

Decoding the domain dynamics of polycrystalline $0.7\text{BiFeO}_3\text{-}0.3\text{BaTiO}_3$

Lixu Xie^{1,2}, Neamul H. Khansur¹, Mingyue Mo², Ahmed Gadelmawla¹, Jie Xing², Zhi Tan², Jianguo Zhu^{2*}, and Kyle G. Webber¹

¹Department of Materials Science and Engineering, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen, Germany

²College of Materials Science and Engineering, Sichuan University, 610064 Chengdu, China

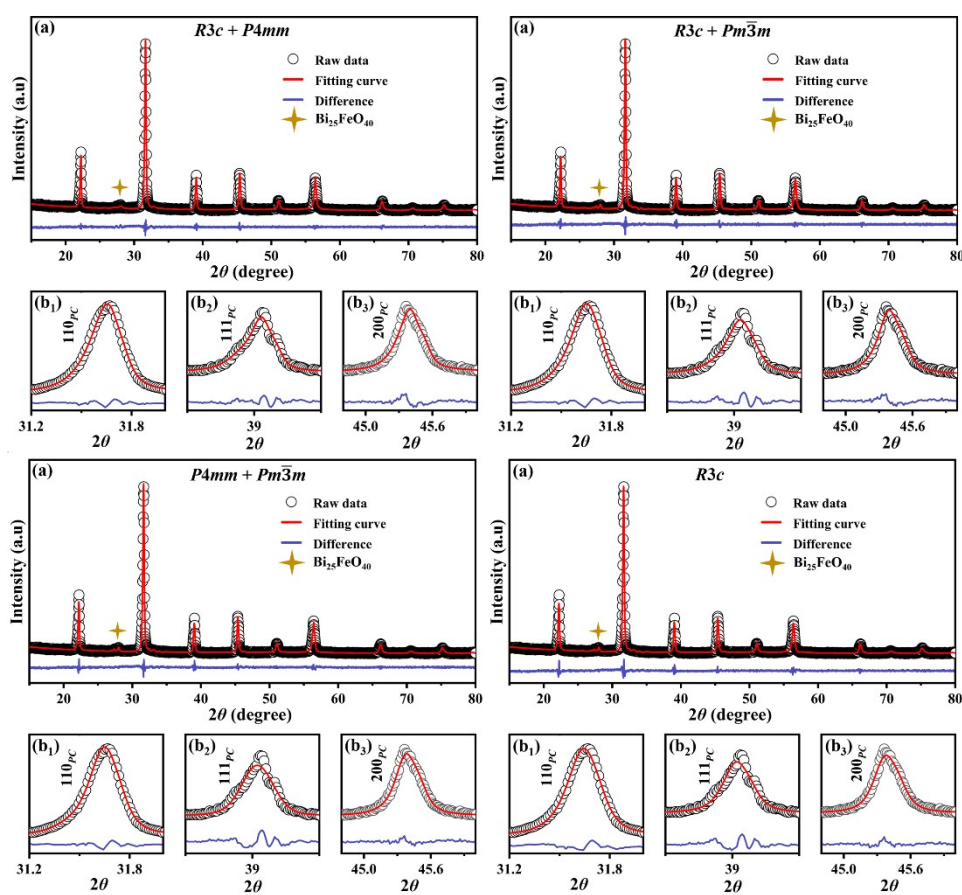


Figure S1. Rietveld refinement XRD patterns of BF30BT with different models.

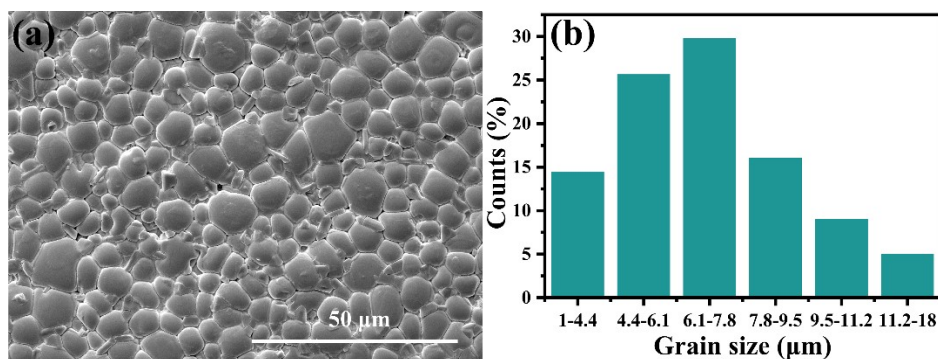


Figure S2. (a) Surface SEM microstructure images of BF30BT and (b) statistics of grain size.

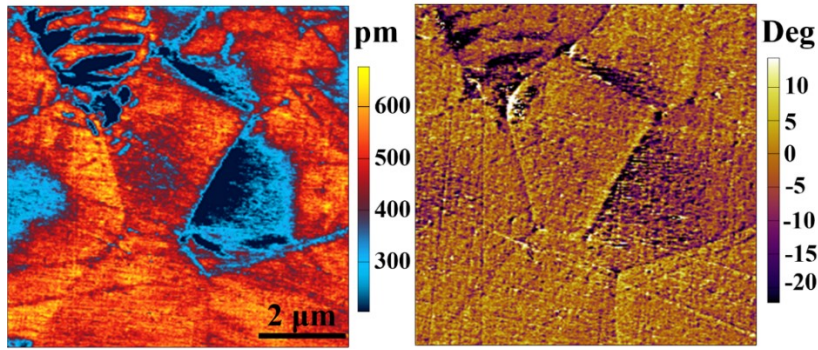


Figure S3. The amplitude and corresponding phase pattern of poled BF30BT ceramic.

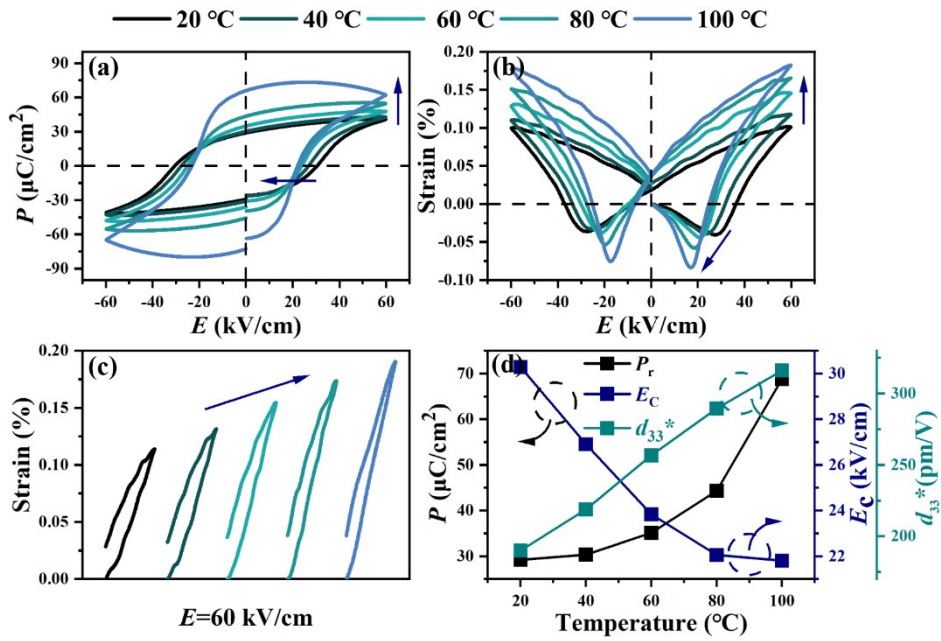


Figure S4. (a) variation of P - E hysteresis loops as a function of temperature in BF30BT (b) bipolar curves of the BF30BT ceramic as a function of temperature; (c) unipolar curves of the BF30BT ceramic as a function of temperature; (d) variation of P_r , E_c , and d_{33}^* as a function of temperature.

The frequency dependence of the piezoelectric response d_{33} at 25 °C is plotted in Figure S4, and its linear relationship is revealed through frequency-dependence Rayleigh analysis.

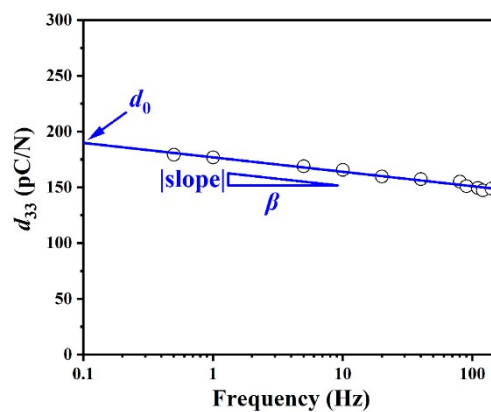


Figure S5. Linear relationship between d_{33} and frequency at 20 °C.

The amplitude dependence of the piezoelectric response d_{33} at 250 °C is plotted in Figure S5, and its linear relationship is revealed through amplitude-dependence Rayleigh analysis.

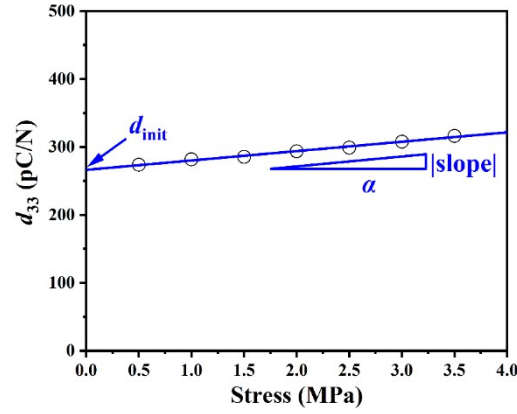


Figure S6. Linear relationship between d_{33} and stress σ_A at 250 °C.

Table S1. Crystal structure parameters of the BF30BT ceramic derived from the Rietveld structure refinement program with different models

Model	Sig	R_{wp} (%)	Symmetry	Space group	Phase ratio	a (Å)	c (Å)	α (°)
$R3c + P4mm$	1.31	4.10	R phase	$R3c$	63.27%	5.6439	13.8192	
			T phase	$P4mm$	31.70%	3.9962	4.0189	
			$Bi_{25}FeO_{40}$	$I23$	5.03%			
$R3c + Pm\bar{3}m$	1.38	4.31	R phase	$R3c$	62.01%	5.6461	13.8229	
			PC phase	$Pm\bar{3}m$	34.50%	4.0010		
			$Bi_{25}FeO_{40}$	$I23$	3.49%			
$R3c$	1.54	4.8	R phase	$R3c$	95.67%	5.6480	13.8301	
			$Bi_{25}FeO_{40}$	$I23$	4.33%			
			T phase	$P4mm$	29.48%	3.9928	4.0497	

			PC phase	$Pm\bar{3}m$	4.97%	3.9927		
			$\text{Bi}_{25}\text{FeO}_{40}$	$I23$	3.17%			

Table S2. Crystal structure parameters of the unpoled BF30BT ceramics derived from the Rietveld structure refinement program with different temperature

Temperature	Sig	R_{wp} (%)	Symmetry	Space group	Phase ratio	a (Å)	c (Å)	α (°)
25 °C	1.32	6.41	R phase	$R3c$	62.14%	5.6282	13.7914	
			T phase	$P4mm$	33.51%	3.9842	4.0052	
			Bi ₂₅ FeO ₄₀	$I23$	4.35%			
	1.59	7.34	R phase	$R3m$	60.17%	3.9727		89.8736
			T phase	$P4mm$	34.71%	3.9861	4.0067	
			Bi ₂₅ FeO ₄₀	$I23$	5.15%			
50 °C	1.35	6.72	R phase	$R3c$	60.29%	5.6314	13.8027	
			T phase	$P4mm$	35.20%	3.9867	4.0063	
			Bi ₂₅ FeO ₄₀	$I23$	4.51%			
	1.57	7.21	R phase	$R3m$	58.29%	3.9734		89.8862
			T phase	$P4mm$	37.10%	3.9869	4.0072	
			Bi ₂₅ FeO ₄₀	$I23$	4.61%			
75 °C	1.37	6.79	R phase	$R3c$	58.43%	5.6340	13.8123	
			T phase	$P4mm$	37.34%	3.9899	4.0092	
			Bi ₂₅ FeO ₄₀	$I23$	4.23%			
	1.54	7.38	R phase	$R3m$	57.42%	3.9760		89.8911
			T phase	$P4mm$	38.45%	3.9884	4.0084	
			Bi ₂₅ FeO ₄₀	$I23$	4.13%			
			R phase	$R3c$	56.11%	5.6365	13.8211	

			T phase	<i>P4mm</i>	38.92%	3.9922	4.0104	
			Bi ₂₅ FeO ₄₀	<i>I23</i>	4.97%			
	1.49	7.09	R phase	<i>R3m</i>	55.72%	3.9809		89.9021
			T phase	<i>P4mm</i>	39.71%	3.9909	4.0105	
			Bi ₂₅ FeO ₄₀	<i>I23</i>	4.57%			
150 °C	1.44	6.83	R phase	<i>R3c</i>	54.37%	5.6393	13.8244	
			T phase	<i>P4mm</i>	40.61%	3.9948	4.0122	
			Bi ₂₅ FeO ₄₀	<i>I23</i>	5.02%			
	1.46	7.17	R phase	<i>R3m</i>	53.91%	3.9839		89.9163
			T phase	<i>P4mm</i>	41.83%	3.9919	4.0113	
			Bi ₂₅ FeO ₄₀	<i>I23</i>	4.26%			
200 °C	1.46	6.92	R phase	<i>R3c</i>	52.76%	5.6411	13.8337	
			T phase	<i>P4mm</i>	42.79%	3.9957	4.0135	
			Bi ₂₅ FeO ₄₀	<i>I23</i>	4.45%			
	1.44	6.98	R phase	<i>R3m</i>	52.98%	3.9861		89.9356
			T phase	<i>P4mm</i>	41.82%	3.9943	4.0121	
			Bi ₂₅ FeO ₄₀	<i>I23</i>	5.20%			
300 °C	1.48	7.01	R phase	<i>R3c</i>	50.91%	5.6421	13.8410	
			T phase	<i>P4mm</i>	44.23%	3.9972	4.0148	
			Bi ₂₅ FeO ₄₀	<i>I23</i>	4.86%			
	1.43	6.92	R phase	<i>R3m</i>	51.85%	3.9921		89.9463
			T phase	<i>P4mm</i>	43.78%	3.9969	4.0131	

			Bi ₂₅ FeO ₄₀	<i>I23</i>	4.37%			
400 °C	1.49	7.11	R phase	<i>R3c</i>	49.98%	5.6481	13.8635	
			T phase	<i>P4mm</i>	45.83%	4.0012	4.0153	
			Bi ₂₅ FeO ₄₀	<i>I23</i>	4.19%			
	1.41	6.83	R phase	<i>R3m</i>	50.26%	3.9961		89.9653
			T phase	<i>P4mm</i>	45.18%	4.0018	4.0157	
			Bi ₂₅ FeO ₄₀	<i>I23</i>	4.56%			
450 °C	1.51	7.19	R phase	<i>R3c</i>	47.96%	5.6504	13.8667	
			T phase	<i>P4mm</i>	43.94%	4.0047	4.0176	
			Bi ₂₅ FeO ₄₀	<i>I23</i>	4.81%			
	1.44	7.01	R phase	<i>R3m</i>	48.72%	3.9986		89.9811
			T phase	<i>P4mm</i>	46.69%	4.0048	4.0174	
			Bi ₂₅ FeO ₄₀	<i>I23</i>	4.59%			
	1.36	6.58	R phase	<i>R3m</i>	37.28%	3.9995		89.9847
			C phase	<i>Pm$\bar{3}$m</i>	57.60%	4.0046		
			Bi ₂₅ FeO ₄₀	<i>I23</i>	5.12%			

Table S3. Crystal structure parameters of the poled BF30BT ceramics derived from the Rietveld structure refinement program with different temperature

Temperature	Sig	R_{wp} (%)	Symmetry	Space group	Phase ratio	a (Å)	c (Å)	α (°)
25 °C	1.21	5.87	R phase	$R3c$	72.23%	5.6299	13.7974	
			T phase	$P4mm$	22.64%	3.9861	4.0105	
			Bi ₂₅ FeO ₄₀	$I23$	5.13%			
	1.49	7.13	R phase	$R3m$	70.38%	3.9767		89.8635
			T phase	$P4mm$	24.77%	3.9856	4.0149	
			Bi ₂₅ FeO ₄₀	$I23$	4.84%			
50 °C	1.26	6.01	R phase	$R3c$	70.86%	5.6305	13.8036	
			T phase	$P4mm$	36.87%	3.9868	4.0108	
			Bi ₂₅ FeO ₄₀	$I23$	4.41%			
	1.47	6.93	R phase	$R3m$	69.94%	3.9734		89.8832
			T phase	$P4mm$	25.87%	3.9878	4.0168	
			Bi ₂₅ FeO ₄₀	$I23$	4.19%			
75 °C	1.27	6.13	R phase	$R3c$	68.97%	5.6314	13.8065	
			T phase	$P4mm$	25.81%	3.9874	4.0108	
			Bi ₂₅ FeO ₄₀	$I23$	5.22%			
	1.47	6.81	R phase	$R3m$	67.81%	3.9843		89.8903
			T phase	$P4mm$	27.04%	3.9885	4.0172	
			Bi ₂₅ FeO ₄₀	$I23$	5.15%			
			R phase	$R3c$	67.01%	5.6319	13.8077	

			T phase	<i>P4mm</i>	27.73%	3.9881	4.0113	
			Bi ₂₅ FeO ₄₀	<i>I23</i>	5.26%			
	1.45	6.77	R phase	<i>R3m</i>	65.72%	3.9851		89.9061
			T phase	<i>P4mm</i>	28.49%	3.9889	4.0175	
			Bi ₂₅ FeO ₄₀	<i>I23</i>	5.79%			
150 °C	1.36	6.54	R phase	<i>R3c</i>	66.07%	5.6330	13.8105	
			T phase	<i>P4mm</i>	30.76%	3.9896	4.0125	
			Bi ₂₅ FeO ₄₀	<i>I23</i>	3.17%			
	1.42	6.68	R phase	<i>R3m</i>	63.89%	3.9856		89.9124
			T phase	<i>P4mm</i>	32.28%	3.9896	4.0181	
			Bi ₂₅ FeO ₄₀	<i>I23</i>	3.83%			
200 °C	1.37	6.59	R phase	<i>R3c</i>	63.91%	5.6341	13.8150	
			T phase	<i>P4mm</i>	35.11%	3.9916	4.0133	
			Bi ₂₅ FeO ₄₀	<i>I23</i>	4.98%			
	1.36	6.49	R phase	<i>R3m</i>	61.71%	3.9871		89.9241
			T phase	<i>P4mm</i>	32.88%	3.9921	4.0201	
			Bi ₂₅ FeO ₄₀	<i>I23</i>	5.41%			
300 °C	1.40	6.72	R phase	<i>R3c</i>	61.39%	5.6436	13.8389	
			T phase	<i>P4mm</i>	33.74%	3.9938	4.0151	
			Bi ₂₅ FeO ₄₀	<i>I23</i>	4.87%			
	1.35	6.71	R phase	<i>R3m</i>	59.99%	3.9919		89.9301
			T phase	<i>P4mm</i>	35.00%	3.9934	4.0213	

			Bi ₂₅ FeO ₄₀	<i>I23</i>	5.01%			
400 °C	1.43	6.81	R phase	<i>R3c</i>	59.01%	5.6468	13.8592	
			T phase	<i>P4mm</i>	36.26%	3.9989	4.0179	
			Bi ₂₅ FeO ₄₀	<i>I23</i>	4.73%			
	1.35	6.67	R phase	<i>R3m</i>	56.81%	3.9944		89.9518
			T phase	<i>P4mm</i>	38.26%	4.0018	4.0223	
			Bi ₂₅ FeO ₄₀	<i>I23</i>	4.93%			
450 °C	1.43	7.01	R phase	<i>R3c</i>	54.29%	5.6512	13.8629	
			T phase	<i>P4mm</i>	40.99%	4.0042	4.0183	
			Bi ₂₅ FeO ₄₀	<i>I23</i>	4.72%			
	1.36	6.70	R phase	<i>R3m</i>	51.39%	3.9978		89.9774
			T phase	<i>P4mm</i>	42.80%	4.0053	4.0245	
			Bi ₂₅ FeO ₄₀	<i>I23</i>	5.81%			
	1.31	6.59	R phase	<i>R3m</i>	43.70%	3.9976		89.9501
			C phase	<i>Pm$\bar{3}$m</i>	51.18%	4.0050		
			Bi ₂₅ FeO ₄₀	<i>I23</i>	5.12%			

Table S4. Electrical properties of BF30BT ceramic at room temperature

d_{33}	k_p	Q_m	$\tan \delta$	P_r	E_c
----------	-------	-------	---------------	-------	-------

165 pC/N	0.32	50	0.02	29.2 $\mu\text{C}/\text{cm}^2$	30.3 kV/cm
----------	------	----	------	--------------------------------	------------