01554
21 paramete.sav:SB-G65-After:Martensite:Atomic Structure:Fe:_atom_site_B_iso_or_equiv value:
22 paramete.sav:SB-G65-After:Austenite:_cell_length_a value:3.6166866 error:5.4276845E-4
23 paramete.sav:SB-G65-After:Austenite:_riet_par_phase_scale_factor value:1.8754184 error:11.
24 paramete.sav:SB-G65-After:Austenite:Popa rules:_riet_par_anisocryst_size0 value:233.2672 e
25 paramete.sav:SB-G65-After:Austenite:Popa rules:_riet_par_anisocryst_size1 value:-28.208872
26 paramete.sav:SB-G65-After:Austenite:Popa rules:_riet_par_aniso_microstrain0 value:0.0 not re
27 paramete.sav:SB-G65-After:Austenite:Popa rules:_riet_par_aniso_microstrain1 value:0.0 not re
28 paramete.sav:SB-G65-After:Ferrite:_cell_length_a value:2.8754842 error:4.183571E-4
29 paramete.sav:SB-G65-After:Ferrite:Popa rules:_riet_par_anisocryst_size0 value:289.03735 er
30 paramete.sav:SB-G65-After:Ferrite:Popa rules:_riet_par_anisocryst_size1 value:-183.53935 er
31 paramete.sav:SB-G65-After:Ferrite:Popa rules:_riet_par_aniso_microstrain0 value:-0.0041583
32 paramete.sav:SB-G65-After:Ferrite:Popa rules:_riet_par_aniso_microstrain1 value:-0.0024848
33 paramete.sav:SB-G65-After:Ferrite:Atomic Structure:Fe:_atom_site_B_iso_or_equiv value:-0.3

Refinement final output indices:

Global Rwp: 0.20510338

Global Rp: 0.12726642

Global Rwpb (no background): 8.558202

Global Rpb (no background): 0.13635594

Total Energy: 0.0

Refinement final output indices for single samples:

Sample SB-G65-After :

Sample Rwp: 0.20510338

Sample Rp: 0.12726642

Sample Rwpb (no background): 8.558202

Sample Rpb (no background): 0.13635594

Refinement final output indices for single datasets:

DataSet SB-G65-after :

DataSet Rwp: 0.20510338

DataSet Rp: 0.12726642

DataSet Rwpb (no background): 8.558202

DataSet Rpb (no background): 0.13635594

Refinement final output indices for single spectra:

Datafile SB-G65.xrdml(0) : Rwp: 0.20510338, Rp: 0.12726642, Rwpb: 8.558202, Rpb: 0.13635594

Sample:SB-G65-After

Phases:

Martensite

Density: 7.649078738428858

Qc: 0.05493051672568076

Austenite

Density: 7.841092894880825

Qc: 0.05561570133096311

Ferrite

Density: 7.800928148673588

Qc: 0.05547307717972451

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 12:46:46 BST 2013

_computing_structure_refinement, Maud, version 2.33

_refine_ls_R_factor_all, 0.12726642

_refine_ls_wR_factor_all, 0.20510338

_refine_ls_goodness_of_fit_all, 0.10646808

_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, 17453.469

_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: Marquadt 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: 10.0
- Parameter: paramete.sav:SB-G65-After:_pd_spec_size_equat Value: 0, minimum: 0.0, maximum: 10.0
- Parameter: paramete.sav:SB-G65-After:_pd_spec_size_thick Value: 0, minimum: 0.0, maximum: 10.0
- Parameter: paramete.sav:SB-G65-After:_pd_spec_size_radius Value: 0, minimum: 0.0, maximum: 10.0
- Parameter: paramete.sav:SB-G65-After:_pd_spec_size_radius_y Value: 0, minimum: 0.0, maximum: 10.0

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: 0.19068563, m
- Parameter: paramete.sav:SB-G65-After:layer1:Volume fraction of Fe4.00 Value: 0.045788053, m
- Parameter: paramete.sav:SB-G65-After:layer1:Volume fraction of ferrite Value: 0.7635263, 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, minin
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:_pd_spec_orientation_phi Value: 0, minin

Parameter loop informations :

Parameter loop number : 0

- Parameter: paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol0 Value: 126.2
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol1 Value: -3.024
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol2 Value: 0.040
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol3 Value: -2.499
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol4 Value: 5.940

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) :

_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: 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 weigth neutron scattering neu

1) Fe Fe 2.0 1.0 0 0 0 2 -0.7952801 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 0 1 8 10446.825712408074 152.95769479755552 0.013904641720076296

2) 1 1 0 4 5220.230861272102 500.3231238331889 0.008030368122631519

3) 0 0 2 2 1909.4263539530568 656.6159159972502 0.010560699317671078
 4) 2 0 0 4 3812.229661930564 597.9974197149604 0.003121796000000001
 5) 1 1 2 8 6058.22832566547 204.07498235029294 0.012517380768396992
 6) 1 2 1 8 6052.328037708738 283.341283344675 0.017560033079617128
 7) 2 1 1 8 6052.328037708738 319.3651104507153 0.0037594575795724737
 8) 2 0 2 8 5090.494768803374 152.95769479755552 0.013904641720076296
 9) 2 2 0 4 2542.7629721364706 500.3231238331889 0.008030368122631519
 10) 1 0 3 8 4473.3481300346 479.54274407128315 0.0031112875209574056
 11) 3 0 1 8 4466.871980127177 433.5375926364733 0.008442145300817397
 12) 1 3 0 4 2233.0324902006287 536.9256168752681 0.015777137867823993
 13) 3 1 0 4 2233.0324902006287 588.7437295197773 0.014661580940237352
 14) 2 2 2 8 4064.567707220201 152.84561373144166 0.014659546424669686
 15) 1 2 3 8 3807.072266479531 188.32315334227283 0.013931133184288074
 16) 2 1 3 8 3807.072266479531 194.96031948627052 0.011604310014627445
 17) 1 3 2 8 3805.427677133676 196.8446533182955 0.017332881499245154
 18) 3 1 2 8 3805.427677133676 223.33164756873222 0.007957073293392427
 19) 2 3 1 8 3804.4441693615763 388.3619105743707 0.015897516992449227
 20) 3 2 1 8 3804.4441693615763 421.42452950291676 0.006576340603232739
 21) 0 0 4 2 913.0190129333212 656.6159159972502 0.010560699317671078
 22) 4 0 0 4 1824.5549278902997 597.9974197149604 0.003121796000000001

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: 2.8928173, minimum:
 - Parameter: paramete.sav:SB-G65-After:Martensite:_cell_length_b Value: 2.8928173, minimum:
 - Parameter: paramete.sav:SB-G65-After:Martensite:_cell_length_c Value: 2.897531, minimum: 5
 - 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

- 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) $-x \mid -y \mid +z$
- 4) $+y \mid -x \mid +z$
- 5) $+x \mid -z \mid +y$
- 6) $+x \mid -y \mid -z$
- 7) $+x \mid +z \mid -y$
- 8) $+z \mid +y \mid -x$
- 9) $-x \mid +y \mid -z$
- 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) $+y+0.5 \mid -x \mid +z+0.5$
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109) $-y+0.5 \mid -z \mid +x+0.5$
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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) $-y+0.5 \mid -x \mid -z+0.5$
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118) $-x+0.5 \mid -z \mid -y+0.5$
119) $+z+0.5 \mid -y \mid +x+0.5$
120) $-z+0.5 \mid -y \mid -x+0.5$
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122) $+y+0.5 \mid -x \mid -z+0.5$
123) $+x+0.5 \mid +y \mid -z+0.5$
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125) $-x+0.5 \mid +z \mid -y+0.5$
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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) $-y+0.5 \mid -x \mid +z+0.5$
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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) $-y+0.5 \mid -z+0.5 \mid +x$
158) $+z+0.5 \mid -x+0.5 \mid -y$
159) $-y+0.5 \mid +z+0.5 \mid -x$
160) $-z+0.5 \mid -x+0.5 \mid +y$
161) $-z+0.5 \mid +x+0.5 \mid -y$
162) $+y+0.5 \mid -z+0.5 \mid -x$
163) $+y+0.5 \mid +x+0.5 \mid -z$
164) $-y+0.5 \mid -x+0.5 \mid -z$
165) $-x+0.5 \mid +z+0.5 \mid +y$
166) $-x+0.5 \mid -z+0.5 \mid -y$
167) $+z+0.5 \mid -y+0.5 \mid +x$
168) $-z+0.5 \mid -y+0.5 \mid -x$
169) $-x+0.5 \mid -y+0.5 \mid -z$
170) $+y+0.5 \mid -x+0.5 \mid -z$
171) $+x+0.5 \mid +y+0.5 \mid -z$
172) $-y+0.5 \mid +x+0.5 \mid -z$
173) $-x+0.5 \mid +z+0.5 \mid -y$
174) $-x+0.5 \mid +y+0.5 \mid +z$
175) $-x+0.5 \mid -z+0.5 \mid +y$
176) $-z+0.5 \mid -y+0.5 \mid +x$
177) $+x+0.5 \mid -y+0.5 \mid +z$
178) $+z+0.5 \mid -y+0.5 \mid -x$
179) $-z+0.5 \mid -x+0.5 \mid -y$
180) $-y+0.5 \mid -z+0.5 \mid -x$
181) $+y+0.5 \mid +z+0.5 \mid -x$
182) $-z+0.5 \mid +x+0.5 \mid +y$
183) $+y+0.5 \mid -z+0.5 \mid +x$
184) $+z+0.5 \mid +x+0.5 \mid -y$
185) $+z+0.5 \mid -x+0.5 \mid +y$
186) $-y+0.5 \mid +z+0.5 \mid +x$
187) $-y+0.5 \mid -x+0.5 \mid +z$
188) $+y+0.5 \mid +x+0.5 \mid +z$
189) $+x+0.5 \mid -z+0.5 \mid -y$
190) $+x+0.5 \mid +z+0.5 \mid +y$
191) $-z+0.5 \mid +y+0.5 \mid -x$
192) $+z+0.5 \mid +y+0.5 \mid +x$

Atom list

n	label	symbol	quantity	occupancy	x	y	z	multiplicity	B	radius	weigh	neutron scattering	neu
1)	Fe	Fe	4.0	1.0	0	0	0	4	-0.7952801	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	42404.09607750988	245.42259792881632	0.0
2)	2	0	0	6	28369.789440173336	215.0341031064658	0.0
3)	2	2	0	12	39871.41354028467	237.8254742240805	0.0
4)	3	1	1	24	65940.99423171686	229.34934446914258	0.0
5)	2	2	2	8	20852.77426257274	245.42259792881632	0.0
6)	4	0	0	6	13226.681852031761	215.0341031064658	0.0
7)	3	3	1	24	48454.09394285307	240.03516394434942	0.0
8)	4	2	0	24	47341.592711758145	229.6205806217392	0.0
9)	4	2	2	24	44276.35867368768	237.82547422333192	0.0

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: 3.6166866, minimum: 5
- Parameter: paramete.sav:SB-G65-After:Austenite:_cell_length_b Value: 3.6166866, minimum: 5
- Parameter: paramete.sav:SB-G65-After:Austenite:_cell_length_c Value: 3.6166866, 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: 0.3012927,
- Parameter: paramete.sav:SB-G65-After:Austenite:_riet_par_phase_scale_factor Value: 1.87541

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 Valu

- Parameter: paramete.sav:SB-G65-After:Austenite:Popa rules:_riet_par_aniso_microstrain1 Valu

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) $-z \mid +y \mid +x$
- 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) $+x+0.5 \mid +y+0.5 \mid +z+0.5$
- 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 | +y+0.5 | +x+0.5
 59) +z+0.5 | +x+0.5 | +y+0.5
 60) +y+0.5 | +z+0.5 | +x+0.5
 61) -y+0.5 | -z+0.5 | +x+0.5
 62) +z+0.5 | -x+0.5 | -y+0.5
 63) -y+0.5 | +z+0.5 | -x+0.5
 64) -z+0.5 | -x+0.5 | +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 -0.3865267 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 0 12 14838.112731935016 318.69549046763325 0.003425368389368737

2) 2 0 0 6 5146.8318351222615 170.4047881476052 0.004158319

3) 2 1 1 24 15536.948779039227 318.6954904627628 0.003425368389368738

4) 2 2 0 12 6214.678089254792 318.69549046763325 0.003425368389368737

5) 3 1 0 24 10394.607176921518 223.78944098281534 0.003910315628785765

6) 2 2 2 8 3002.6612608627106 368.12572456691964 0.003143298559676089

7) 3 2 1 48 16077.19344463152 318.695490465258 0.0034253683893687385

8) 4 0 0 6 1837.51140979798 170.4047881476052 0.004158319

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: 2.8754842, minimum: 5.0,

- Parameter: paramete.sav:SB-G65-After:Ferrite:_cell_length_b Value: 2.8754842, minimum: 5.0,

- Parameter: paramete.sav:SB-G65-After:Ferrite:_cell_length_c Value: 2.8754842, 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: 1.0306509

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: 28

- Parameter: paramete.sav:SB-G65-After:Ferrite:Popa rules:_riet_par_anisocryst_size1 Value: -1

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: 0
- Parameter: paramete.sav:SB-G65-After:Ferrite:Atomic Structure:Fe:_atom_site_aniso_B_11 Value: 0
- Parameter: paramete.sav:SB-G65-After:Ferrite:Atomic Structure:Fe:_atom_site_aniso_B_22 Value: 0
- Parameter: paramete.sav:SB-G65-After:Ferrite:Atomic Structure:Fe:_atom_site_aniso_B_33 Value: 0
- Parameter: paramete.sav:SB-G65-After:Ferrite:Atomic Structure:Fe:_atom_site_aniso_B_23 Value: 0
- Parameter: paramete.sav:SB-G65-After:Ferrite:Atomic Structure:Fe:_atom_site_aniso_B_13 Value: 0
- Parameter: paramete.sav: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 :