Supplementary Information

Table 1S: Rietveld refined parameters of $BaTi_{0.85}Fe_{0.15}O_3$ using two phase model

Parameters	Values pertaining to the different phases	
Phases	Tetragonal	Hexagonal
Vol. Fraction (%)	80.58 ± 2.83	19.42 ± 1.90
Space group	P4/mmm	P63/mmc
	Unit cell parameters	
a(Å)	4.00550 ± 0.001	5.70990 ± 0.002
c(Å)	4.01749 ± 0.002	14.03939 ± 0.007
c/a	1.003	2.459
V(Å)^3	64.457 ± 0.040	396.401 ± 0.271
Cal. density (g/cm³)	6.018	5.872
Refinement	Rietveld refinement (Fulprof)	
Profile	Pseudo-Voigt	
	Atom Parameters	
Ba1	0.00000, 0.00000, 0.00000	0.00000, 0.00000, 0.25000
Ba2		0.33330, 0.66670, 0.09384
Ti1	0.50000, 0.50000, 0.50000	0.00000, 0.00000, 0.00000
Ti2		0.33330, 0.66670, 0.85288
O1	0.50000, 0.50000, 0.00000	0.51850, 0.03700, 0.25000
O2	0.50000, 0.00000, 0.50000	0.83490, 0.66980, 0.08020
Fe1	0.50000, 0.50000, 0.50000	0.00000, 0.00000, 0.00000
Fe2		0.33330, 0.66670, 0.85288
	Reliability Factors	
R_B, R_F	4.37, 2.78	13.0, 8.84
R_p, R_{wp}, χ^2	10.5, 14.3, 0.07	
Bond Distances (Å)	Tetragonal phase	Hexagonal phase
Ti/Fe-O	4 x 2.0028(5) 2 x 2.0085(10)	3 x 1.9105(6) 6 x 1.9834(6) 3 x 2.0574(6)
Ba-O	4 x 2.8323(5) 8 x 2.8364(8)	6 x 2.8609(10) 6 x 2.8894(10) 3 x 2.8565(9) 6 x 2.8612(10) 3 x 2.9562(11)

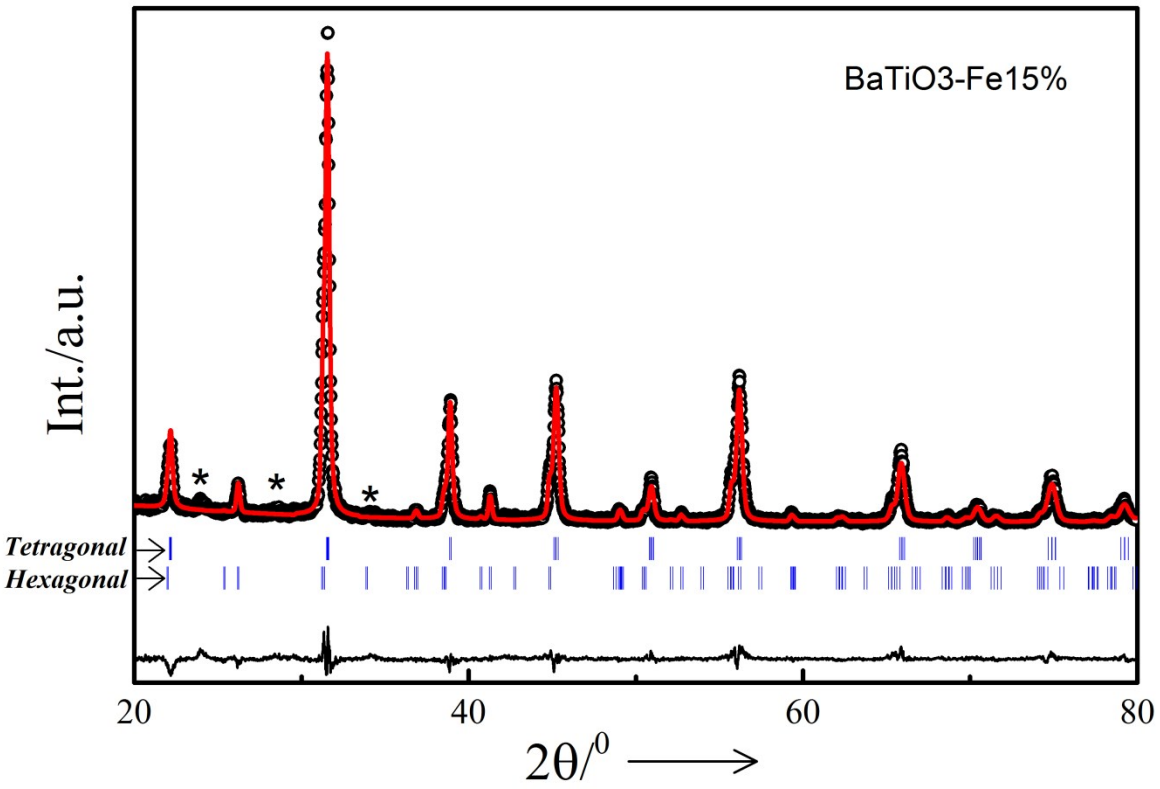

Figure 1S: XRD refinement of $BaTi_{0.85}Fe_{0.15}O_3$ sample. The dashed lines are experimental data, while the solid curves are the calculation results. The vertical bars indicate the peak positions that are calculated by refinement, and the bottom solid lines indicate the differences between experimental and calculation results.