Novel BaTiO3-based, Ag/Pd compatible lead-free relaxors with superior energy storage performance

YANG, Hui-Jing, LU, Zhilun, LI, Linhao, BAO, Weichao, JI, Hongfen, LI, Jinglei, FETEIRA, Antonio <http://orcid.org/0000-0001-8151-7009>, XU, Fangfang, ZHANG, Yong, SUN, Huajun, HUANG, Zhichao, LOU, Weichao, SONG, Kaixin, SUN, Shikuan, WANG, Ge, WANG, Dawei and REANEY, Ian M

Published version

YANG, Hui-Jing, LU, Zhilun, LI, Linhao, BAO, Weichao, JI, Hongfen, LI, Jinglei, FETEIRA, Antonio, XU, Fangfang, ZHANG, Yong, SUN, Huajun, HUANG, Zhichao, LOU, Weichao, SONG, Kaixin, SUN, Shikuan, WANG, Ge, WANG, Dawei and REANEY, Ian M (2020). Novel BaTiO3-based, Ag/Pd compatible lead-free relaxors with superior energy storage performance. ACS Applied Materials and Interfaces.

Copyright and re-use policy

Supporting information

Novel $BaTiO_3$-based, Ag/Pd compatible lead-free relaxors with superior energy storage performance

Huijing Yang[a,b#] , Zhilun Lu[a#], Linhao Li[a#], Weichao Bao[c#], Hongfen Ji[a,d], Jinglei Li[e], Antonio Feteira[f], Fangfang Xu[c], Yong Zhang[g], Huajun Sun[g], Zhichao Huang[f,h], Weichao Lou[f,h], Kaixin Song[h], Shikuan Sun[a], Ge Wang[a]*, Dawei Wang[a]*, Ian M. Reaney[a]

[a]Department of Materials Science and Engineering, University of Sheffield, Sheffield, S1 3JD, UK

[b]Department of Physics, Tangshan Normal University, Tangshan, 063000, China

[c]State Key Laboratory of High Performance Ceramics and Superfine Microstructure, Shanghai Institute of Ceramics, Shanghai, 200050, China

[d]Laboratory of Thin Film Techniques and Optical Test, Xi'an Technological University, Xi'an, 710032, China

[e]Electronic Materials Research Laboratory, Key Laboratory of the Ministry of Education and International Center for Dielectric Research, Xi'an Jiaotong University, Xi'an, 710049, China.

[f]Materials and Engineering Research Institute, Sheffield Hallam University, Sheffield, S1 1WB, UK

[g]State Key Laboratory of Silicate Materials for Architectures, School of Materials Science and Engineering, Wuhan University of Technology, Wuhan, 430070, China.

[h]College of Electronics Information, Hangzhou Dianzi University, Hangzhou, 310018, China

*Corresponding authors. E-mail address: g.wang@sheffield.ac.uk, dawei.wang@sheffield.ac.uk

#Author Contributions: H. Y., Z. L., L. Li. and W. Bao contributed equally to this work.

Figure S-1. Full-pattern refinement of $xB_{2/3}MN$-BT ceramics

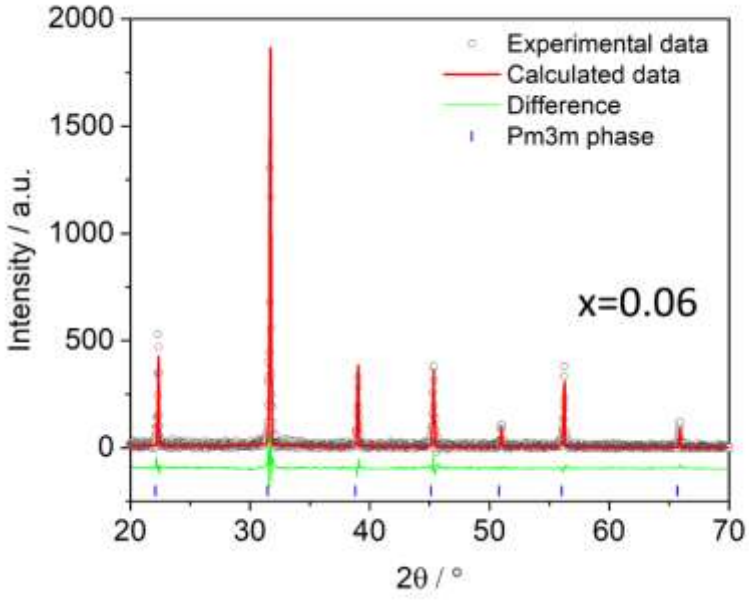

Figure S-2. P-E loop for BT ceramics at 60 kV cm^{-1}

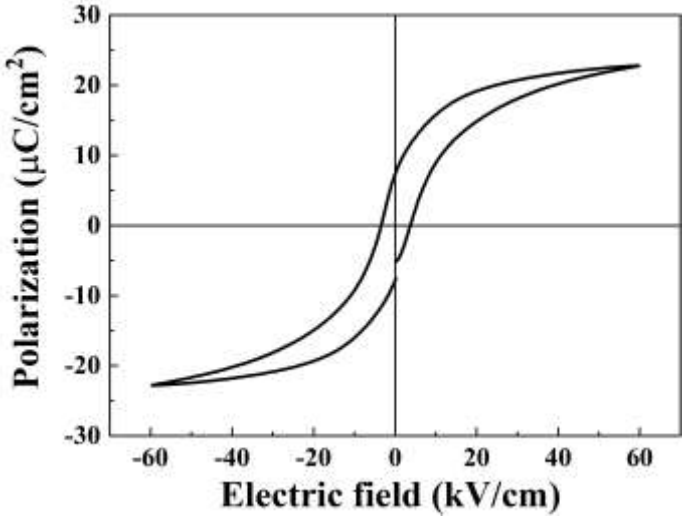

Figure S-3. (a-f) The frequency-dependent dielectric properties for $xB_{2/3}MN$-BT ($x=0.00 \leq x \leq 0.10$) ceramics.

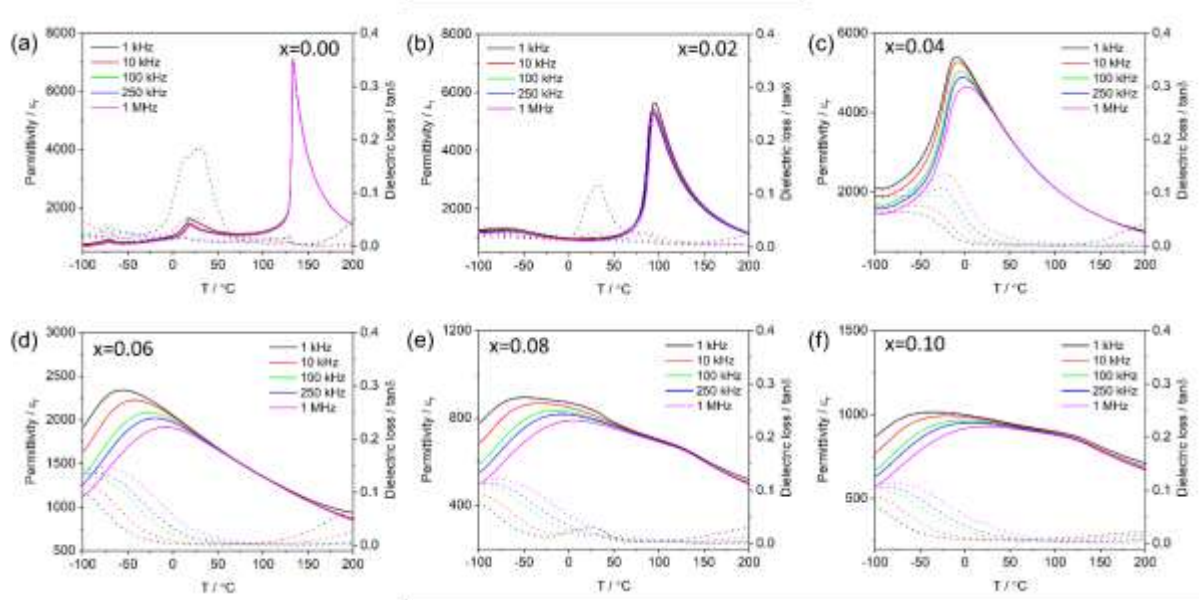

Figure S-4. (a-f) The SEM image of thermal-etched surfaces for $xB_{2/3}MN$-BT ($x=0.00 \leq x \leq 0.10$) ceramics.

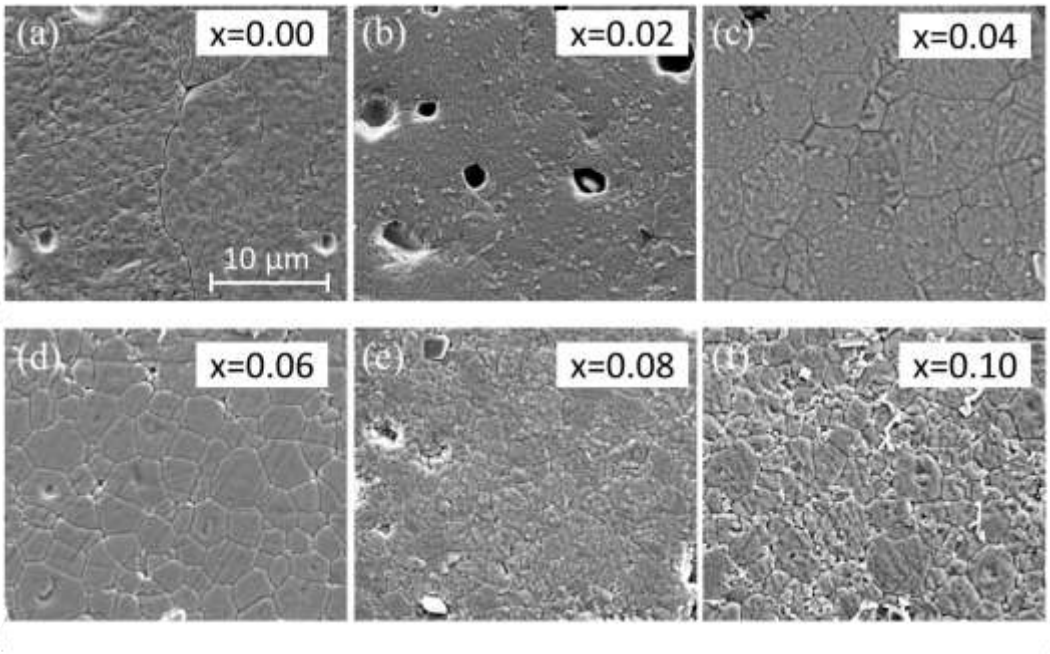

Figure S-5. (a-d) Unipolar P-E loops under E_{max} and (e-h) calculated energy storage properties (W_{rec} and η) at different electric field for x$B_{2/3}$MN-BT ceramics.

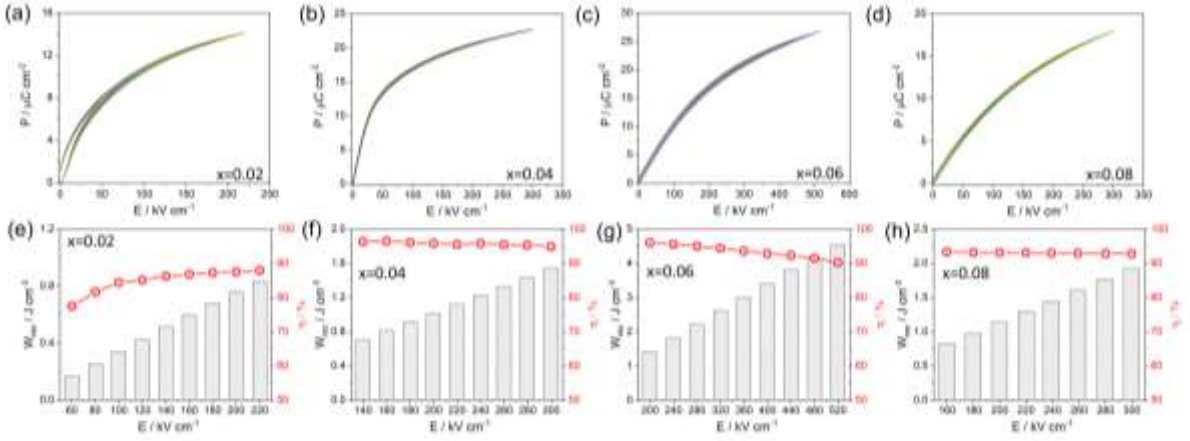

Figure S-6. (a) Changes of E_{max} and ΔP for $xB_{2/3}MN$-BT ceramics. (b) Change of W_{rec} and η as function of x concentration.

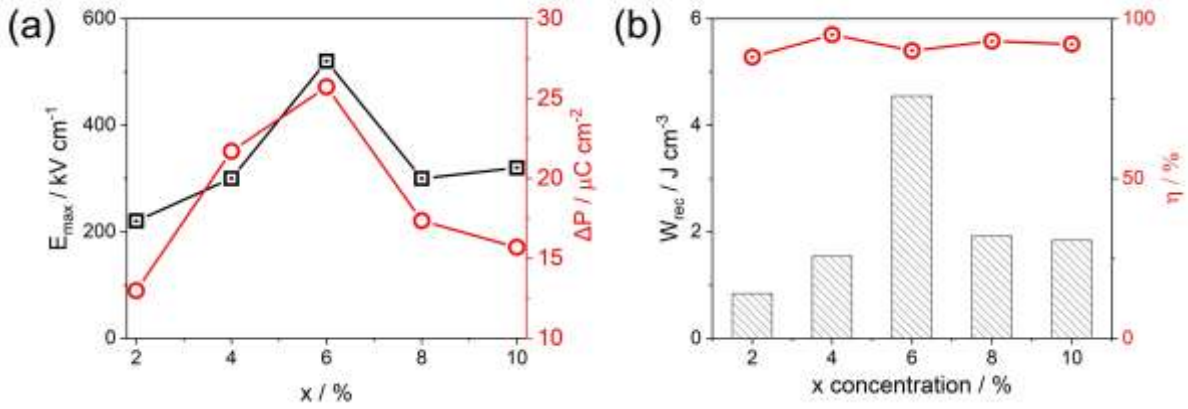

Table S-1. Refined crystallography details for BT-x$B_{2/3}$MN ceramics.

Composition / x	0.00		0.02	0.04	0.06
GOF	1.31	2.19	1.34	1.55	1.86
R_{exp}	9.03	16.25	6.75	7.79	8.02
R_{wp}	11.84	39.59	9.08	12.05	14.99
Space group	*P4mm*	*Pm3m*	*P4mm*	*Pm3m*	*Pm3m*
Cell mass	233.19	234.642	233.57	234.64	235.73
Cell volume	64.40(4)	64.49(4)	64.52(7)	64.69(4)	64.93(4)
Crystal density	6.013(4)	6.023(4)	6.018(8)	6.023(4)	6.029(9)
Lattice parameter a / Å	3.9946(12)	4.0144(8)	3.9901(13)	4.0144(8)	4.0192(8)
Lattice parameter c / Å	4.0358(12)	N/A	4.0211(8)	N/A	N/A
c/a ratio	1.0103	N/A	1.0083	N/A	N/A

Refined atoms position details								
	site	NP	x	y	z	Atom	Occ	Beq
0.00	Ba	1	0.0000	0.0000	0.0000	Ba+2	1.000	0.012
	Ti	1	0.5000	0.5000	0.5370	Ti+4	1.000	0.019
	O1	1	0.50000	0.5000	-0.3700	O-2	1.000	0.062
	O2	2	0.5000	0.00000	0.5180	O-2	1.000	0.042
0.02	Ba	1	0.0000	0.0000	0.0000	Ba+2	0.980	0.025
						Bi+3	0.013	0.025
	Ti	1	0.5000	0.5000	0.5370	Ti+4	0.980	0.033
						Mg+2	0.007	0.033
						Nb+5	0.013	0.033
	O1	1	0.5000	0.5000	-0.3700	O-2	1.000	0.051
	O2	2	0.5000	0.0000	0.5180	O-2	1.000	0.033
0.04	Ba	1	0.0000	0.0000	0.0000	Ba+2	0.960	0.015
						Bi+3	0.027	0.015
	Ti	1	0.5000	0.5000	0.5000	Ti+4	0.960	0.015
						Mg+2	0.013	0.015
						Nb+5	0.027	0.015
	O1	3	0.0000	0.5000	0.5000	O-2	1.000	0.004
0.06	Ba	1	0.0000	0.0000	0.0000	Ba+2	0.940	0.022
						Bi+3	0.040	0.022
	Ti	1	0.5000	0.5000	0.5000	Ti+4	0.940	0.025
						Mg+2	0.020	0.025
						Nb+5	0.040	0.025
	O1	3	0000	0.5000	0.5000	O-2	1.000	0.012

Table S-2. Average grain size for $xB_{2/3}MN$-BT ceramics

Composition	Average grain size / μm
x=0.00	25.2 ± 0.6
x=0.02	16.6 ± 0.5
x=0.04	7.2 ± 0.6
x=0.06	2.8 ± 0.3
x=0.08	2.4 ± 0.5
x=0.10	2.3 ± 0.4