

Jacobi matrix :

#	0	1	2	3	4	5	6	7	8	9
0	2507692.2									
1	-246374.5	86884.0								
2	3592.6372	-1276.1143	84.67144							
3	324394.38	-140945.6	7359.2637	767487.7						
4	3.4994032E7	-1.7245776E7	767444.44	8.8043624E7	1.06920499E10					
5	4.27084032E9	-2.22585037E9	8.8111664E7	1.07009321E10	1.3498214E12	1.7512494E12				
6	5.5946419E11	-2.95995867E11	1.06990469E10	1.34966385E12	1.74959167E14	2.317321E14				
7	18316.172	523.8354	228.75922	23301.273	2661922.0	3.25703488E8	4.1531E8			
8	-118137.97	37527.19	650.99603	72630.305	8836166.0	1.12863782E9	1.4851E9			
9	-4.7548896E7	2.0294676E7	-1057626.2	-1.07768712E8	-1.2529623E10	-1.55359353E10				
10	-2.040891E7	8630332.0	-490322.8	-4.791268E7	-5.3951432E9	-6.515825E11	-8.1512E11			
11	-81840.03	17084.713	-1315.49	-145813.12	-1.7572902E7	-2.22148966E9	-2.891E9			
12	421198.78	-529857.9	-2241.8594	-212723.34	-2.2216594E7	-2.49297178E9	-2.91E9			

Correlation matrix:

#	0	1	2	3	4	5	6	7	8	9
0	1.0									
1	1.1751893	1.0								
2	0.42526707	-0.1670979	-1.0							
3	1.258324	1.0099288	-0.2738267	1.0						
4	0.53791285	-0.07935931	-1.0387174	-0.19515719	-1.0					
5	-0.23105137	1.5052675	3.036433	2.4390202	0.76435906	1.0				
6	-0.33958802	-1.2744426	-1.7741631	-1.7281758	-0.24029419	-1.1024015	1.0			
7	-1.1799556	-0.9827144	0.16194984	-0.95280474	0.053861182	-1.5217013	1.261E0			
8	-0.9955566	-0.74439114	0.30940676	-0.72007984	0.24462657	-1.9859627	1.511E0			
9	-1.5113814	-1.2644243	0.13668431	-1.1763899	-0.044447266	-1.1248474	0.977E0			
10	1.3991673	1.2607695	-0.116668664	1.3212786	-0.02242499	1.1998217	-1.001E0			
11	-1.0746449	-1.0630059	-0.26125854	-0.9779618	-0.45981416	0.99319106	-0.511E0			
12	0.27902523	-0.30741775	-0.49669504	-0.83587193	-0.26544273	1.4853995	-0.911E0			

Correlation matrix from Choleski decomposition :

#	0	1	2	3	4	5	6	7	8	9
0	1.0									
1	1.1751893	1.0								
2	0.42526707	-0.1670979	-1.0							
3	1.258324	1.0099288	-0.2738267	1.0						
4	0.53791285	-0.07935931	-1.0387174	-0.19515719	-1.0					
5	-0.23105137	1.5052675	3.036433	2.4390202	0.76435906	1.0				
6	-0.33958802	-1.2744426	-1.7741631	-1.7281758	-0.24029419	-1.1024015	1.0			
7	-1.1799556	-0.9827144	0.16194984	-0.95280474	0.053861182	-1.5217013	1.261E0			
8	-0.9955566	-0.74439114	0.30940676	-0.72007984	0.24462657	-1.9859627	1.511E0			
9	-1.5113814	-1.2644243	0.13668431	-1.1763899	-0.044447266	-1.1248474	0.977E0			
10	1.3991673	1.2607695	-0.116668664	1.3212786	-0.02242499	1.1998217	-1.001E0			

11 -1.0746449 -1.0630059 -0.26125854 -0.9779618 -0.45981416 0.99319106 -0.5
12 0.27902523 -0.30741775 -0.49669504 -0.83587193 -0.26544273 1.4853995 -0.9
Analysis title: Put a title here

Refined parameters:

0 SB-G65-after:SB-G65-After:layer1:_pd_phase_atom_%1 value:0.056260906 error:0.001892386
1 SB-G65-after:SB-G65-After:layer1:_pd_phase_atom_%2 value:0.3393475 error:0.016494544
2 SB-G65-after:SB-G65-After:SB-G65-after:_riet_par_background_pol0 value:133.9654 error:2.86
3 SB-G65-after:SB-G65-After:SB-G65-after:_riet_par_background_pol1 value:-3.827515 error:0.2
4 SB-G65-after:SB-G65-After:SB-G65-after:_riet_par_background_pol2 value:0.055667497 error:0
5 SB-G65-after:SB-G65-After:SB-G65-after:_riet_par_background_pol3 value:-3.7103452E-4 erro
6 SB-G65-after:SB-G65-After:SB-G65-after:_riet_par_background_pol4 value:8.8297435E-7 error
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:2.8921866 error:6.8584835E-4
10 SB-G65-after:SB-G65-After:Martensite:_cell_length_c value:2.858315 error:0.0017808267
11 SB-G65-after:SB-G65-After:Martensite:Atomic Structure:Fe:_atom_site_B_iso_or_equiv value:
12 SB-G65-after:SB-G65-After:Ferrite:_cell_length_a value:2.874254 error:3.5672108E-4

Refinement final output indices:

Global Rwp: 0.19918479

Global Rp: 0.11845177

Global Rwpb (no background): 8.025218

Global Rpb (no background): 0.123766206

Total Energy: 0.0

Refinement final output indices for single samples:

Sample SB-G65-After :

Sample Rwp: 0.19918479

Sample Rp: 0.11845177

Sample Rwpb (no background): 8.025218

Sample Rpb (no background): 0.123766206

Refinement final output indices for single datasets:

DataSet SB-G65-after :

DataSet Rwp: 0.19918479

DataSet Rp: 0.11845177

DataSet Rwpb (no background): 8.025218

DataSet Rpb (no background): 0.123766206

Refinement final output indices for single spectra:

Datafile SB-G65.xrdml(0) : Rwp: 0.19918479, Rp: 0.11845177, Rwpb: 8.025218, Rpb: 0.123766206

Sample:SB-G65-After

Phases:

Martensite

Density: 7.75740609318666

Qc: 0.05531811618508623

Austenite

Density: 7.829752891451307

Qc: 0.05557547030419097

Ferrite

Density: 7.810948985225203

Qc: 0.0555086952641765

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 15:12:31 BST 2013

_computing_structure_refinement, Maud, version 2.33

_refine_ls_R_factor_all, 0.11845177

_refine_ls_wR_factor_all, 0.19918479

_refine_ls_goodness_of_fit_all, 0.106705524

_publ_contact_author_name, Luca Lutterotti

_publ_section_title, Put a title here

_pd_proc_ls_extract_int, never

_pd_proc_ls_texture_comp, never

_computing_reduce_memory_occ, true

_pd_proc_ls_theoretical_weight, false

_pd_proc_ls_extract_pos, never

_pd_proc_ls_strain_comp, never

_pd_proc_ls_extract_Fhkl, end of iteration

_pd_proc_ls_Fhkl_comp, end of iteration

_pd_proc_ls_weight_scheme, sqrt

_refine_ls_weighting_scheme, WgtSS

_refine_ls_WSS_factor, 16460.705

_maud_store_spectra_with_analysis, false

_riet_remove_phases_under, 0.001

_riet_refine_cell_over, 0.1

_riet_refine_sizestrain_over, 0.1

_riet_refine_crystal_structure_over, 0.1

_riet_refine_texture_over, 0.15

_riet_refine_strain_over, 0.25

_pd_proc_ls_interpolation_comp, end of iteration

Subordinate objects :

Subordinate object number 0 :

Object: Marqardt Least Squares

String informations (CIF term, value) :
_refine_ls_number_iteration, 5
_riet_refine_ls_precision, 0.00000001
_riet_refine_ls_derivative_step, 0.0001
_riet_refine_ls_double_derivative, false

Loops of subordinate objects :

Object loop number 0 :

Object number 0 :

Object: SB-G65-After

String informations (CIF term, value) :
_pd_spec_description, Sample description
_riet_thin_film_phase_refinement, films

Parameter informations :

- Parameter: SB-G65-after:SB-G65-After:_pd_spec_orientation_omega Value: 0, minimum: 0.0, maximum: 360.0
- Parameter: SB-G65-after:SB-G65-After:_pd_spec_orientation_chi Value: 0, minimum: 0.0, maximum: 90.0
- Parameter: SB-G65-after:SB-G65-After:_pd_spec_orientation_phi Value: 0, minimum: 0.0, maximum: 360.0
- Parameter: SB-G65-after:SB-G65-After:_riet_par_spec_displac_x Value: 0, minimum: 0.0, maximum: 0.0
- Parameter: SB-G65-after:SB-G65-After:_riet_par_spec_displac_y Value: 0, minimum: 0.0, maximum: 0.0
- Parameter: SB-G65-after:SB-G65-After:_riet_par_spec_displac_z Value: 0, minimum: 0.0, maximum: 0.0
- Parameter: SB-G65-after:SB-G65-After:_pd_spec_size_axial Value: 0, minimum: 0.0, maximum: 0.0
- Parameter: SB-G65-after:SB-G65-After:_pd_spec_size_equat Value: 0, minimum: 0.0, maximum: 0.0
- Parameter: SB-G65-after:SB-G65-After:_pd_spec_size_thick Value: 0, minimum: 0.0, maximum: 0.0
- Parameter: SB-G65-after:SB-G65-After:_pd_spec_size_radius Value: 0, minimum: 0.0, maximum: 0.0
- Parameter: SB-G65-after:SB-G65-After:_pd_spec_size_radius_y Value: 0, minimum: 0.0, maximum: 0.0

Subordinate objects :

Subordinate object number 0 :

Object: flat_sheet

Subordinate object number 1 :

Object: None Layer workout

Subordinate object number 2 :

Object: No precession

Loops of subordinate objects :

Object loop number 0 :

Object number 0 :

Object: layer1

Parameter informations :

- Parameter: 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: 0.6043916, minimum
- Parameter: SB-G65-after:SB-G65-After:layer1:_pd_phase_atom_%1 Value: 0.056260906, minimum
- Parameter: SB-G65-after:SB-G65-After:layer1:_pd_phase_atom_%2 Value: 0.3393475, 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: 133.96
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:_riet_par_background_pol1 Value: -3.827
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:_riet_par_background_pol2 Value: 0.0556
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:_riet_par_background_pol3 Value: -3.710
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:_riet_par_background_pol4 Value: 8.8297

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_of

Subordinate objects :

Subordinate object number 0 :

Object: none cal

Subordinate object number 1 :

Object: Instrument disalignment

Subordinate object number 2 :

Object: Bragg-Brentano

String informations (CIF term, value) :

_diffn_radiation_monochromator, Filtered
_pd_instr_2theta_monochr_post, 0
_pd_instr_dist_src/samp, 175.0
_pd_instr_monochr_pre_spec, none
_pd_instr_2theta_monochr_pre, 0
_pd_instr_divg_ax_src/samp, 0.0
_pd_instr_divg_slit_auto, false

Parameter informations :

- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:Diffraction Instrument:Bragg-Brentano:_dif
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:Diffraction Instrument:Bragg-Brentano:_dif

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: 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 : 1

- 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: 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.xrxml(0):_pd_meas_counts_moni
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:SB-G65.xrxml(0):_riet_par_spec_displac_
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:SB-G65.xrxml(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 -0.5714244 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 5081.550183633465 1249.127682077458 0.008399206813394731

2) 1 0 1 8 10114.68329444858 209.52889703960878 0.004711933051142504

3) 2 0 0 4 3612.7092068176303 1092.1279698148635 0.005187216000000001

4) 0 0 2 2 1781.4107797401387 1319.9663126250769 0.016439313224825433

5) 1 2 1 8 5567.118618548756 750.6543058117412 0.012306162086904658

6) 2 1 1 8 5567.118618548756 523.1480890956926 0.0027646921061226797

7) 1 1 2 8 5522.566994209275 382.0493595608394 0.005294225190339795

8) 2 2 0 4 2284.0319358986385 1249.127682077458 0.008399206813394731

9) 2 0 2 8 4529.93749116169 209.52889703960878 0.004711933051142504

10) 1 3 0 4 1952.8877581795236 1313.7566730543972 0.01111888288459059
 11) 3 1 0 4 1952.8877581795236 983.5390594043979 0.01035746972559776
 12) 3 0 1 8 3899.3719054646062 749.3021490019709 0.0033793589074570625
 13) 1 0 3 8 3849.203147561322 945.1076324900006 0.013622874811854759
 14) 2 2 2 8 3441.7826084429066 343.9594435448726 0.009360594534002125
 15) 2 3 1 8 3150.755742488094 1058.4912470628183 0.012111555723545804
 16) 3 2 1 8 3150.755742488094 848.6087124729767 2.681334318502316E-4
 17) 1 3 2 8 3141.8776040798843 447.0092851405311 0.010962322193581118
 18) 3 1 2 8 3141.8776040798843 280.8029066215578 0.0019878772929345537
 19) 1 2 3 8 3127.3478558354536 362.42031899094394 0.0023569581204208167
 20) 2 1 3 8 3127.3478558354536 321.56270998623546 0.005841677046888565
 21) 4 0 0 4 1472.7532122956989 1092.1279698148635 0.005187216000000001
 22) 0 0 4 2 728.5794353306084 1319.9663126250769 0.016439313224825433

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: 2.8921866, minimum:
 - Parameter: SB-G65-after:SB-G65-After:Martensite:_cell_length_b Value: 2.8921866, minimum:
 - Parameter: SB-G65-after:SB-G65-After:Martensite:_cell_length_c Value: 2.858315, minimum: 5
 - 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, minimum:
 - 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) $-x \mid +y \mid -z$
- 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) $+y+0.5 \mid -x \mid +z+0.5$
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) $-y+0.5 \mid -z+0.5 \mid +x$
 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 weigth neutron scattering neu

1) Fe Fe 4.0 1.0 0 0 0 4 -0.5714244 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 41345.037103238166 156.13226340182888 0.0011898097855989414
- 2) 2 0 0 6 27427.45379832801 127.14182989696118 0.0020608109999999999
- 3) 2 2 0 12 37256.610341604 148.88465502642458 0.0014572134328438306
- 4) 3 1 1 24 60057.95415501339 140.79848039106793 0.0017068074304245403
- 5) 2 2 2 8 18830.643188203914 156.13226340182888 0.0011898097855989414
- 6) 4 0 0 6 11541.930707180818 127.14182989696118 0.0020608109999999999
- 7) 3 3 1 24 41208.51204706162 150.9926851633674 0.0013847722918190614
- 8) 4 2 0 24 39918.41651460394 141.05723797981776 0.0016993882854869512
- 9) 4 2 2 24 36073.639716851365 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_equi 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) $-z \mid -x \mid +y$
- 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) $-z+0.5 \mid +y+0.5 \mid +x+0.5$
- 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 | -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 -0.5714244 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 15168.408594383314 351.10910702138517 0.002394770409058374
2) 2 0 0 6 5379.525046902681 234.2359219287546 0.0034314161
3) 2 1 1 24 16605.333168342582 351.1091070175466 0.002394770409058373
4) 2 2 0 12 6792.074033489078 351.10910702138517 0.002394770409058374
5) 3 1 0 24 11617.457161227045 276.31026856210167 0.0030984395493883167
6) 2 2 2 8 3431.9561144851264 390.0668353797713 0.0019291694929051046
7) 3 2 1 48 18792.630542972103 351.10910701951315 0.0023947704090583727
8) 4 0 0 6 2196.6229843814303 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: 2.874254, minimum: 5.0, maximum: 5.0
- Parameter: SB-G65-after:SB-G65-After:Ferrite:_cell_length_b Value: 2.874254, minimum: 5.0, maximum: 5.0
- Parameter: SB-G65-after:SB-G65-After:Ferrite:_cell_length_c Value: 2.874254, minimum: 5.0, maximum: 5.0
- Parameter: SB-G65-after:SB-G65-After:Ferrite:_cell_angle_alpha Value: 90, minimum: 90.0, maximum: 90.0
- Parameter: SB-G65-after:SB-G65-After:Ferrite:_cell_angle_beta Value: 90, minimum: 90.0, maximum: 90.0
- Parameter: SB-G65-after:SB-G65-After:Ferrite:_cell_angle_gamma Value: 90, minimum: 90.0, maximum: 90.0
- Parameter: SB-G65-after:SB-G65-After:Ferrite:_riet_par_strain_thermal Value: 0, minimum: -0.1, maximum: 0.1
- Parameter: SB-G65-after:SB-G65-After:Ferrite:_exptl_absorpt_cryst_size Value: 0, minimum: 0.0, maximum: 0.0
- Parameter: SB-G65-after:SB-G65-After:Ferrite:_riet_par_phase_scale_factor Value: 1.6610774, minimum: 1.6610774, maximum: 1.6610774

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 :