

Supporting material:

Alignment of strontium hexaferrite, by cold compaction of anisotropic non-magnetically interacting crystallites

Jack Thomas-Hunt,^{1,2} Amalie Povlsen,¹ Harikrishnan Vijayan,¹ Cecilie Grønvaldt Knudsen,¹ Frederik H. Gjørup,¹ Mogens Christensen.¹

¹ Department of Chemistry & iNANO, Aarhus University, Aarhus C-8000, Denmark

² School of Chemistry, Cardiff University, Park Place, Cardiff, CF10 3AT Wales, United Kingdom

Logscale plot of refined data:

Logscale plot of the powder diffraction pattern of the 5 pellers are shown in Figure S1.

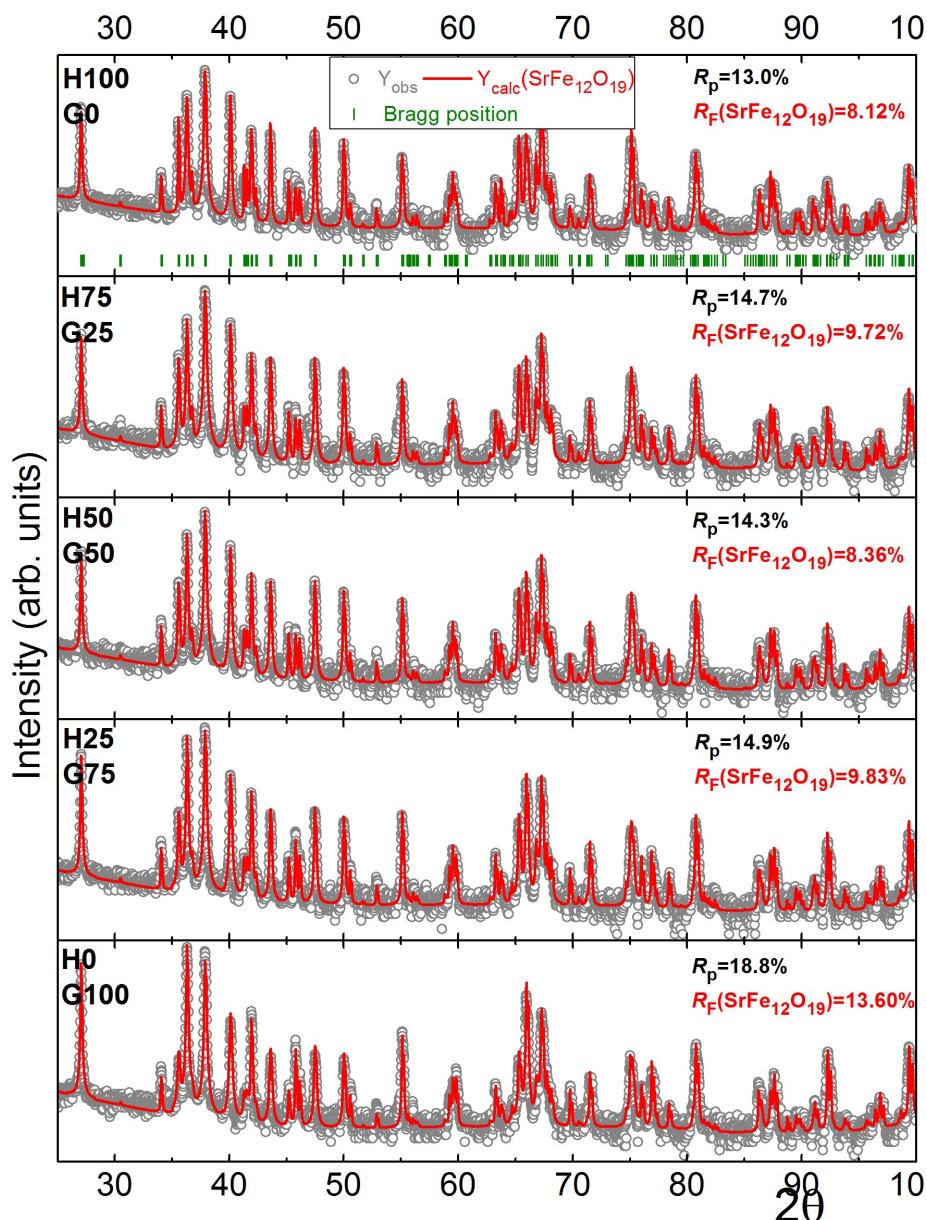


Figure S1 Powder diffraction patterns and Rietveld models for the calcinated pellets shown on a logscale to enhance potential weak features. Gray circles are the observed data, while the red line is calculated model and green tick marks are the Bragg positions.

Different strain models:

Three different models were tested with respect to the strain in the pressed pellet: 1) No strain, 2) equal strain for all 5 samples and 3) Independently refined strain. It is due to the strong texture in the samples not possible to refine an anisotropic strain. All samples are phase pure $\text{SrFe}_{12}\text{O}_{19}$.

Table S1) No strain:

Sample	R_B (%)	R_F (%)	R_p (%)	R_{wp} (%)	G_1	Strain (%%)	AB (nm)	C (nm)
100H0G	8.81	8.0	12.8	17.1	0.593(4)	-	*	*
75H25G	11.8	9.7	14.6	19.4	0.614(4)	-	70(3)	84(8)
50H50G	10.5	8.4	14.2	18.7	0.586(4)	-	69(3)	96(10)
25H75G	11.5	9.8	14.8	19.1	0.505(3)	-	61(3)	105(13)
0H100G	19.1	13.6	18.7	24.0	0.434(2)	-	40(2)	110(20)

- strain was not refined, * the size parameters could not be refined.

Table S2) Equal strain:

Sample	R_B (%)	R_F (%)	R_p (%)	R_{wp} (%)	G_1	Strain (%%)	AB (nm)	C (nm)
100H0G	10.4	9.1	11.0	14.1	0.610(4)	0.164(3)	*	*
75H25G	13.4	10.6	13.8	18.2	0.611(4)	0.164(3)	159(17)	185(35)
50H50G	20.2	14.0	13.2	17.2	0.583(4)	0.164(3)	156(17)	247(63)
25H75G	18.5	12.8	13.8	17.8	0.503(3)	0.164(3)	127(12)	297(95)
0H100G	43.3	20.0	18.4	23.2	0.432(2)	0.164(3)	64(4)	315(156)

* The size parameters could not be refined. The extracted size parameters are outside the resolution instrumental resolution, therefore the absolute values cannot be trusted.

Table S3) Independently refined strain:

Sample	R_B (%)	R_F (%)	R_p (%)	R_{wp} (%)	G_1	Strain (%%)	AB (nm)	C (nm)
100H0G	9.49	8.63	11.0	14.1	0.610(4)	*	*	*
75H25G	33.9	19.9	13.9	18.3	0.611(4)	0.14(1)	225(52)	252(82)
50H50G	26.9	19.0	13.1	17.2	0.583(4)	0.16(1)	273(77)	466(278)
25H75G	20.9	14.3	13.8	17.8	0.504(3)	0.12(1)	132(17)	316(126)
0H100G	40.5	17.1	18.3	23.1	0.432(2)	0.09(1)	55(4)	222(85)

* The size parameters could not be refined. The extracted size parameters are outside the resolution instrumental resolution, therefore the absolute values cannot be trusted.

The refinement of the strain parameters results in a reduction of the R_p and R_{wp} , while the R_B and R_F increases very substantially in some cases. In conclusion the absolute size extracted from the refinements cannot be trusted and there is no clear trend to be seen in the relative size changes. It is noteworthy that all samples see an increase in the thickness of the pellets

Unconstrained refinement of unit cell

The refinement of the 5 pellets were investigated using two models, 1) a single constrained unit cell parameter is used to refine all powder diffraction data. 2) the unit cell parameter is allowed to refine freely for the 5 pellets. Model 2 introduces an additional 8 parameters with only very slight influence of the R_{wp} . However the obtained preferred orientation parameter G_1 is unaffected by the used model.

Table S4 showing the results of a constrained vs freely refined unit cell. The refined unit cell contains an additional 8 parameters for conducting the refinements. The refined SyCos values have been recalculated into a meaningful displacement using the equation: $s = \pi/180*R*SyCos$, [FullProf_Manual.pdf] where R is the radius of the diffractometer R = 350 mm. The constrained refined unit cell was $a = b = 5.8787(1)\text{\AA}$, $c = 23.0577(2)\text{\AA}$.

Sample	Constrained unit cell				Freely refined unit cell					
	2θ offset (°)	R_{wp} (%)	s (μm)	G_1	2θ offset (°)	R_{wp} (%)	a (Å)	c (Å)	s (μm)	G_1
100H0G	0.127(2)	17.10	0.11(1)	0.593(4)	0.136(3)	16.80	5.8801(1)	23.0597(5)	0.03(2)	0.593(4)
75H25G		19.40	0.91(1)	0.614(4)		19.40	5.8792(1)	23.0596(4)	0.28(2)	0.614(4)
50H50G		18.70	1.38(1)	0.586(4)		18.70	5.8783(1)	23.0581(4)	0.30(2)	0.586(4)
25H75G		19.10	2.60(1)	0.505(3)		18.90	5.8775(1)	23.0555(3)	0.20(2)	0.505(3)
0H100G		24.00	7.14(1)	0.435(2)		23.80	5.8760(3)	23.0522(10)	0.01(46)	0.434(2)