

Jacobi matrix :

#	0	1	2	3
0	8.1479385E10			
1	3.6250911E10	1.61349571E10		
2	5.08153E7	2.2530708E7	1.1532539E7	
3	8.4090648E7	4.124276E7	3321332.2	1.36996848E8

Correlation matrix:

#	0	1	2	3
0	-1.0			
1	1275.3706	1.0		
2	-58.967865	-10.836459	1.0	
3	10.836459	-58.967865	1275.3706	-1.0

Correlation matrix from Choleski decomposition :

#	0	1	2	3
0	-1.0			
1	1275.3706	1.0		
2	-58.967865	-10.836459	1.0	
3	10.836459	-58.967865	1275.3706	-1.0

Analysis title: Put a title here

Refined parameters:

0 SB-G65-after:SB-G65-After:Martensite:_cell_length_a value:2.891856 error:3.3643094E-4
1 SB-G65-after:SB-G65-After:Martensite:_cell_length_c value:2.859399 error:7.5606065E-4
2 SB-G65-after:SB-G65-After:Austenite:_cell_length_a value:3.6186302 error:5.700771E-4
3 SB-G65-after:SB-G65-After:Ferrite:_cell_length_a value:2.874111 error:1.665778E-4

Refinement final output indices:

Global Rwp: 0.20574842

Global Rp: 0.1318583

Global Rwpb (no background): 7.356876

Global Rpb (no background): 0.14155146

Total Energy: 0.0

Refinement final output indices for single samples:

Sample SB-G65-After :

Sample Rwp: 0.20574842

Sample Rp: 0.1318583

Sample Rwpb (no background): 7.356876

Sample Rpb (no background): 0.14155146

Refinement final output indices for single datasets:

DataSet SB-G65-after :

DataSet Rwp: 0.20574842
DataSet Rp: 0.1318583
DataSet Rwpb (no background): 7.356876
DataSet Rpb (no background): 0.14155146

Refinement final output indices for single spectra:

Datafile SB-G65.xrdml(0) : Rwp: 0.20574842, Rp: 0.1318583, Rwpb: 7.356876, Rpb: 0.14155146

Sample:SB-G65-After

Phases:

Martensite

Density: 7.756238354036137

Qc: 0.05531395245043086

Austenite

Density: 7.828465107633181

Qc: 0.05557089978099704

Ferrite

Density: 7.81211493317909

Qc: 0.055512838028055456

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 15:48:37 BST 2013

_computing_structure_refinement, Maud, version 2.33

_refine_ls_R_factor_all, 0.1318583

_refine_ls_wR_factor_all, 0.20574842

_refine_ls_goodness_of_fit_all, 0.10680712

_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, 17563.422

_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: 0.6687906, minimum
- Parameter: SB-G65-after:SB-G65-After:layer1:_pd_phase_atom_%1 Value: 0.056937348, minimum
- Parameter: SB-G65-after:SB-G65-After:layer1:_pd_phase_atom_%2 Value: 0.27427205, 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,
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:_riet_par_background_exp_thermal_shift
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:_pd_spec_orientation_omega Value: 0, m
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:_pd_spec_orientation_chi Value: 0, minim
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:_pd_spec_orientation_phi Value: 0, minim

Parameter loop informations :

Parameter loop number : 0

- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:_riet_par_background_pol0 Value: 133.51
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:_riet_par_background_pol1 Value: -3.867
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:_riet_par_background_pol2 Value: 0.0564
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:_riet_par_background_pol3 Value: -3.706
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:_riet_par_background_pol4 Value: 8.2404

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) :

_diffrn_radiation_monochromator, Filtered

_pd_instr_2theta_monochr_post, 0

_pd_instr_dist_src/samp, 175.0

_pd_instr_monochr_pre_spec, none

_pd_instr_2theta_monochr_pre, 0

_pd_instr_divg_ax_src/samp, 0.0

_pd_instr_divg_slit_auto, false

Parameter informations :

- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:Diffraction Instrument:Bragg-Brentano:_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.xrdml(0):_pd_meas_counts_moni
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:SB-G65.xrdml(0):_riet_par_spec_displac
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:SB-G65.xrdml(0):_riet_par_spec_displac

Parameter loop informations :

Object loop number 2 :

Object number 0 :

Object: Martensite

General position

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

Atom list

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

1) Fe Fe 2.0 1.0 0 0 0 2 -0.5939843 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 4 5094.809033951408 1244.1353817627619 0.008177597333938618
- 2) 1 0 1 8 10143.42781850497 203.58515290672665 0.00450575237699068
- 3) 2 0 0 4 3631.765963913191 1086.3471853154338 0.0052106989999999975
- 4) 0 0 2 2 1792.074580935267 1318.080429462003 0.016737103237360034
- 5) 1 2 1 8 5612.295967258142 744.6603493147046 0.0122858326346203
- 6) 2 1 1 8 5612.295967258142 517.9865082112511 0.003225282555518811
- 7) 1 1 2 8 5569.776850873804 376.82237072987175 0.005675712942341837
- 8) 2 2 0 4 2308.4380703740826 1244.1353817627619 0.008177597333938618
- 9) 2 0 2 8 4580.523266502667 203.58515290672665 0.00450575237699068
- 10) 1 3 0 4 1979.0952274966346 1307.600500515134 0.011124340626119946
- 11) 3 1 0 4 1979.0952274966346 978.7013715578097 0.010505050942351645
- 12) 3 0 1 8 3952.0973080930135 743.4287177536537 0.0033646907582132843
- 13) 1 0 3 8 3904.324846837511 941.8102305684234 0.013904442719414125
- 14) 2 2 2 8 3498.6084138940146 338.27299314081796 0.009245140870403467
- 15) 2 3 1 8 3210.637453862183 1052.8384362281397 0.01204572831700182
- 16) 3 2 1 8 3210.637453862183 843.7638011249137 0.0019281143235860769
- 17) 1 3 2 8 3202.268083412332 440.8262548718082 0.01095210756034303
- 18) 3 1 2 8 3202.268083412332 275.1885642719239 0.0014315862214296878
- 19) 1 2 3 8 3188.565546587221 356.98484697976556 0.0030183561130907996
- 20) 2 1 3 8 3188.565546587221 316.2382759578533 0.006173610597915068
- 21) 4 0 0 4 1504.7235633479706 1086.3471853154338 0.0052106989999999975
- 22) 0 0 4 2 745.0906585204035 1318.080429462003 0.016737103237360034

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: 2.891856, minimum: 5
- Parameter: SB-G65-after:SB-G65-After:Martensite:_cell_length_b Value: 2.891856, minimum: 5
- Parameter: SB-G65-after:SB-G65-After:Martensite:_cell_length_c Value: 2.859399, 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: 1.2, mi

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 Valu
- Parameter: SB-G65-after:SB-G65-After:Martensite:Atomic Structure:Fe:_atom_site_fract_y Valu
- Parameter: SB-G65-after:SB-G65-After:Martensite:Atomic Structure:Fe:_atom_site_fract_z Valu

- 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
- 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 :

General position

- 1) $+x \mid +y \mid +z$
- 2) $-y \mid +x \mid +z$
- 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) $+y \mid +x \mid -z$
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- 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) $-x \mid -y+0.5 \mid +z+0.5$
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- 87) $+y \mid -z+0.5 \mid +x+0.5$
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- 94) $+x \mid +z+0.5 \mid +y+0.5$
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189) $+x+0.5 \mid -z+0.5 \mid -y$

190) +x+0.5 | +z+0.5 | +y
 191) -z+0.5 | +y+0.5 | -x
 192) +z+0.5 | +y+0.5 | +x

Atom list

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

1) Fe Fe 4.0 1.0 0 0 0 4 -0.5939843 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 41453.803438210154 156.13226340182888 0.0011898097855989418

2) 2 0 0 6 27523.52243277038 127.14182989696118 0.002060811

3) 2 2 0 12 37516.912245462576 148.88465502642458 0.0014572134328438297

4) 3 1 1 24 60634.40535114096 140.79848039106793 0.0017068074304245403

5) 2 2 2 8 19027.780800519435 156.13226340182888 0.0011898097855989418

6) 4 0 0 6 11702.991670006486 127.14182989696118 0.002060811

7) 3 3 1 24 41891.42747324692 150.9926851633674 0.0013847722918190607

8) 4 2 0 24 40614.81996692324 141.05723797981776 0.0016993882854869512

9) 4 2 2 24 36829.19698797046 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: 3.6186302, minimum: 5

- Parameter: SB-G65-after:SB-G65-After:Austenite:_cell_length_b Value: 3.6186302, minimum: 5

- Parameter: SB-G65-after:SB-G65-After:Austenite:_cell_length_c Value: 3.6186302, 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: 0.42649165
- Parameter: SB-G65-after:SB-G65-After:Austenite:_riet_par_phase_scale_factor Value: 4.8, min

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 Valu
- Parameter: SB-G65-after: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: 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
- Parameter: SB-G65-after:SB-G65-After:Austenite:Atomic Structure:Fe:_atom_site_aniso_B_13
- Parameter: SB-G65-after:SB-G65-After:Austenite: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 2 :

Object: Ferrite

General position

- 1) +x | +y | +z
- 2) -y | +x | +z
- 3) -x | -y | +z
- 4) +y | -x | +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) $+z \mid +x \mid +y$
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 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 weigth neutron scattering neu
 1) Fe Fe 2.0 1.0 0 0 0 2 -0.5939843 1.27 55.847

Atomic #, atom #, isotope #, weight, radius, symbol for tables: 26, 54, 80, 55.847, 1.27, Fe
 Neutron sf: 9.45
 Magnetic sf: 0.0706 35.0085 0.3589 15.3583 0.5819 5.5606 -0.0114
 Electron sf: 0.1929 0.8239 1.8689 2.3694 1.906 0.1087 1.0806 4.7637 22.85
 Neutron abs: 0.525525525525254
 Electron abs: 0.0
 X-ray sf: 0.493002 0.322912 0.140191 0.04081 10.5109 26.1257 3.14236 57.7997 0.003038 0.48
 X-ray disp and abs: 0.0 0.0 0.0 0.0 0.002 0.002 0.008 0.008 0.018 0.035 0.0 0.059 0.09 0.09 0.09

Reflection list

n	h	k	l	multiplicity	meanFhkl	crystallite(Angstrom)	microstrain
1)	1	1	0	12	15209.278696604917	371.4639470734107	0.002600832086883338
2)	2	0	0	6	5408.671231497536	241.9638617221973	0.0038593502
3)	2	1	1	24	16740.807431985268	371.4639470691573	0.0026008320868833386
4)	2	2	0	12	6866.195556640339	371.4639470734107	0.002600832086883338
5)	3	1	0	24	11776.379728002234	288.5838924486342	0.0034594351640537964
6)	2	2	2	8	3488.4374618271495	414.6306421840285	0.002013514854709522
7)	3	2	1	48	19154.305000024946	371.4639470713364	0.0026008320868833386
8)	4	0	0	6	2245.0430434522664	241.9638617221973	0.0038593502

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: 2.874111, minimum: 5.0, maximum: 5.0
- Parameter: SB-G65-after:SB-G65-After:Ferrite:_cell_length_b Value: 2.874111, minimum: 5.0, maximum: 5.0
- Parameter: SB-G65-after:SB-G65-After:Ferrite:_cell_length_c Value: 2.874111, 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: 3.2, minimum: 3.2, maximum: 3.2

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: 34

- 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 :