Supporting Information

Large Piezoelectricity in $NaNbO_3$-based Lead-free Ceramics via Tuning Oxygen Octahedral Tilt

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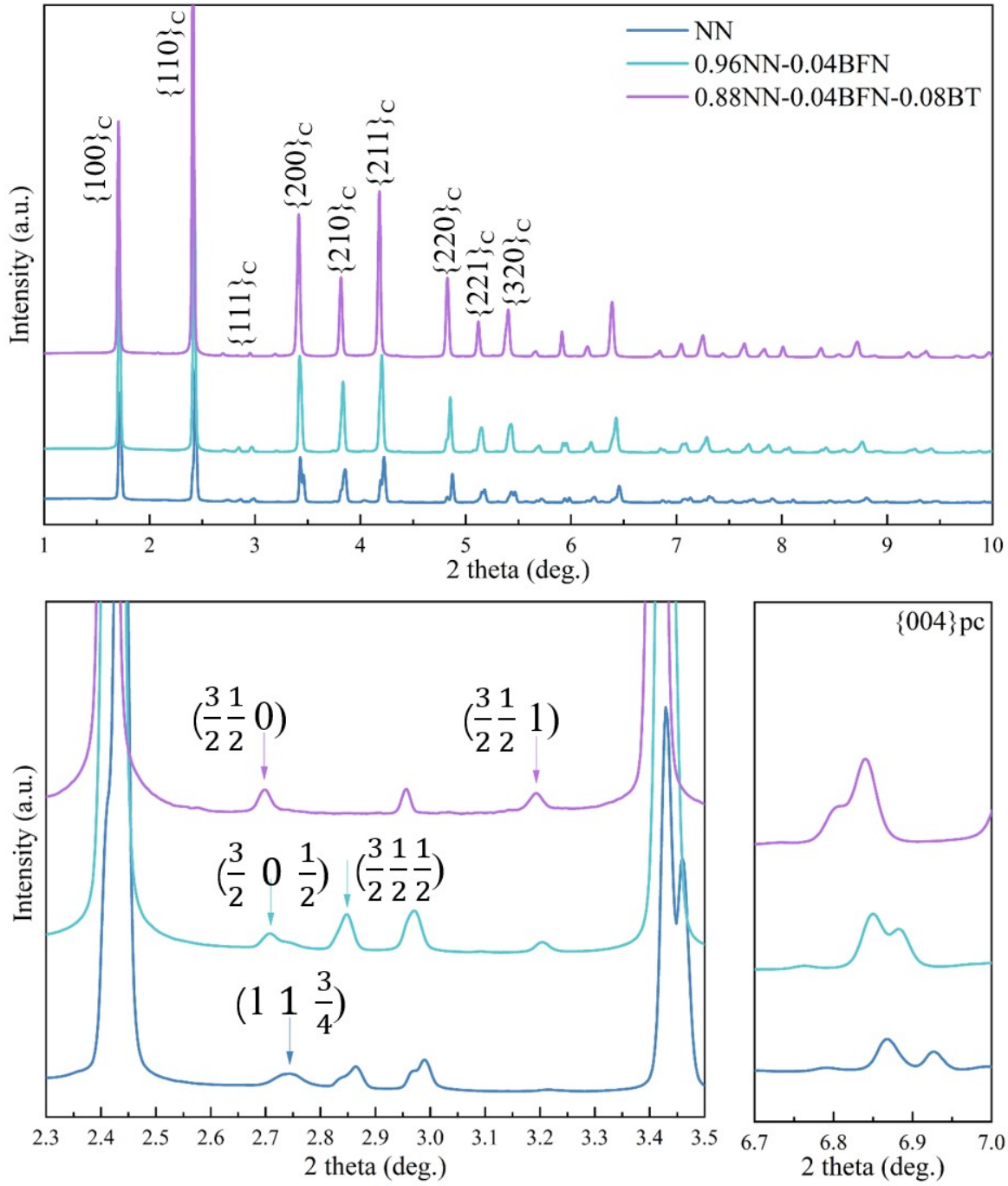

Figure S1. The composition dependence of SXRD patterns.

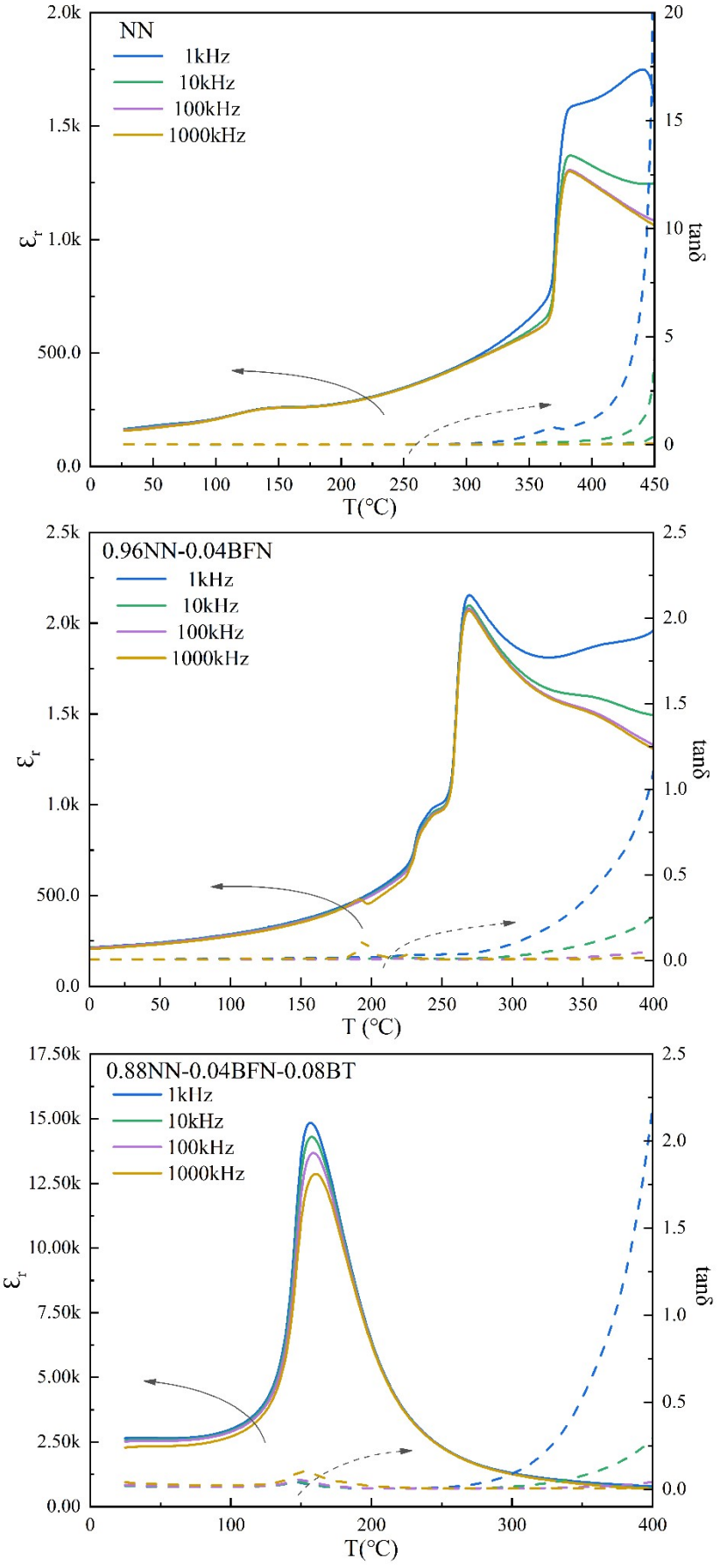

Figure S2. Dielectric permittivity and loss tangent with variable temperature and frequency at different compositions.

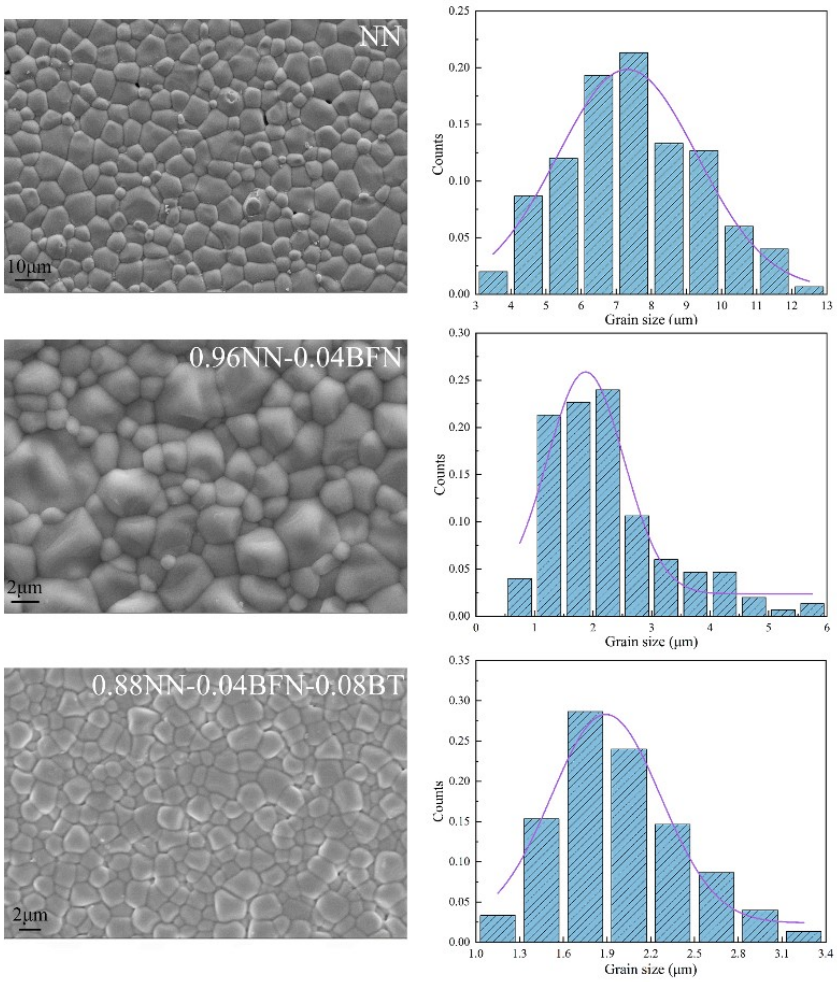

Figure S3. SEM micrograph of the as-sintered surface for NN, 0.96NN-0.04BFN, 0.88NN-0.04BFN-0.08BT and the grain size distribution at different compositions.

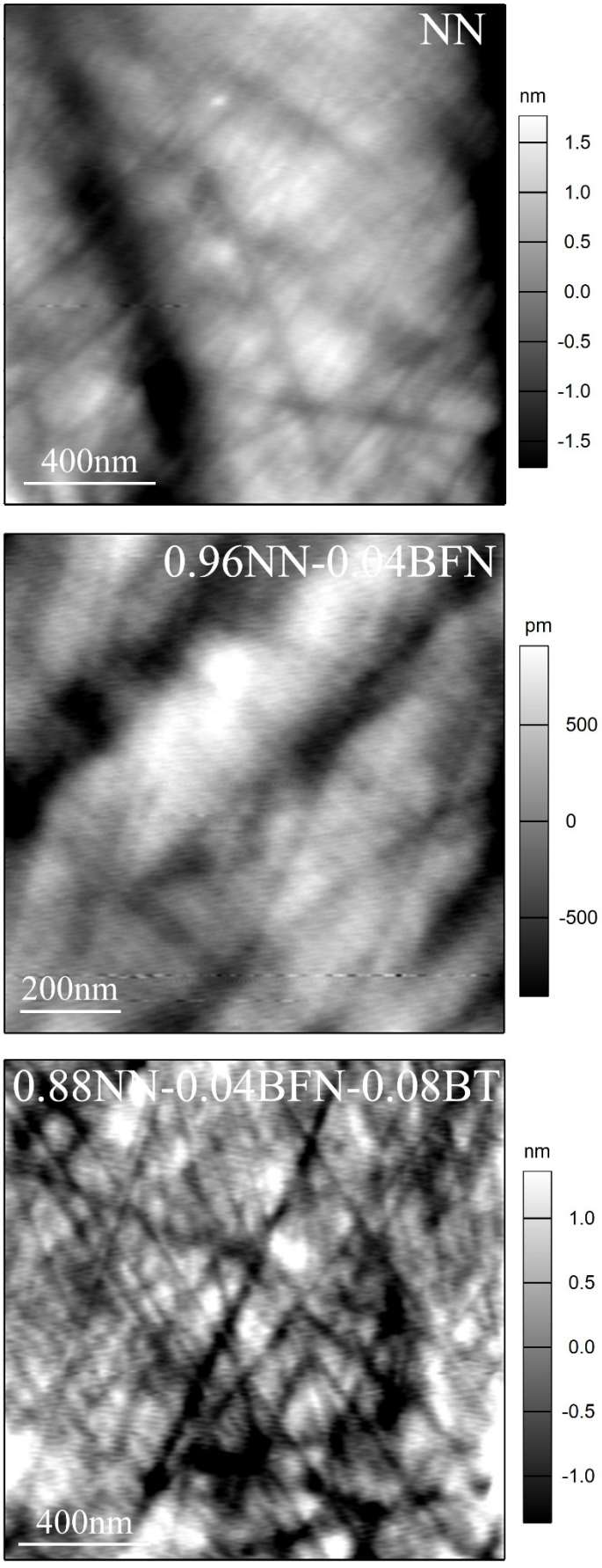

Figure S4. PFM surface topography with different compositions.

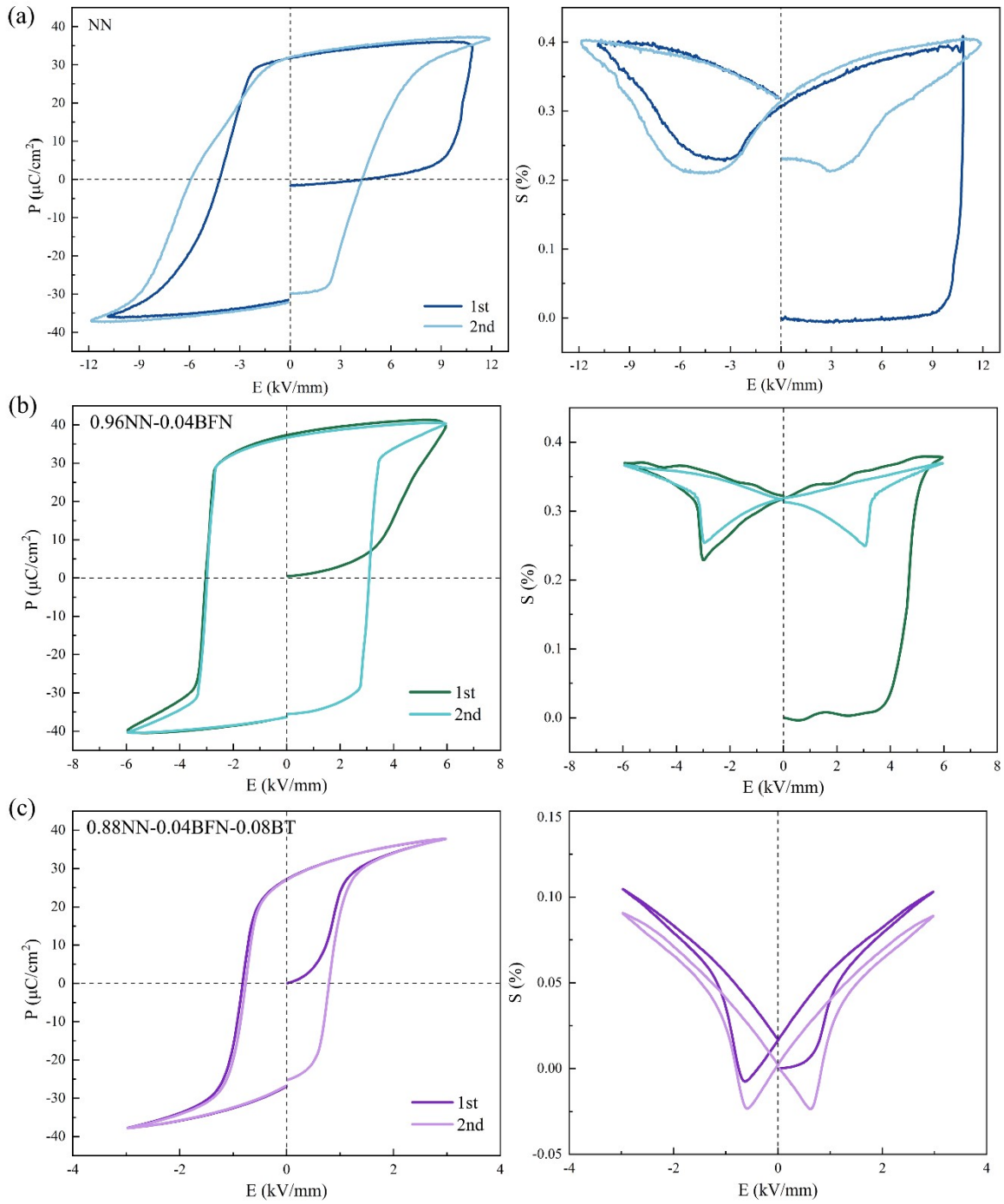

Figure S5. Polarization loops with first and second circle of unpoled ceramic disks for (a) NN, (b) 0.96NN-0.04BFN and (c) 0.88NN-0.04BFN-0.08BT and the corresponding bipolar strain curves.

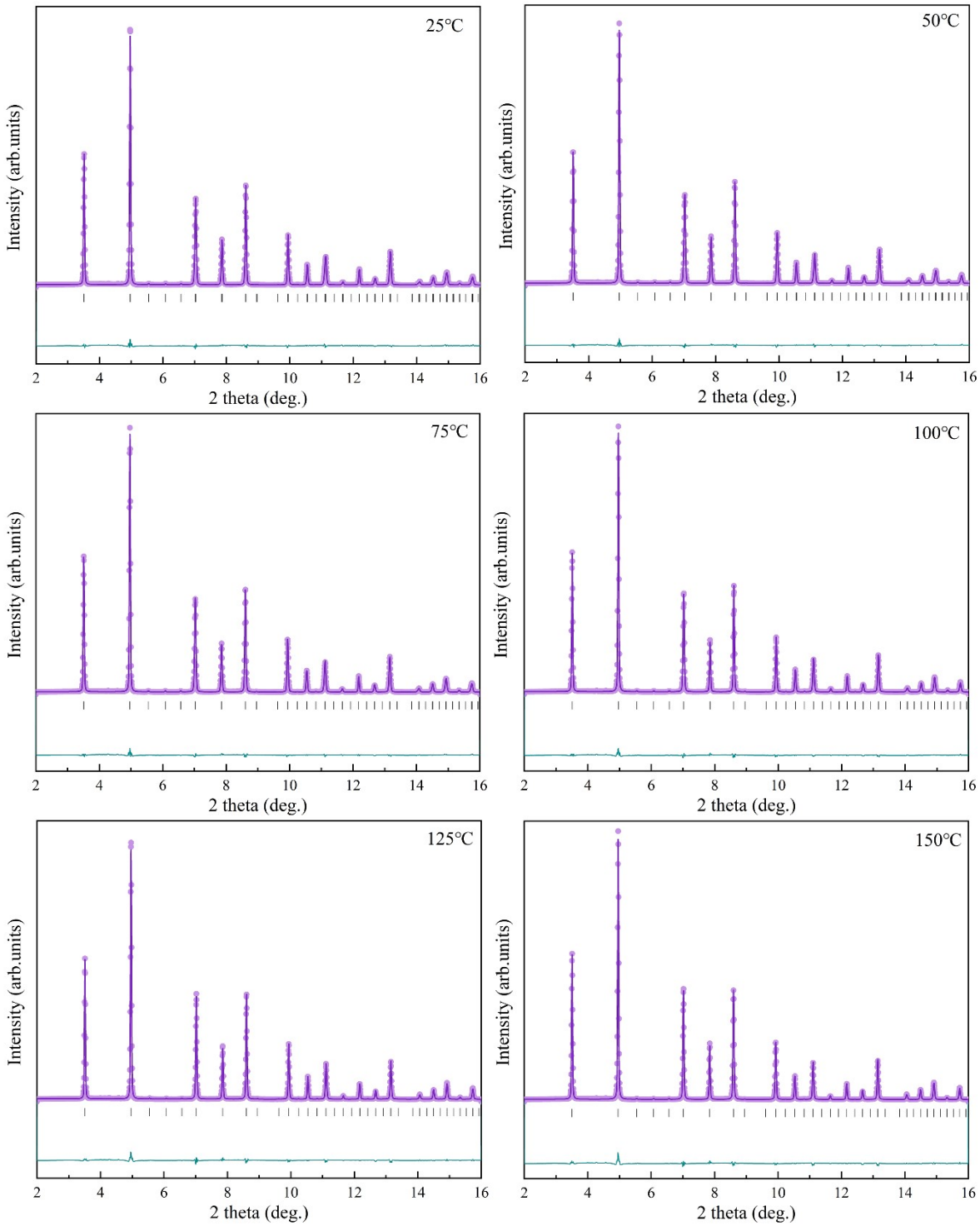

Figure S6. Structure refinement of temperature-dependent SXRD in 0.88NN-0.04BFN-0.08BT with increasing temperature (25°C-150°C).

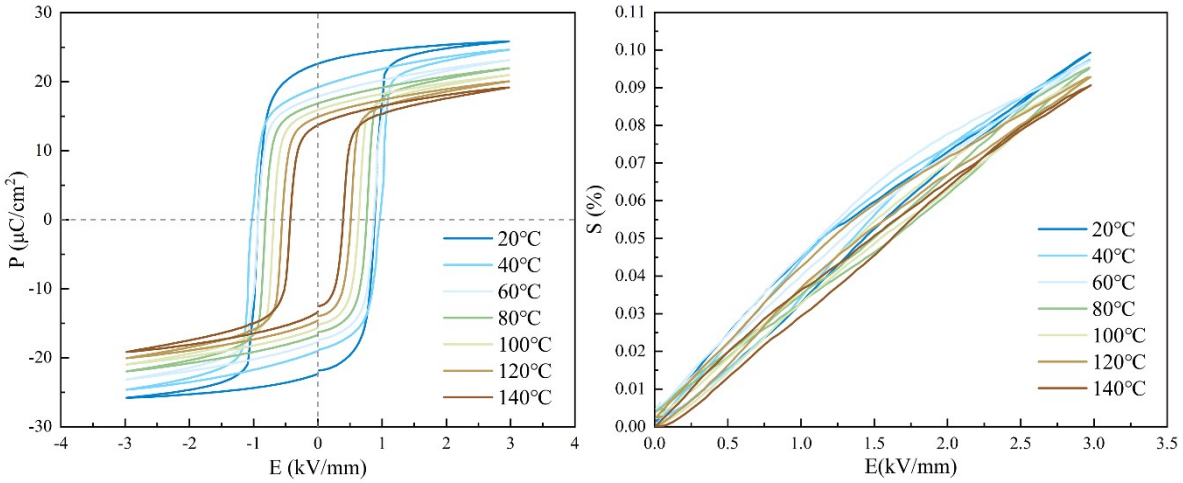

Figure S7. (a) temperature-dependent polarization loops and (b) unipolar strain of the 0.88NN-0.04BFN-0.08BT composition under 3kV mm^{-1} in the range of 20 - 140°C

Table S1. Detailed structural parameters for different compositions refined by the Rietveld method.

NN				
Space group			*Pbcm*	
a = 5.504(1) Å		*b* = 5.568(9) Å	*c* = 15.519(4) Å	
Atom	X	Y	Z	Occ
Na1	0.2246(5)	0.25	0	0.5
Na2	0.2219(7)	0.2110(5)	0.25	0.5
Nb	0.2521(1)	0.7357(1)	0.1261(1)	1
O1	0.6845(4)	0.25	0	0.5
O2	0.1769(2)	0.7408(3)	0.25	0.5
O3	0.4740(6)	0.4670(4)	0.1420(2)	1
O4	0.0326(2)	0.0334(0)	0.1118(2)	1

0.96NN-0.04BFN				
Space group			$Pb2_1m$	
a = 5.490(4) Å		*b* = 5.547(7) Å	*c* = 7.824(7) Å	
Atom	X	Y	Z	Occ
Na1	0.7060(2)	0.1950(1)	0.25	0.5
Na2	0.7250(3)	0.1960(5)	0.25	0.5
Nb	0.2371(2)	0.2100(1)	0	0.98
Fe	0.2371(2)	0.2100(1)	0.5	0.02
O1	0.2900(1)	0.2510(4)	0	0.5
O2	0.1940(5)	0.2370(3)	0.5	0.5
O3	0.5288(6)	-0.0010(6)	0.2796(5)	1
O4	0.0190(4)	-0.0030(7)	0.2190(2)	1

0.88NN-0.04BFN-0.08BT				
Space group			*P4bm*	
a = *b* = 5.564(8) Å			*c* = 3.927(1) Å	
Atom	X	Y	Z	Occ
Na	0	0.5	0.5023(2)	0.88
Ba	0	0.5	0.5023(2)	0.12
Nb	0	0	0	0.90
Fe	0	0	0	0.02
Ti	0	0	0	0.08
O1	0.2749(7)	0.2250(3)	0.0620(4)	2
O2	0	0	0.4497(2)	1

Table S2. Structural parameters change for tetragonal 0.88NN-0.04BFN-0.08BT with increasing temperature.

Space group			*P4bm*	
T (°C)	*a* (Å)	*c* (Å)	*c/a*	*ω* (°)
25	5.564(8)	3.927(1)	1.002(13)	5.71
50	5.565(6)	3.929(6)	1.001(64)	5.44
75	5.566(1)	3.932(4)	1.001(01)	5.145
100	5.566(7)	3.935(1)	1.000(45)	4.915
125	5.568(1)	3.937(1)	1.000(21)	4.55
150	5.570(4)	3.938(9)	1.000(15)	4.12