

Supplementary Information for

Simultaneously enhanced piezoelectric properties and thermal stability of Pb(Zr, Ti)O₃-based ceramics by composition design strategy

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Table S1 Lattice parameters obtained from the Rietveld structural refinements.

x	Space group	Lattice parameters				Cell volume (\AA^3)	Phase content (%)	Tetragonality (c/a)
		a (\AA)	b (\AA)	c (\AA)	Angle ($^\circ$)			
0	$P4mm$	4.0506	4.0506	4.1213	$\alpha = \beta = \gamma = 90$	67.618	13.34	1.017
	$R3m$	4.0737	4.0737	4.0737	$\alpha = \beta = \gamma = 89.707$	67.602	86.66	
0.005	$P4mm$	4.0487	4.0487	4.1208	$\alpha = \beta = \gamma = 90$	67.550	70.13	1.018
	$R3m$	4.0736	4.0736	4.0736	$\alpha = \beta = \gamma = 89.713$	67.596	29.97	
0.01	$P4mm$	4.0475	4.0475	4.1206	$\alpha = \beta = \gamma = 90$	67.504	53.24	1.018
	$R3m$	4.0735	4.0735	4.0735	$\alpha = \beta = \gamma = 89.715$	67.594	46.76	
0.015	$P4mm$	4.0466	4.0466	4.1199	$\alpha = \beta = \gamma = 90$	67.465	60.91	1.018
	$R3m$	4.0730	4.0730	4.0730	$\alpha = \beta = \gamma = 89.719$	67.564	39.09	
0.02	$P4mm$	4.0465	4.0465	4.1209	$\alpha = \beta = \gamma = 90$	67.468	66.35	1.018
	$R3m$	4.0725	4.0725	4.0725	$\alpha = \beta = \gamma = 89.7357$	67.522	33.65	
0.025	$P4mm$	4.0451	4.0451	4.1215	$\alpha = \beta = \gamma = 90$	67.443	77.09	1.019
	$R3m$	4.0719	4.0719	4.0719	$\alpha = \beta = \gamma = 89.769$	67.514	22.91	

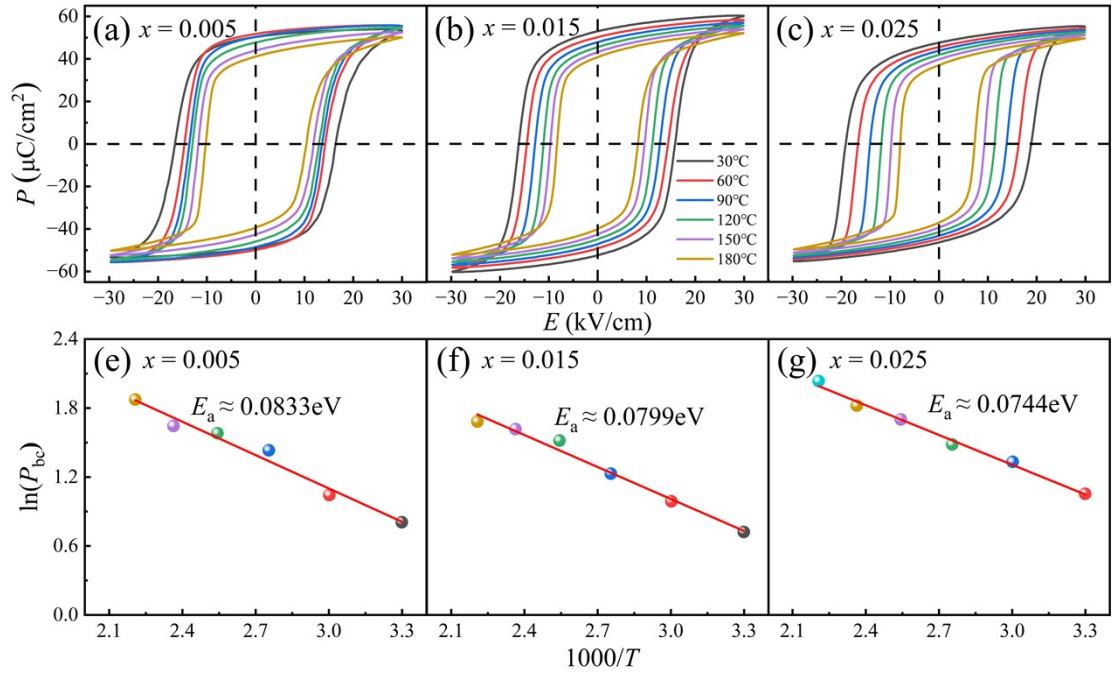


Fig.S1 (a)-(c) The P - E loops dependence of Nd_2O_3 content for the PNZTN- x ceramics; (d)-(f) Plot of $\ln(P_{bc})$ versus $1000/T$.

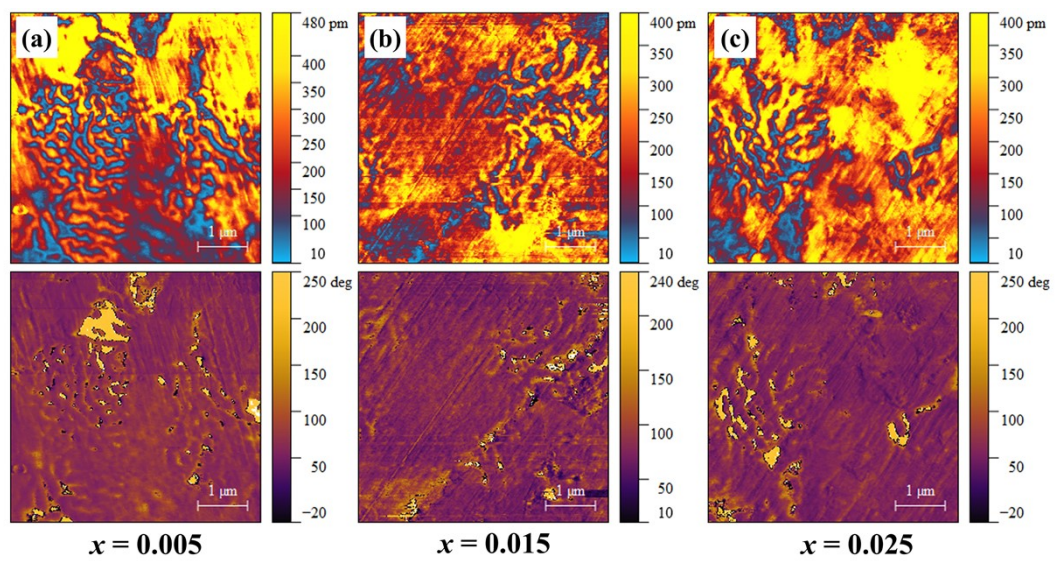


Fig.S2 PFM measurements for the PNZTN- x ceramics with (a) $x = 0.005$, (b) $x = 0.015$, (c) $x = 0.025$.