

Electronic Supplementary Material

Table S1. Experimental parameters for X-ray powder diffraction of BZT, BSmZT and BLaZT ceramics

Chemical formula	BZT	BSmZT	BLadZT
Crystal system	Tetragonal	Tetragonal	Tetragonal
Space group	P4mm	P4mm	P4mm
a (Å) = b (Å)	3.9868(5)	3.9779(4)	3.9762(6)
c (Å)	4.0214(5)	3.9998(4)	4.0068(7)
c/a	1.0087	1.0055	1.0077
Volume (Å ³)	63.918(14)	63.291(10)	63.348(18)
Z	1	1	1
Density (g/cm ³)	6.0701	6.0842	6.0848
Temperature (°C)	25	25	25
CuK α Radiations (Å)	1.54056	1.54056	1.54056
Measuring range (°)	$10 \leq 2\theta \leq 110$	$10 \leq 2\theta \leq 110$	$10 \leq 2\theta \leq 110$
Step (2 θ)	0.031	0.031	0.031
Rietveld data			
Program	Jana 2006	Jana 2006	Jana 2006
Profile fonction	Pseudo-Voigt	Pseudo-Voigt	Pseudo-Voigt
Caglioti parameters	U = 0.597	U = 0.496	U = 0.438
	V = -0.415	V = -0.492	V = -0.381
	W = 0.179	W = 0.201	W = 0.135
Rp (%)	9.19	6.34	7.64
Rwp (%)	12.72	8.23	10.19
Rexp (%)	7.29	6.45	6.65
GOF	1.74	1.28	1.53

Table S2. Refined structural parameters for BZT, BSmZT and BLaZT powder from X-ray diffraction data.

Compound	Wyckoff position	Atom	x	y	z	Uiso (Å ²)	Occupies
BZT	1a	Ba	0.5	0.5	0.5074(13)	0.027(2)	1
	1b	Ti/Zr	0	0	-0.0127(19)	0.031(2)	0.99/0.01
	1c	O1	0.5	0	0.028(5)	0.027(3)	1
	1d	O2	0	0	0.534(7)	0.027(3)	1
BSmZT	1a	Ba/Sm	0.5	0.5	0.5216	0.0253(13)	0.95/0.034
	1b	Ti/Zr	0	0	0.001(4)	0.0262(15)	0.99/0.01
	1c	O1	0.5	0	0.104(5)	0.0204	1
	1d	O2	0	0	0.52(3)	0.0204	1
BLaZT	1a	Ba/La	0.5	0.5	0.5251(7)	0.0207(16)	0.95/0.034
	1b	Ti/Zr	0	0	-0.007(3)	0.021(2)	0.99/0.01
	1c	O1	0.5	0	0.096(4)	0.006(3)	1
	1d	O2	0	0	0.516(19)	0.006(3)	1

Table S3. Selected bond distances (Å) for BZT, BSmZT and BLaZT powder from X-ray diffraction data.

Bond distances (Å)	BZT	BSmZT	BLaZT
4(Ti/Zr-O ₁)	2.0054 (17)	2.032 (4)	2.024(3)
1(Ti/Zr-O ₂)	2.20 (3)	2.09 (13)	2.06(9)
1(Ti/Zr-O ₂)	1.83 (3)	1.91 (13)	1.95(9)
4(Ba/Ln-O ₁)	2.780 (14)	2.594 (12)	2.627(10)
4(Ba/Ln-O ₁)	2.899 (15)	3.064 (14)	3.032(11)
4(Ba/Ln-O ₂)	2.8285 (11)	2.8116 (5)	2.8119(14)

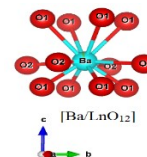
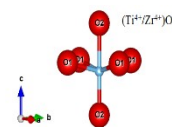


Table S4. Equivalent circuit electrical parameters obtained from a complex impedance spectrum for BZT, BSmZT and BLaZT ceramics.

Composition	T(°C)	$R_{gb}(k\Omega)$	$C_{gb}(nF)$	CPE_{gb} ($nF.s^{\alpha-1}$)	α_{gb}	$R_g(k\Omega)$	$C_g(nF)$	CPE_g ($nF.s^{\alpha-1}$)	α_g
BZT	300	659.786	1.100	9.11	0.7271	12.083	0.5938	53.2000	0.4967
	310	489.401	1.054	9.652	0.7314	09.770	0.5706	18.3100	0.5838
	320	339.272	0.905	9.623	0.7534	07.374	0.5574	5.9950	0.6725
	330	258.826	0.908	10.33	0.7504	05.842	0.5372	5.0750	0.6312
	340	186.763	0.814	11.26	0.7542	04.683	0.5189	4.3880	0.7149
	350	144.011	0.5869	10.95	0.7773	03.685	0.5208	0.6398	0.8682
	360	108.708	0.605	12.41	0.7658	03.014	0.3960	0.8895	0.9016
	370	083.813	0.5698	13.85	0.7591	02.466	0.3355	1.2370	0.900
	380	063.399	0.4953	15.28	0.7564	01.963	0.3653	1.5210	0.9393
	390	050.915	0.2113	16.88	0.7627	01.642	0.8769	1.5430	0.9367
BSmZT	400	038.333	0.1261	18.54	0.7596	01.383	0.1124	1.6310	0.9786
	300	719.779	0.6889	6.706	0.7212	14.225	0.9456	0.8148	0.9398
	310	538.326	0.6014	6.401	0.7444	11.529	1.3390	1.0900	0.9401
	320	422.629	0.6713	6.926	0.7300	09.375	1.5110	1.1983	0.9413
	330	337.523	0.6598	7.093	0.7306	07.767	1.7125	1.5190	0.9766
	340	290.585	0.5445	7.421	0.7404	06.368	1.2350	0.7101	0.9686
	350	237.338	0.6696	13.51	0.6557	05.385	0.1686	1.6310	0.9574
	360	198.575	0.7076	26.58	0.5748	04.532	0.3340	2.0110	0.9512
	370	173.496	0.6992	41.99	0.5278	03.846	0.5527	2.3960	0.8819
	380	146.834	0.6322	50.04	0.5207	03.230	0.9110	32.0200	0.6417
BLaZT	390	129.603	0.5621	51.84	0.5229	02.682	1.1500	39.1200	0.6353
	400	110.810	0.4991	53.73	0.5258	02.230	1.5000	44.8700	0.6288
	300	1333	0.6416	8.276	0.6561	24.989	0.5856	3.282	0.7073
	310	1036	0.5667	8.302	0.6718	19.590	0.5651	0.4827	0.8935
	320	819.011	0.5285	8.503	0.6788	15.888	0.2331	0.5954	0.9803
	330	667.223	0.4658	8.662	0.6894	13.195	0.5155	0.2561	0.987
	340	569.339	0.4506	9.371	0.6837	10.888	0.5951	0.1687	0.9922
	350	476.143	0.4406	10.77	0.6712	08.643	0.6330	0.1067	0.9999
	360	410.313	0.4343	12.67	0.6551	06.866	0.7427	0.1461	0.8944
	370	358.419	0.4309	14.82	0.6399	05.690	0.7402	0.2402	0.7772
380	304.330	0.4262	16.57	0.6301	04.589	0.7152	0.3800	0.4531	
390	263.907	0.4381	21.34	0.6036	03.751	0.6803	0.1930	0.5507	
400	221.422	0.4257	20.82	0.6067	03.151	0.6821	0.4126	0.4647	

Table S5. Parameters obtained from plot for BZT, BSmZT and BLaZT ceramics.

Composition	T(°C)	$\sigma_{dc}(\Omega.m)^{-1}$	$A_1 (\Omega^{-1} m^{-1} rad^{-s})$	n_1	$A_2(\Omega^{-1} m^{-1} rad^{-s})$	n_2
BZT	300	$2.11827 \cdot 10^{-5}$	$2.38222 \cdot 10^{-4}$	0.10936	$2.41525 \cdot 10^{-9}$	0.89043
	320	3.9889810^{-5}	$3.51436 \cdot 10^{-5}$	0.29756	$1.00449 \cdot 10^{-8}$	0.80088
	340	$7.1533 \cdot 10^{-5}$	$4.63637 \cdot 10^{-5}$	0.29856	$4.62008 \cdot 10^{-8}$	0.70671
	360	1.2139710^{-4}	$7.65681 \cdot 10^{-6}$	0.51168	$1.2957 \cdot 10^{-6}$	0.50165
	380	$2.06372 \cdot 10^{-4}$	$3.000171 \cdot 10^{-6}$	0.63875	$9.1723 \cdot 10^{-5}$	0.2551
	400	3.4104310^{-4}	$5.79406 \cdot 10^{-7}$	0.83669	$4.692 \cdot 10^{-4}$	0.01691
BSmZT	300	1.4929910^{-5}	$1.16326E-7$	0.63998	$4.14008 \cdot 10^{-6}$	0.32183
	320	2.5325110^{-5}	$2.16823 \cdot 10^{-8}$	0.81456	$1.79789 \cdot 10^{-5}$	0.25405
	340	$3.66786 \cdot 10^{-5}$	$9.99681 \cdot 10^{-9}$	0.88976	$6.41151 \cdot 10^{-5}$	0.19676
	360	$4.41447 \cdot 10^{-5}$	$6.3933 \cdot 10^{-9}$	0.90021	$1.59699 \cdot 10^{-4}$	0.15974
	380	$4.72069 \cdot 10^{-5}$	$3.999 \cdot 10^{-9}$	0.94781	$2.57557 \cdot 10^{-4}$	0.14335
	400	$4.9064 \cdot 10^{-5}$	$3.60856 \cdot 10^{-9}$	0.96738	$3.45475 \cdot 10^{-4}$	0.13063
BLaZT	300	1.2433510^{-5}	$2.47142 \cdot 10^{-9}$	0.59858	$3.4077 \cdot 10^{-5}$	0.34585
	320	$2.19264 \cdot 10^{-5}$	$8.03615 \cdot 10^{-9}$	0.71897	$4.1397 \cdot 10^{-5}$	0.11809
	340	$3.66786 \cdot 10^{-5}$	$2.66647 \cdot 10^{-9}$	0.82855	$6.02951 \cdot 10^{-5}$	0.09254
	360	4.416410^{-5}	$1.40432 \cdot 10^{-9}$	0.88744	$7.71349 \cdot 10^{-5}$	0.08554
	380	$5.84267 \cdot 10^{-5}$	$1.04544 \cdot 10^{-9}$	0.90915	$9.07504 \cdot 10^{-5}$	0.08309
	400	7.9373410^{-5}	9.4895310^{-10}	0.91514	$1.07504 \cdot 10^{-5}$	0.07097

Table S6.Parameters obtained from plot for BZT, BLaZT and BSmZT ceramics.

Composition	T(°C)	M_{max}^{gb}	f_{max}^{gb}	β_{gb}	M_{max}^g	f_{max}^g	β_g
BZT	300	0.43905	264.63743	0.47856	3.43004	25507.72669	0.89575
	310	0.4407	355.38291	0.46143	3.33417	31507.58249	0.87862
	320	0.43717	520.37911	0.44147	3.24325	41195.19434	0.86489
	330	0.43271	695.19616	0.42825	3.16443	49964.37188	0.85481
	340	0.42066	1000.11272	0.41497	3.03124	62856.08699	0.84461
	350	0.41514	1327.58268	0.39424	2.91035	75218.54733	0.82376
	360	0.43377	1828.61887	0.39610	2.73445	91910.67632	0.78043
	370	0.45956	2424.26831	0.40289	2.49964	112131.65118	0.72097
	380	0.47949	3608.87109	0.38248	2.25119	140970.77156	0.66964
	390	0.50292	5397.59779	0.35713	2.02868	183782.59316	0.62305
	400	0.52939	10550.05084	0.29794	1.72061	302246.45614	0.57425
BSmZT	300	1.42958	306.57564	0.58889	2.47676	9219.36089	0.74511
	310	1.38766	395.70674	0.58539	2.39642	12452.60271	0.72007
	320	1.36185	487.18009	0.58923	2.35801	16006.98902	0.70552
	330	1.34548	610.70714	0.58542	2.31876	20271.70059	0.69527
	340	1.33977	755.72604	0.56956	2.26626	24339.39729	0.69173
	350	1.34544	998.5457	0.53772	2.18073	30041.73775	0.69066
	360	1.36644	1268.76576	0.50313	2.07388	35503.82654	0.69858
	370	1.39957	1586.09663	0.47426	1.96733	40918.16552	0.71152
	380	1.43806	2007.10734	0.45154	1.86074	47054.3747	0.72991
	390	1.50876	2174.47012	0.44659	1.67031	45281.61518	0.71422
	400	1.51779	2611.97553	0.43967	1.60641	49941.45751	0.72326
BLaZT	300	0.89129	225.30536	0.50994	2.72621	8311.79714	0.78624
	310	0.91039	302.64429	0.52703	2.79416	10755.90801	0.80038
	320	0.93654	398.35198	0.54410	2.83893	13667.07317	0.80824
	330	0.95035	495.3434	0.53382	2.75176	17350.0067	0.79252
	340	0.96793	603.90378	0.52101	2.68314	21511.99619	0.78192
	350	0.98671	764.51363	0.50640	2.61981	27281.81677	0.77643
	360	1.00431	963.76800	0.48773	2.58010	34249.84634	0.78144
	370	1.01808	1198.44674	0.47078	2.56509	42018.02714	0.79364
	380	1.03519	1515.34752	0.45554	2.57604	51790.73531	0.81295
	390	1.04961	1888.96968	0.44100	2.60892	62550.38401	0.83791
	400	1.06092	2330.37117	0.43051	2.63668	74327.73236	0.86520