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Supplementary Information

Solvothermal synthesis of nanoscale $BaTiO_3$ in benzyl alcohol-water mixtures and effects of manganese oxide coating to enhance the PTCR effect

Min Zhang,[a] Thomas Caldwell,[a] Andrew L. Hector,[a] Nuria Garcia-Araez [a,b] and Joseph Falvey [a]

[a] School of Chemistry, University of Southampton, Highfield, Southampton SO17 1BJ, UK

[b] The Faraday Institution, Quad One, Harwell Campus, Didcot OX11 0RA, UK

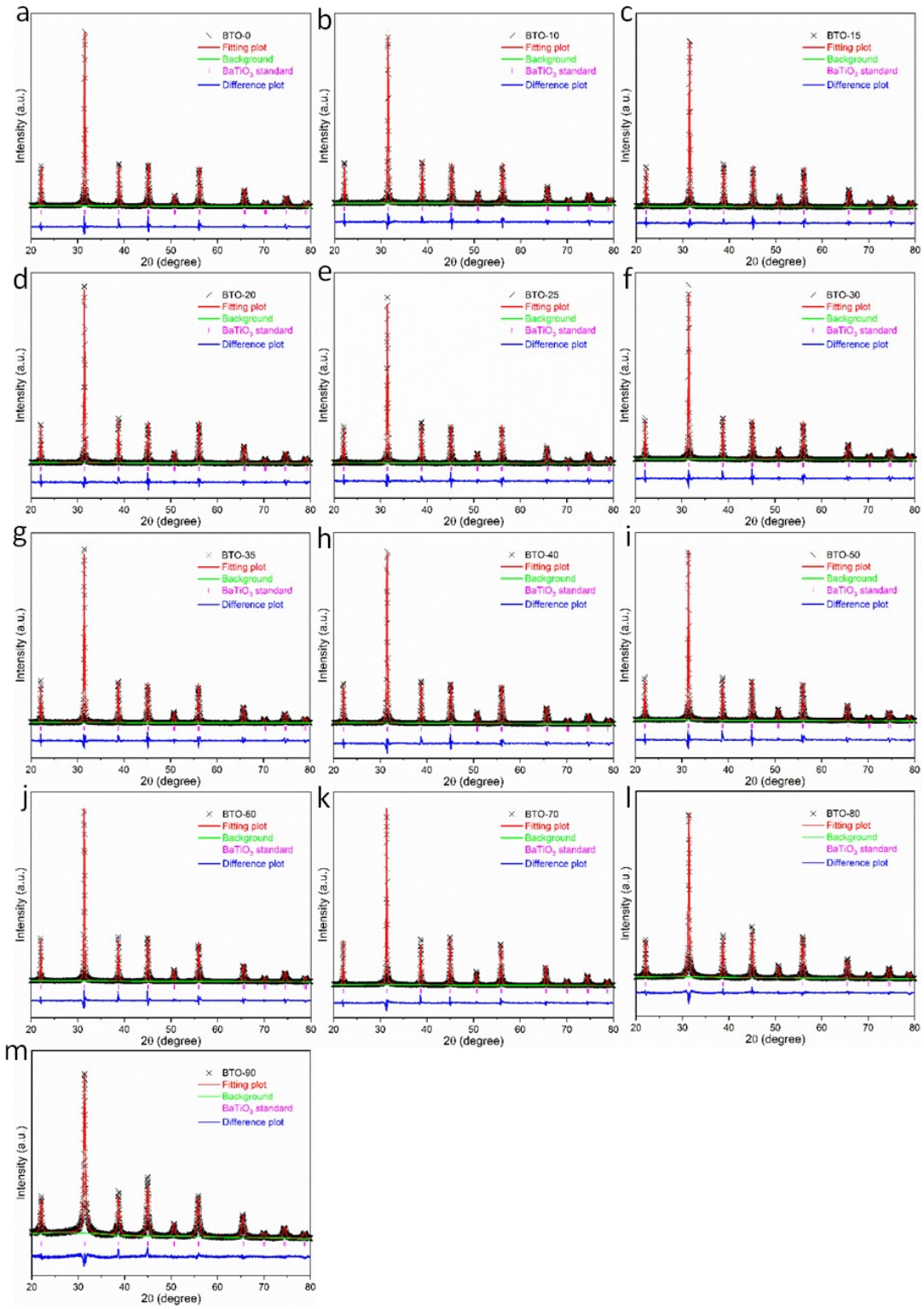

Fig. S1 Rietveld fits to the XRD patterns of (a) BTO-0, (b) BTO-10, (c) BTO-15, (d) BTO-20, (e) BTO-25, (f) BTO-30, (g) BTO-35, (h) BTO-40, (i) BTO-50, (j) BTO-60, (k) BTO-70, (l) BTO-80 and (m) BTO-90 samples (sample labels explained in Table 1). The data points and Rietveld fits are overlaid as black crosses and red lines, respectively. The difference plots and backgrounds are shown in blue and green, respectively. The pink tick marks represent the allowed reflection positions for the tetragonal $BaTiO_3$ structure with space group *P4mm*.

Table S1 Lattice parameters (*a*, *c*), tetragonality (*c/a*), Lorentzian crystallite size broadening term (L_x) and reliability factors (R_{wp}, R_p) obtained from the Rietveld fits to the XRD patterns of $BaTiO_3$ samples (sample labels explained in Table 1).

Sample	Lattice parameter		Tetragonality	Crystallite size broadening	Reliability factor	
	a [Å]	*c* [Å]	*c/a*	L_x	R_{wp}	R_p
BTO-0	4.01277(14)	4.0254(2)	1.0031	8.23(9)	0.1029	0.0810
BTO-10	4.0109(2)	4.0261(2)	1.0038	6.11(11)	0.1408	0.1068
BTO-15	4.0120(2)	4.0261(2)	1.0035	6.39(11)	0.1366	0.1009
BTO-20	4.0113(2)	4.0261(2)	1.0037	6.10(11)	0.1390	0.1051
BTO-25	4.0119(2)	4.0276(3)	1.0039	6.94(13)	0.1506	0.1138
BTO-30	4.0132(2)	4.0279(2)	1.0037	6.20(11)	0.1458	0.1111
BTO-35	4.0136(2)	4.0290(3)	1.0038	6.79(12)	0.1500	0.1151
BTO-40	4.0155(2)	4.0301(2)	1.0036	7.34(10)	0.1197	0.0918
BTO-50	4.0190(2)	4.0327(2)	1.0034	7.09(11)	0.1297	0.1005
BTO-60	4.02402(14)	4.0340(2)	1.0025	7.47(10)	0.1219	0.0941
BTO-70	4.02742(15)	4.0323(3)	1.0012	5.87(8)	0.1075	0.0838
BTO-80	4.0255(4)	4.0258(8)	1.0001	12.94(11)	0.0967	0.0748
BTO-90	4.0291(5)	4.0319(11)	1.0007	28.06(22)	0.0846	0.0677

Table S2 Mass losses of $BaTiO_3$ samples synthesised via a solvothermal method with various benzyl alcohol percentages (0, 20%, 40%, 60%, 80% and 90%) in benzyl alcohol/water solvent mixtures.

Percentage of benzyl alcohol (%)	Mass loss (%)
0	1.2
20	0.3
40	0.9
60	0.8
80	5.0
90	7.6

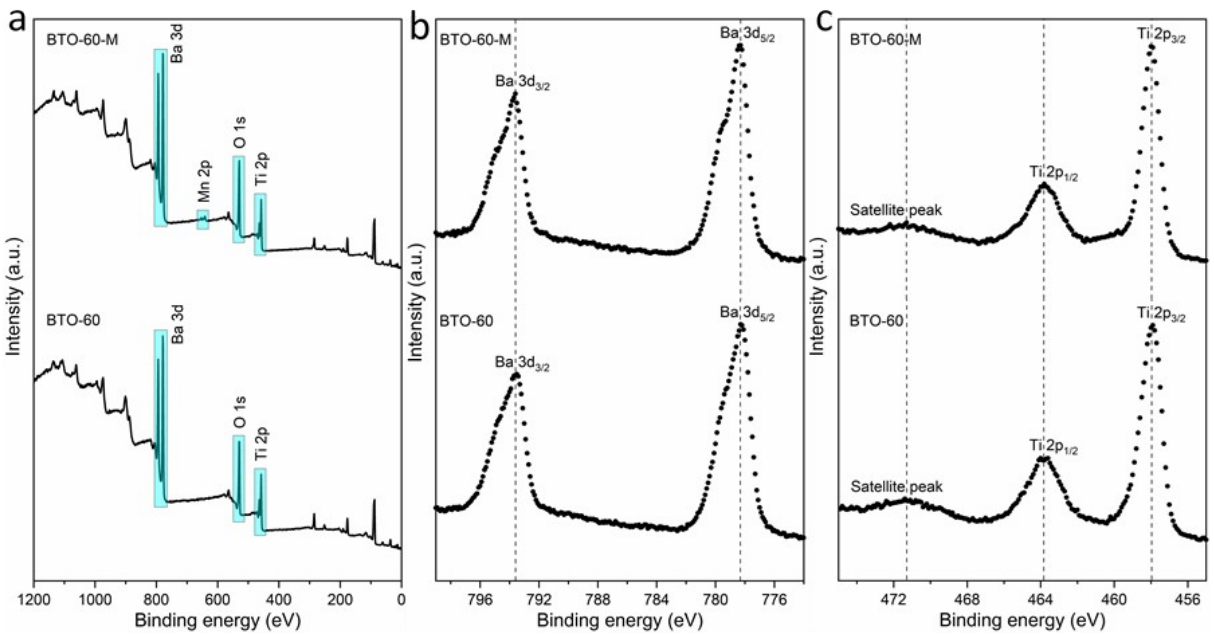

Fig. S2 XPS spectra of BTO-60 and BTO-60-M samples: (a) survey spectra, (b) Ba 3*d* and (c) Ti 2*p* (sample labels explained in Table 2).

Table S3 Lattice parameters (*a*, *c*), tetragonality (*c/a*), Lorentzian crystallite size broadening term (L_x) and reliability factors (R_{wp}, R_p) obtained from the Rietveld fits to the XRD patterns of the uncoated and manganese oxide coated $BaTiO_3$ samples (sample labels explained in Table 2).

Sample	Lattice parameter		Tetragonality	Crystallite size broadening	Reliability factor	
	a [Å]	*c* [Å]	*c/a*	L_x	R_{wp}	R_p
BTO-60	4.02402(14)	4.0340(2)	1.0025	7.47(10)	0.1219	0.0941
BTO-60-M	4.00688(12)	4.0135(2)	1.0017	6.84(8)	0.0943	0.0718