Support information

The Effect of Nb_2O_5 Precursor on KNN-Based Ceramics' Piezoelectricity and Strain Temperature Stability

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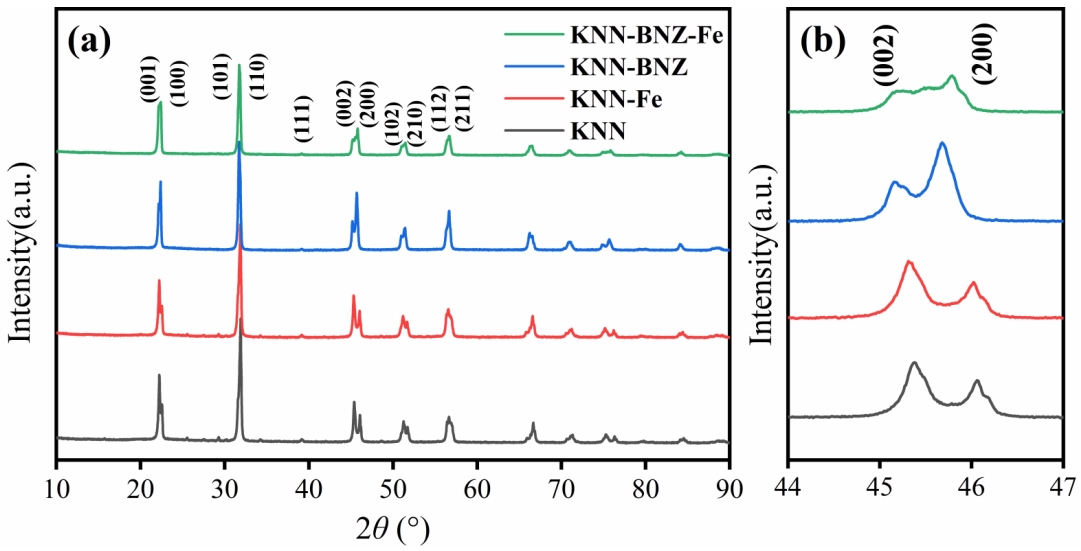

Figure S1 XRD patterns of KNN, KNN-Fe, KNN-BNZ, KNN-BNZ-Fe and KNN-UN from (a) 20 °<θ < 90°, (b) 44°<θ <47°

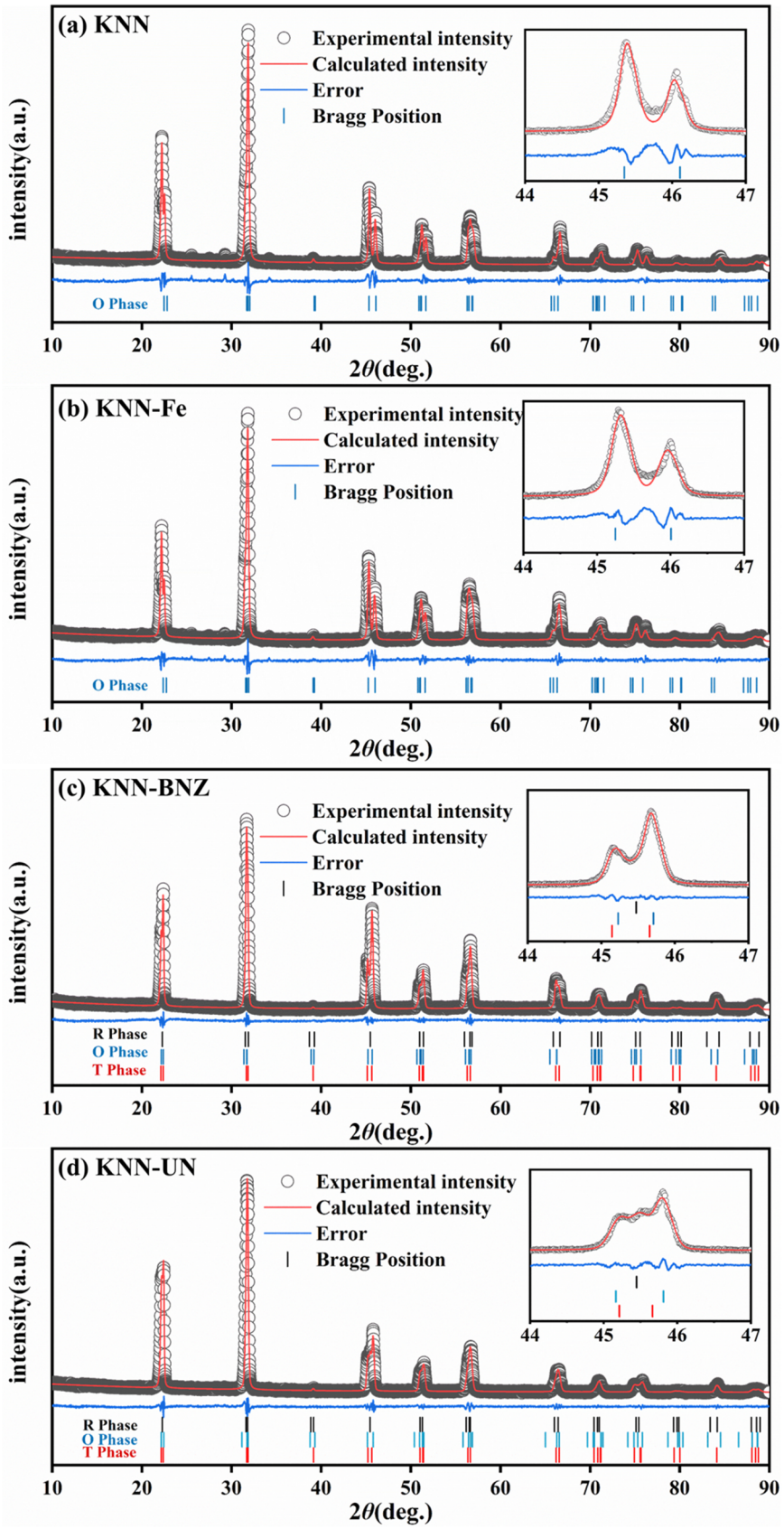

Figure S2 (a)-(d) The Rietveld refinement for KNN, KNN-Fe, KNN-BNZ, KNN-UN ceramics

Table S1 Parameters of KNN, KNN-Fe, KNN-BNZ and KNN-UN ceramics obtained from Rietveld refinement

Parameters	KNN	KNN-Fe	KNN-BNZ			KNN-UN		
sig	1.98	1.99	1.88			1.52		
R_w(%)	4.38	4.93	3.96			4.06		
Symmetry	O Phase	O Phase	R Phase	O Phase	T Phase	R Phase	O Phase	T Phase
proportion	100%	100%	34.2%	29.8%	36.0%	33.5%	46.7%	19.8%
Space group	*Amm*2	*Amm*2	*R*3*m*	*Amm*2	*P*4*mm*	*R*3*m*	*Amm*2	*P*4*mm*
a(Å)	3.9399	3.9931	3.9863	3.9667	3.9709	3.9885	3.9581	3.9704
b(Å)	5.6634	5.6630	3.9863	5.6957	3.9709	3.9885	5.7336	3.9704
c(Å)	5.6292	5.6281	3.9863	5.6367	4.0136	3.9885	5.6151	4.0077
Alpha(°)	90.0000	90.0000	89.4240	90.0000	90.0000	89.6780	90.0000	90.0000
A (*x,y,z*)	0.0000, 0.0000, 0.0138	0.0000, 0.0000, 0.0138	0.0134, 0.0134, 0.0134	-0.0002, -0.0001, 0.0135	0.0000, 0.0000, 0.0177	0.0129, 0.0129, 0.0129	0.0000, 0.0001, 0.0137	0.0000, 0.0000, 0.0178
B (*x,y,z*)	0.5001, 0.0000, 0.4998	0.5002, 0.0000, 0.4993	0.4922, 0.4922, 0.4922	0.5002, 0.0002, 0.4923	0.5000, 0.5000, 0.4922	0.4949, 0.4949, 0.4949	0.5000, 0.0000, 0.4949	0.5000, 0.5000, 0.4950
O1 (*x,y,z*)	0.0000, 0.0000, 0.5361	0.0000, 0.0000, 0.5358	0.5217, 0.5217, 0.0321	0.0002, 0.0000, 0.5278	0.5000, 0.5000, 0.0433	0.5247, 0.5247, 0.0324	0.0000, -0.0001 0.5309	0.4998, 0.4995, 0.0434
O2 (*x,y,z*)	0.5000, 0.2476, 0.2841	0.4997, 0.2470, 0.2820	-	0.4916, 0.2434, 0.2794	0.5000, 0.0000, 0.5316	-	0.4997, 0.2449, 0.2812	0.4999, -0.0026 0.5345

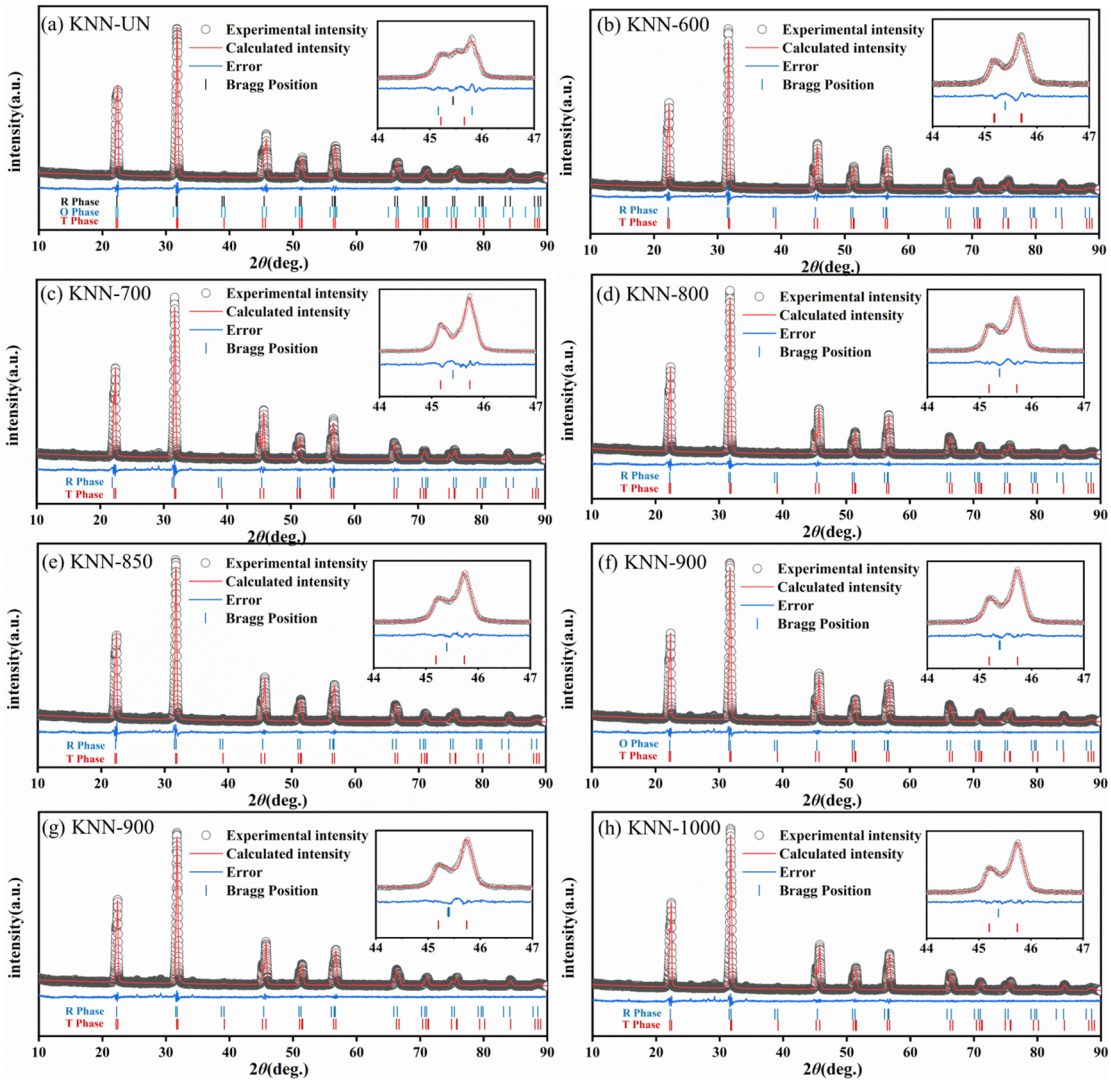

Figure S3 (a)-(h) The Rietveld refinement for KNN-UN, KNN-600, KNN-700, KNN-800, KNN-850, KNN-900, KNN-950, KNN-1000

Table S2 Parameters of KNN-UN ~ KNN-1000 obtained from Rietveld refinement

Parameters	KNN-UN			KNN-600		KNN-700		KNN-800		KNN-850		KNN-900		KNN-950		KNN-1000	
sig	1.52			1.61		1.70		1.58		1.59		1.65		1.60		1.70	
R_w(%)	4.06			4.34		4.54		4.23		4.27		4.41		4.49		4.55	
Symmetry	R Phase	O Phase	T Phase	R Phase	T Phase	R Phase	T Phase	R Phase	T Phase	R Phase	T Phase	R Phase	T Phase	R Phase	T Phase	R Phase	T Phase
proportion	33.5%	46.7%	19.8%	39.4%	60.6%	41.3%	58.7%	47.4%	52.6%	48.7%	51.3%	46.9%	53.1%	44.9%	55.1%	43.8%	56.2%
Space group	*R*3*m*	*Amm*2	*P*4*mm*	*R*3*m*	*P*4*mm*	*R*3*m*	*P*4*mm*	*R*3*m*	*P*4*mm*	*R*3*m*	*P*4*mm*	*R*3*m*	*P*4*mm*	*R*3*m*	*P*4*mm*	*R*3*m*	*P*4*mm*
a(Å)	3.9885	3.9581	3.9704	3.9931	3.9671	3.9343	3.9648	3.9937	3.9664	3.9926	3.9644	3.9934	3.9650	3.9929	3.9641	3.9944	3.9642
b(Å)	3.9885	5.7336	3.9704	3.9931	3.9671	3.9343	3.9648	3.9937	3.9664	3.9926	3.9644	3.9934	3.9650	3.9929	3.9641	3.9944	3.9642
c(Å)	3.9885	5.6151	4.0077	3.9931	4.0102	3.9343	4.0111	3.9937	4.0104	3.9926	4.0094	3.9934	4.0101	3.9929	4.0090	3.9944	4.0088
Alpha(°)	89.6780	90.0000	90.0000	89.6165	90.0000	89.5387	90.0000	89.5922	90.0000	89.5541	90.0000	89.5871	90.0000	89.5808	90.000	89.5114	90.000
A (*x*,*y*,*z*)	0.0129,	0.0000,	0.0000,	0.0129,	0.0000,	0.0133,	0.0000,	0.0135,	0.0000,	0.0129,	0.0003	0.0133,	0.0000,	0.0134,	0.0001,	0.0133,	0.0001
	0.0129,	0.0001,	0.0000,	0.0129,	-0.0002	0.0133,	-0.0002	0.0135,	-0.000,	0.0129,	-0.0002	0.0133,	-0.0002	0.0134,	-0.0002	0.0133,	0.0002
	0.0129	0.0137	0.0178	0.0129	0.0179	0.0133	0.0175	0.0135	0.0177	0.0129	0.0180	0.0133	0.0177	0.0134	0.0177	0.0133	0.0176
B (*x*,*y*,*z*)	0.4949,	0.5000,	0.5000,	0.4941,	0.5000	0.4819,	0.5001	0.4892,	0.5001	0.4945,	0.5003	0.4871,	0.5001	0.4881,	0.5000	0.4846,	0.5000
	0.4949,	0.0000,	0.5000,	0.4941,	0.5001,	0.4819,	0.5001,	0.4892,	0.5001,	0.4945,	0.5003,	0.4871,	0.5001,	0.4881,	0.5001,	0.4846,	0.5001,
	0.4949	0.4949	0.4950	0.4941	0.4946	0.4819	0.4825	0.4892	0.4898	0.4945	0.4956	0.4871	0.4877	0.4881	0.4889	0.4846	0.4851
O1 (*x*,*y*,*z*)	0.5247,	0.0000,	0.4998,	0.5244,	0.5004	0.5115,	0.5001	0.5192,	0.5001	0.5243,	0.4919	0.5170,	0.4999	0.5181,	0.5001	0.5143,	0.5001
	0.5247,	-0.0001	0.4995,	0.5244,	0.4999,	0.5115,	0.4997,	0.5192,	0.4997,	0.5243,	0.4905,	0.5170,	0.4996,	0.5181,	0.4999,	0.5143,	0.4997
	0.0324	0.5309	0.0434	0.0328	0.0437	0.0321	0.0426	0.0326	0.0432	0.0329	0.0403	0.0325	0.0429	0.0325	0.0431	0.0323	0.0428
O2 (*x*,*y*,*z*)		0.4997,	0.4999,		0.4995,		0.4995,		0.4995,		0.4924,		0.4996,		0.4997,		0.4996
	-	0.2449,	-0.0026	-	0.0003,	-	0.0001,	-	0.0001,	-	0.0002,	-	0.0001,	-	0.0001,	-	0.0002
		0.2812	0.5345		0.5337		0.5205		0.5283		0.5312		0.5261		0.5273		0.5234

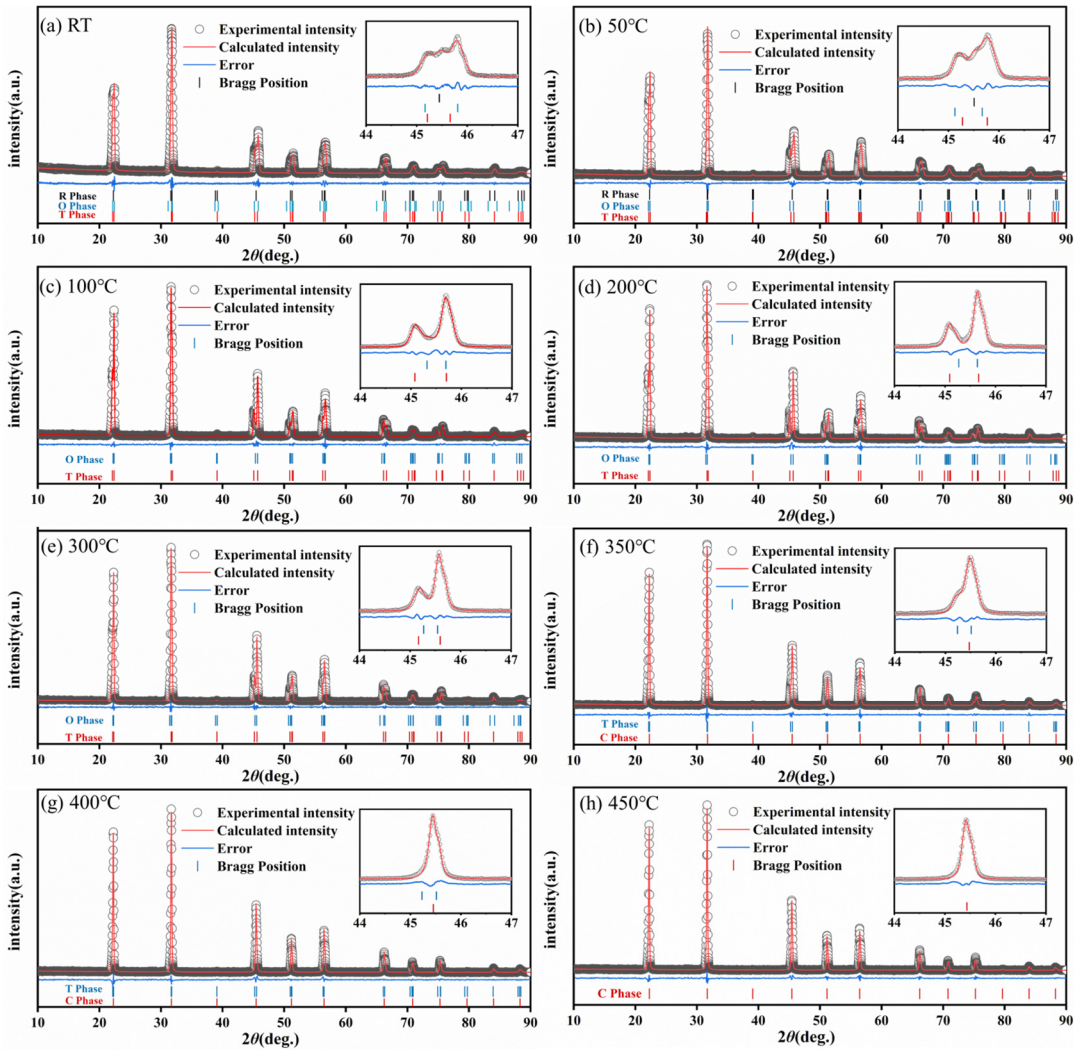

Figure S4 (a)-(h) the Rietveld refinement for KNN-UN from room temperature to 450℃

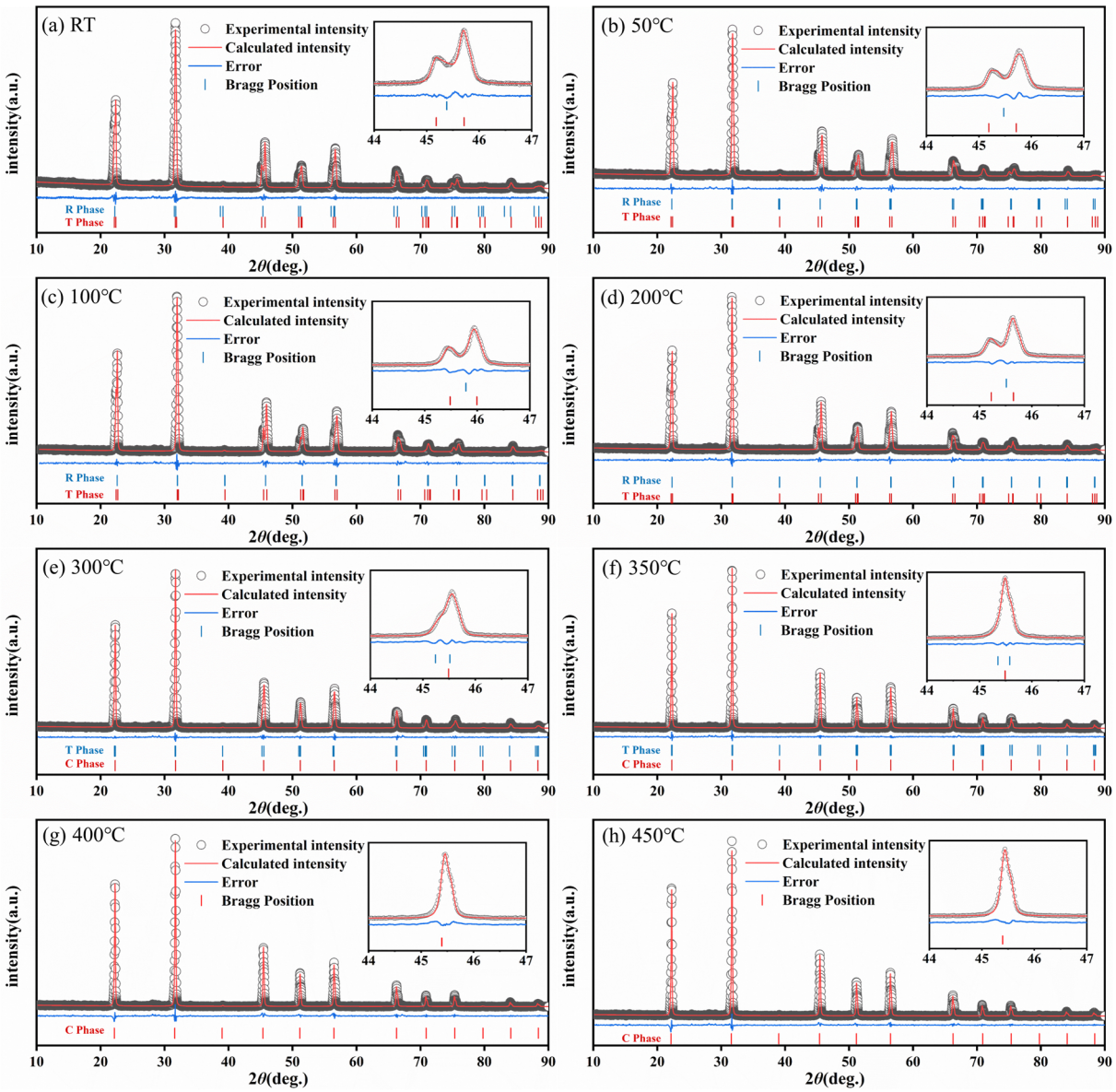

Figure S5 (a)-(h) the Rietveld refinement for KNN-800 from room temperature to 450℃

Table S3 Parameters of KNN-UN from room temperature to 450 ℃ obtained from Rietveld refinement

Parameters	Room temperature				50℃		100℃		200℃		300℃		350℃		400℃		450℃
sig		1.52			1.67		1.59		1.60		1.58		1.74		1.57		1.92
R_w(%)		4.06			8.57		8.15		8.22		8.13		8.99		8.12		9.98
Symmetry	R Phase	O Phase	T Phase	R Phase	O Phase	T Phase	O Phase	T Phase	O Phase	T Phase	O Phase	T Phase	T Phase	C Phase	T Phase	C Phase	C Phase
proportion	33.5%	46.7%	19.8%	2.3%	66.1%	31.6%	44.5%	53.5%	32.3%	67.7%	11.7%	81.3%	64.3%	35.7%	8.7%	91.3%	100%
Space group	*R*3*m*	*Amm*2	*P*4*mm*	*R*3*m*	*Amm*2	*P*4*mm*	*Amm*2	*P*4*mm*	*Amm*2	*P*4*mm*	*Amm*2	*P*4*mm*	*P*4*mm*	*P*23	*P*4*mm*	*P*23	*P*23
a(Å)	3.9885	3.9581	3.9704	3.9831	3.9618	3.9700	3.9680	3.9673	3.9723	3.9701	3.9802	3.9759	3.9827	3.9860	3.9826	3.9876	3.9893
b(Å)	3.9885	5.7336	3.9704	3.9831	5.6693	3.9700	5.6673	3.9673	5.6405	3.9701	5.6916	3.9759	3.9827	3.9860	3.9826	3.9876	3.9893
c(Å)	3.9885	5.6151	4.0077	3.9831	5.6511	4.0148	5.6432	4.0192	5.6813	4.0179	5.6312	4.0115	4.0055	3.9860	4.0065	3.9876	3.9893
Alpha(°)	89.6780	90.0000	90.0000	89.8527	90.0000	90.0000	90.0000	90.0000	90.0000	90.0000	90.0000	90.0000	90.0000	90.0000	90.0000	90.0000	90.0000
A (*x*,*y*,*z*)	0.0129,	0.0000,	0.0000,	0.0132,	0.0000,	0.0000,	0.0000,	0.0000,	0.0000,	0.0000,	0.0000,	0.0000,	-0.0029,	0.0003,	-0.0012	0.0000,	0.0000,
	0.0129,	0.0001,	0.0000,	0.0128,	0.0000,	-0.0002	0.0002,	0.0000,	0.0001,	0.0000,	0.0003,	0.0000,	-0.0043,	0.0002,	-0.0012	0.0000,	0.0000,
	0.0129	0.0137	0.0178	0.0127	0.0137	0.0179	0.0137	0.0178	0.0139	0.0180	0.0138	0.0181	0.0168	0.0182	0.0175	0.0180	0.0180
B (*x*,*y*,*z*)	0.4949,	0.5000,	0.5000,	0.5001,	0.5000,	0.5001,	0.5000,	0.5000,	0.5000,	0.5000,	0.5000,	0.5000,	0.5022,	0.4973,	0.5013,	0.4987,	0.5000,
	0.4949,	0.0000,	0.5000,	0.5001,	0.0000,	0.5001,	0.0000,	0.5000,	0.0000,	0.5000,	0.0000,	0.5000,	0.5022,	0.4973,	0.5013,	0.4987,	0.5000,
	0.4949	0.4949	0.4950	0.5001	0.4989	0.4989	0.4963	0.4950	0.5009	0.5009	0.5003	0.5002	0.5011	0.4973	0.5003	0.4987,	0.5000,
O1 (*x*,*y*,*z*)	0.5247,	0.0000,	0.4998,	0.5298,	-0.0002	0.4996,	-0.0002	0.4998,	-0.0004	0.5001,	-0.0004,	0.5001,	0.4995,	0.5004,	0.5025	0.5002,	0.5000,
	0.5247,	-0.0001	0.4995,	0.5298,	-0.0003	0.4996,	-0.0001	0.4995,	-0.0002	0.5000,	-0.0003,	0.4993,	0.4916,	0.5004,	0.5025	0.5002,	0.5000,
	0.0324	0.5309	0.0434	0.0331	0.5347	0.0435	0.5320	0.0434	0.5374	0.0441	0.5360	0.0439	0.0418	0.0442	0.0434	0.0441	0.0440
O2 (*x*,*y*,*z*)		0.4997,	0.4999,		0.4999,	0.4998,	0.4951,	0.4999,	0.5004,	0.4999,	0.4986,	0.4998,	0.4950,	0.5012,	0.4992,	0.5001,	0.5000,
	-	0.2449,	-0.0026	-	0.2468,	-0.0001	0.2452,	-0.0026	0.2477,	0.0000,	0.2470,	0.0003,	0.0017,	0.0005,	0.0001,	0.0001,	0.0000,
		0.2812	0.5345		0.2833	0.5384	0.2820	0.5345	0.2845	0.5409	0.2840	0.5398	0.5370	0.5403	0.5388	0.5400	0.5400

Table S4 Parameters of KNN-800 from room temperature to 450 ℃ obtained from Rietveld refinement

Parameters	Room temperature		50℃		100℃		200℃		300℃		350℃		400℃	450℃
sig	1.58		1.73		1.60		1.86		1.79		1.81		1.99	1.92
R_w(%)	4.23		9.40		8.22		9.71		9.82		9.95		9.95	9.90
Symmetry	R Phase	T Phase	R Phase	T Phase	R Phase	T Phase	R Phase	T Phase	T Phase	C Phase	T Phase	C Phase	C Phase	C Phase
proportion	47.4%	52.6%	51.4%	48.6%	22.5%	77.5%	17.7%	86.3%	61.3%	38.7%	6.7%	93.3%	100%	100%
Space group	*R*3*m*	*P*4*mm*	*R*3*m*	*P*4*mm*	*R*3*m*	*P*4*mm*	*R*3*m*	*P*4*mm*	*P*4*mm*	*P*23	*P*4*mm*	*P*23	*P*23	*P*23
a(Å)	3.9937	3.9664	3.9860	3.9663	3.9853	3.9679	3.9829	3.9715	3.9773	3.9842	3.9774	3.9848	3.9759	3.9759
b(Å)	3.9937	3.9664	3.9860	3.9663	3.9853	3.9769	3.9829	3.9715	3.9773	3.9842	3.9774	3.9848	3.9759	3.9759
c(Å)	3.9937	4.0104	3.9860	4.0097	3.9853	4.0103	3.9829	4.0067	4.0010	3.9842	3.9961	3.9848	4.0115	4.0115
Alpha(°)	89.5922	90.0000	89.8595	90.0000	90.0405	90.0000	89.9544	90.0000	90.0000	90.0000	90.0000	90.0000	90.0000	90.0000
A (*x,y,z*)	0.0135,	0.0000,	0.0136,	0.0000,	0.0141,	0.0000,	0.0134,	0.0000,	-0.0006,	0.0000,	-0.0001,	0.0000,	0.0000,	0.0000,
	0.0135,	-0.0002,	0.0136,	0.0000,	0.0141,	-0.0002,	0.0134,	-0.0001,	-0.0006,	0.0000,	-0.0003,	0.0000,	0.0000,	0.0000,
	0.0135	0.0177	0.0136	0.181	0.0141	0.0188	0.0134	0.0180	0.0175	0.0180	0.0178	0.0180	0.0181	0.0181
B (*x,y,z*)	0.4892,	0.5001	0.5022,	0.5000,	0.5245,	0.5001,	0.5000,	0.5001,	0.5003,	0.4992,	0.5002,	0.4992,	0.5000,	0.5000,
	0.4892,	0.5001,	0.5022,	0.5000,	0.5245,	0.5001,	0.5001,	0.5001,	0.5004,	0.4992,	0.5003,	0.4992,	0.5000,	0.5000,
	0.4892	0.4898	0.5022	0.5028	0.5245	0.5048	0.5001	0.5001	0.5003	0.4992	0.5002	0.4992	0.5002	0.5002
O1 (*x,y,z*)	0.5192,	0.5001	0.5338,	0.5000,	0.5563,	0.4997,	0.5300,	0.4997,	0.5031,	0.5002,	0.4991,	0.5002,	0.5001,	0.5001,
	0.5192,	0.4997,	0.5338,	0.5000,	0.5563,	0.4997,	0.5299,	0.4997,	0.5031,	0.5002,	0.4991,	0.5002,	0.4993,	0.4993,
	0.0326	0.0432	0.0328	0.0442	0.0347	0.0458	0.0330	0.0437	0.0441	0.0439	0.0435	0.0441	0.0439	0.0439
O2 (*x,y,z*)		0.4995,		0.5000,		0.4998,		0.4997,	0.4971,	0.5000,	0.4993,	0.5000,	0.4998,	0.4998,
	-	0.0001,	-	0.0000,	-	0.0002,	-	0.0003,	-0.0001,	0.0001,	0.0000,	0.0001,	0.0003,	0.0003,
		0.5283		0.5430		0.5663		0.5396	0.5388	0.5400	0.5394	0.5400	0.5398	0.5398

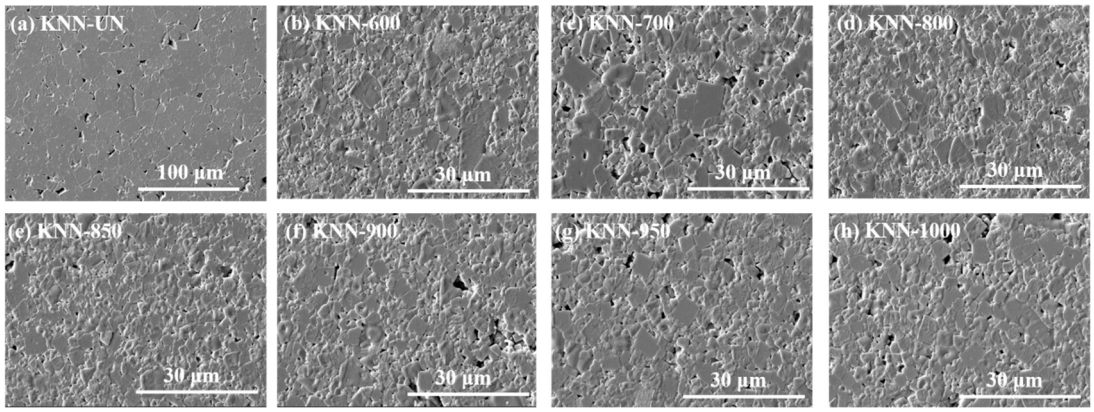

Figure S6 (a)-(h) Scanning Electron Microscopy (SEM) micrographs for KNN-UN, KNN-600, KNN-700, KNN-800, KNN-850, KNN-900, KNN-950, KNN-1000

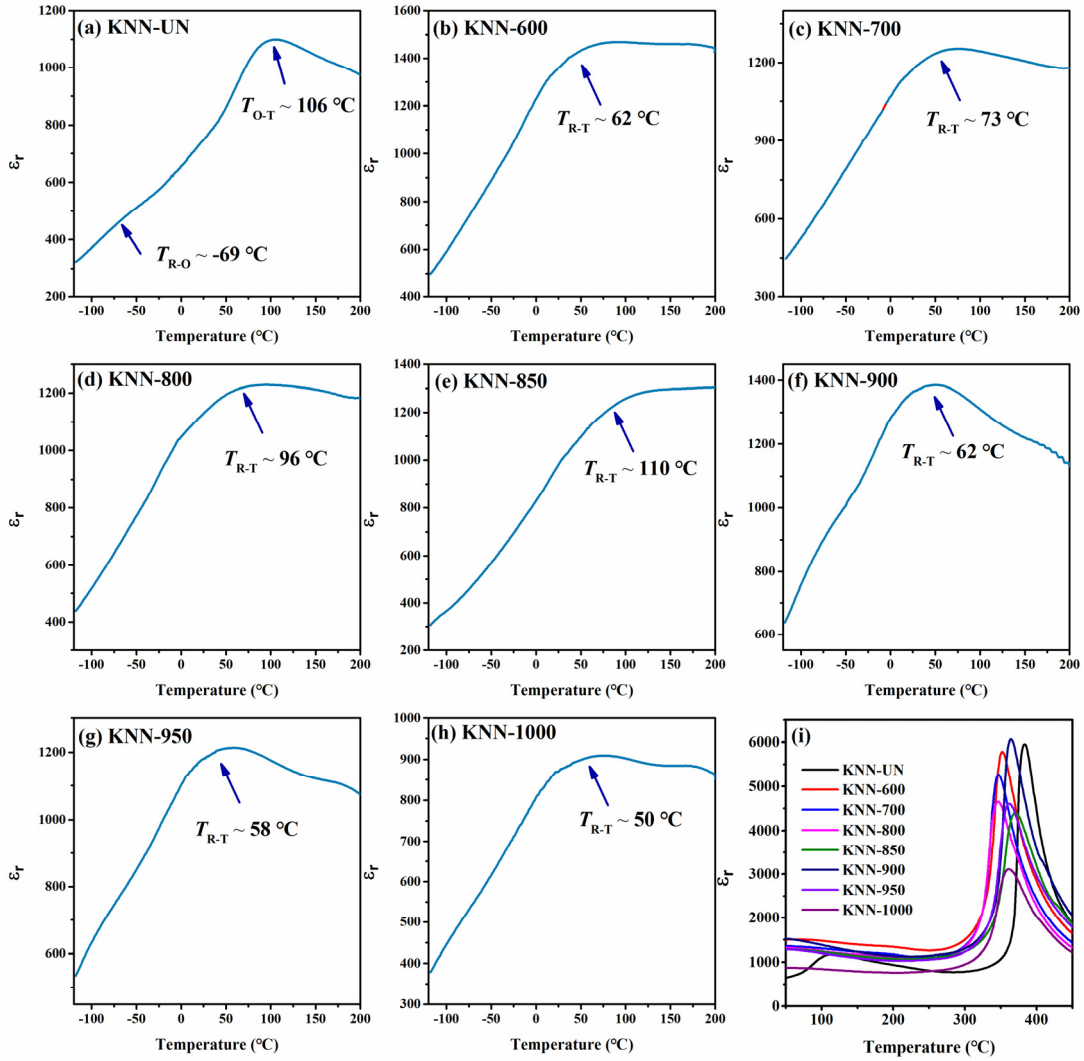

Figure S7 (a)-(h) The ε_r-T curves of KNN-UN, KNN-600, KNN-700, KNN-800, KNN-850, KNN-900, KNN-950, KNN-1000 from -120 °C to 200 °C; (i) the ε_r-T curves of KNN-UN, KNN-600, KNN-700, KNN-800, KNN-850, KNN-900, KNN-950, KNN-1000 from room temperature to 450 °C

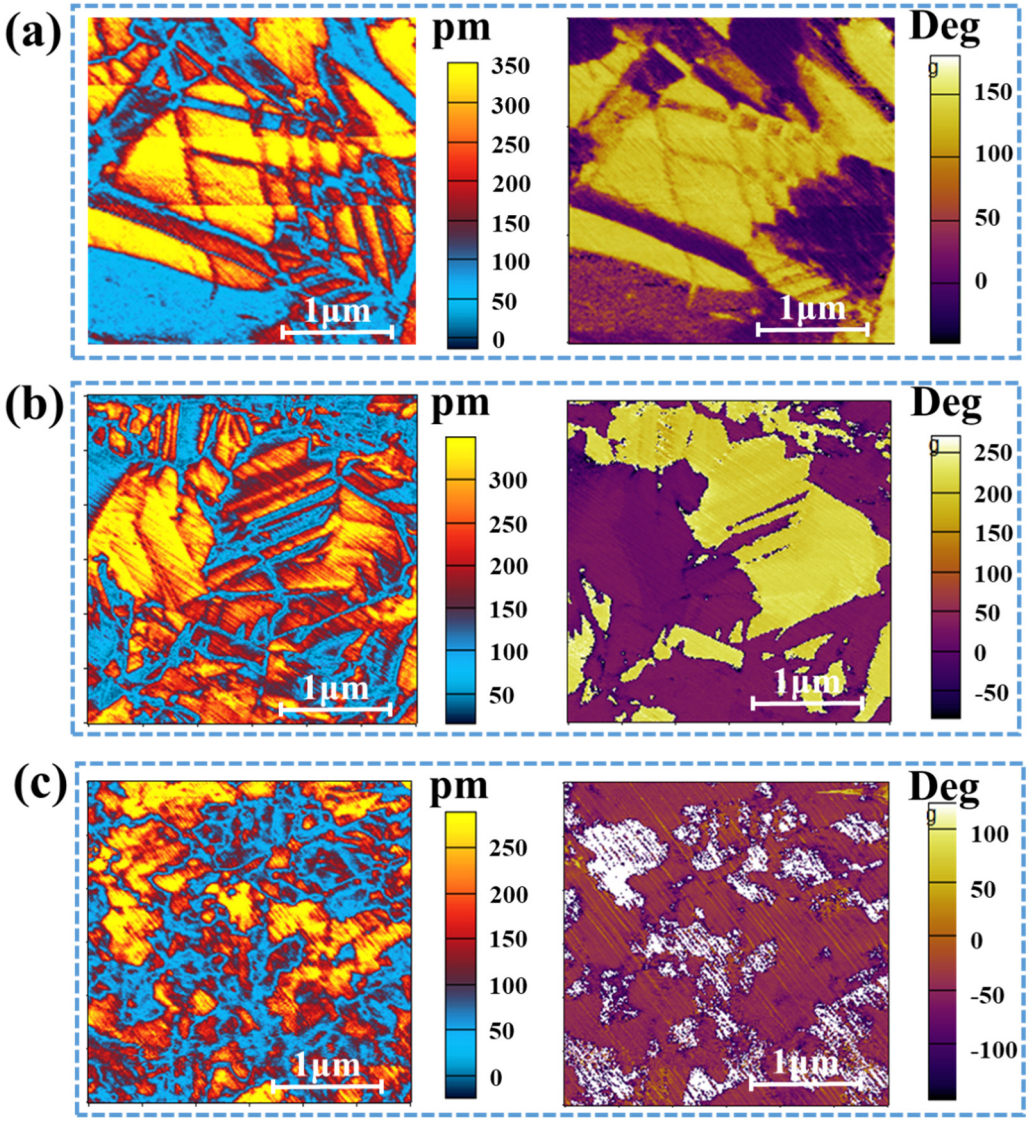

Figure S8 (a) The piezo-response force microscopy (PFM) amplitude and phase images of KNN with a scan area of 3×3 μm; (b) the piezo-response force microscopy (PFM) amplitude and phase images of KNN-Fe with a scan area of 3×3 μm; (c) the piezo-response force microscopy (PFM) amplitude and phase images of KNN-BNZ with a scan area of 3×3 μm