Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supplementary Information

Enhancing the Thermoelectric Power Factor of $Sr_{0.9}Nd_{0.1}TiO_3$ through Control of the Nanostructure and Microstructure

D. Ekren [a], A. Golinia [a], F. Azough [a], S. J. Day [b],

D. Hernandez. Maldonado [c], D.M. Kepaptsoglou [c], Q. M. Ramasse [c], R. Freer [a]

[a] School of Materials, University of Manchester, Manchester, M13 9PL, UK.

[b] Diamond Light Source, Harwell Science and Innovation Campus, Oxfordshire, OX11 0DE, UK

[c] SuperSTEM Laboratory, STFC Daresbury Campus, Daresbury WA4 4AD, U.K.

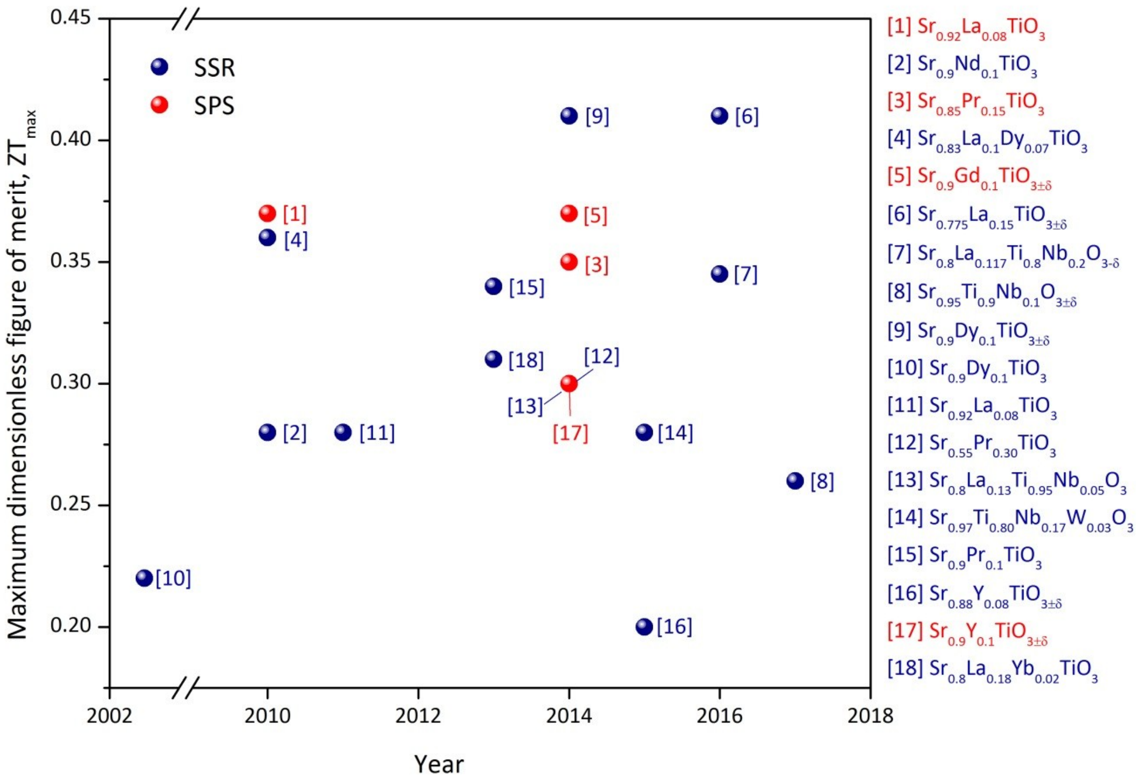

Figure S.1 *Thermoelectric dimensionless figure of merit of $SrTiO_3$ ceramics prepared with different A-site and B-site dopants using solid state reaction (SSR) and spark plasma sintering (SPS)*[1–18]

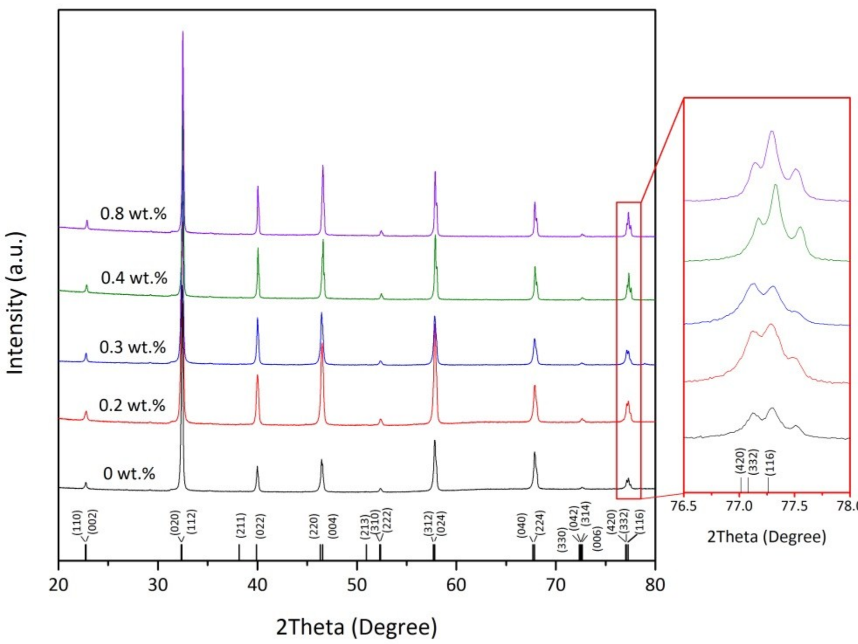

***Figure S.2** X-Ray diffraction patterns for $Sr_{0.9}Nd_{0.1}TiO_3$ samples prepared with different amounts of ZrO_2*

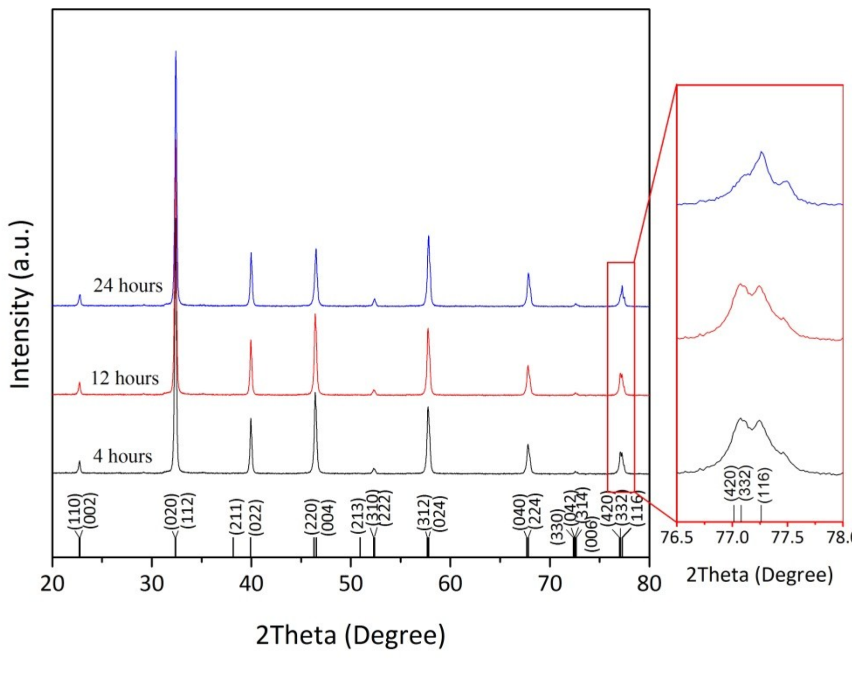

***Figure S.3** X-Ray diffraction patterns for 3Z samples illustrating the effect of sintering time.*

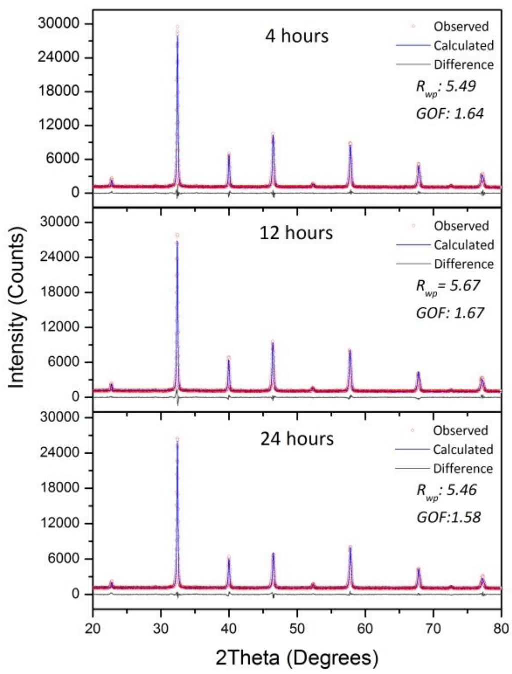

Figure S.4 *Full profile Rietveld refinement from laboratory XRD data (λ=1.540598 Å) for 3Z samples sintered for 4-24 hours*

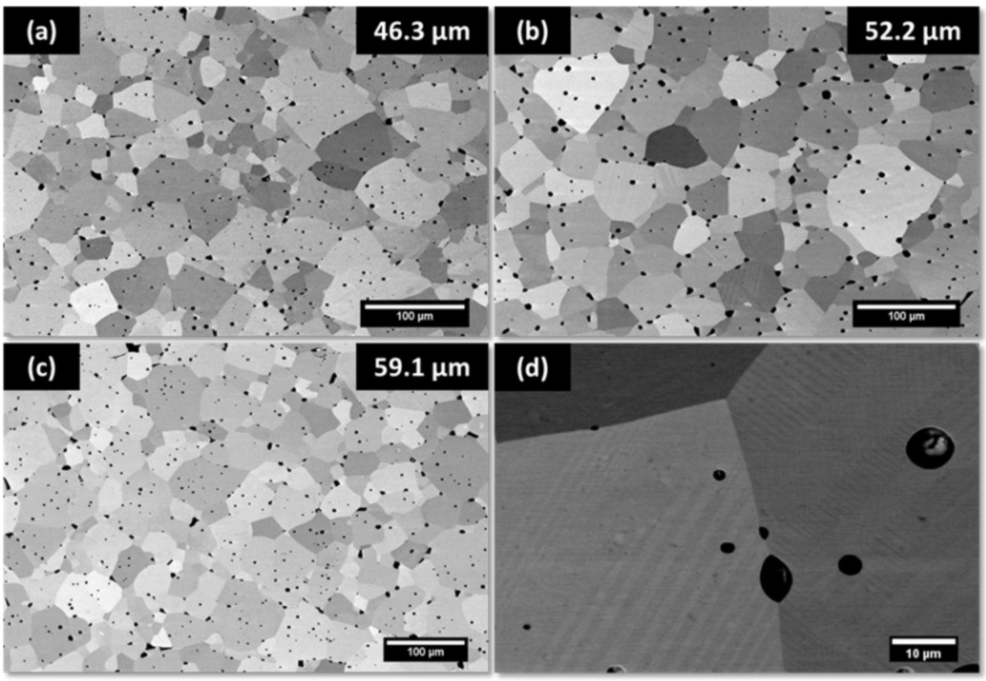

Figure S.5 *BSE-SEM micrographs for 3Z samples after* ***(a)*** *4 hours,* ***(b)*** *12 hours and* ***(c-d)*** *24 hours of sintering. The values for the average grain size in shown in the top right inset of the figures.*

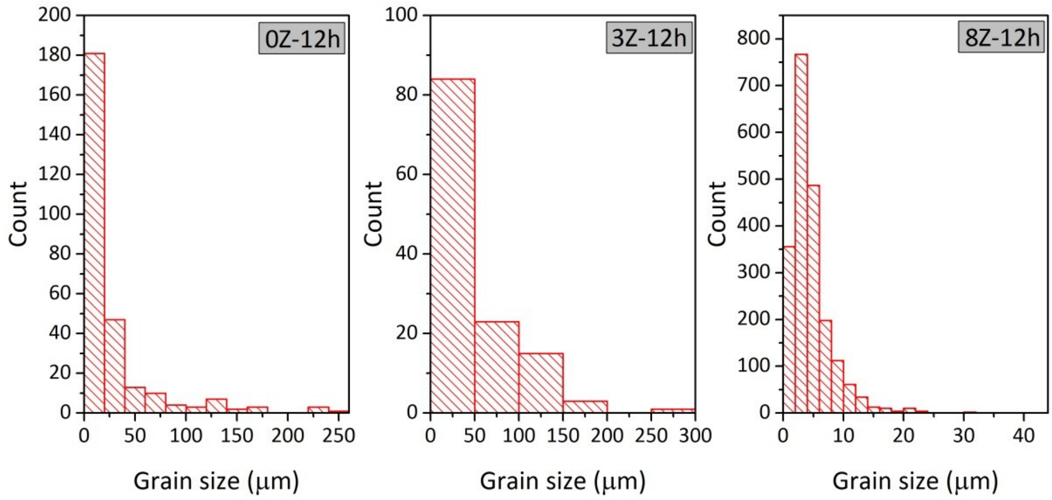

Figure S.6 *Grain size distribution data obtained from multiple SEM micrographs for 0Z-12h, 3Z-12h and 8Z-12 samples*

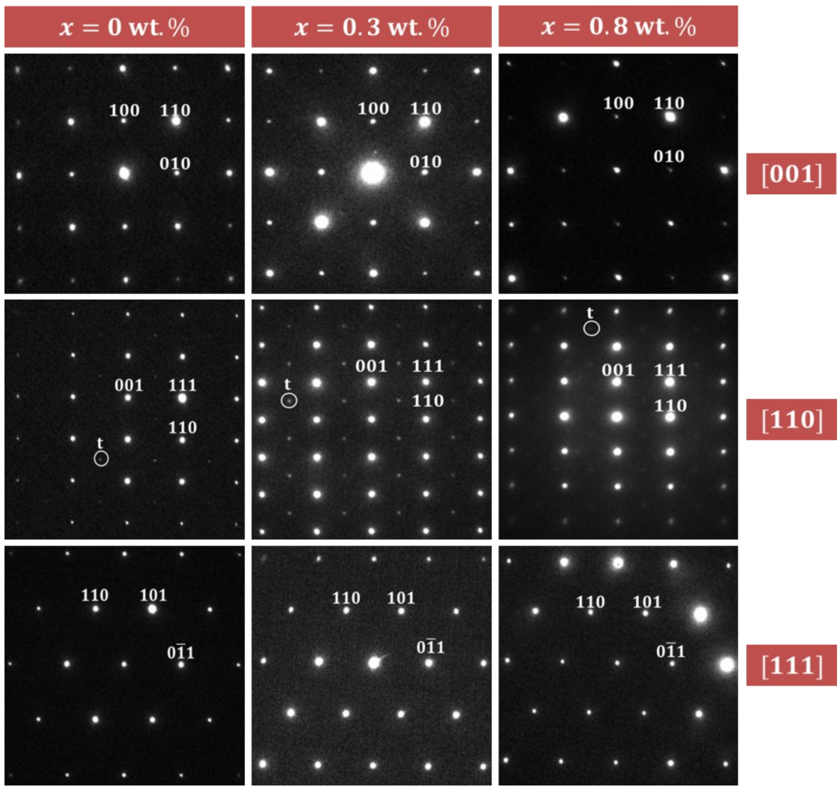

Figure S.7 *SAED patterns along major zone axes for 0.5 wt% B_2O_3 doped $Sr_{0.9}Nd_{0.1}TiO_3$ samples co-doped with different amounts of ZrO_2*

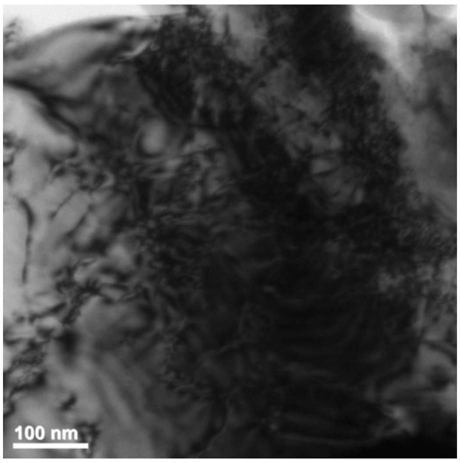

Figure S.8 *Low magnification TEM data showing high density of dislocations in 3Z-12h sample without ZrO_2 addition*

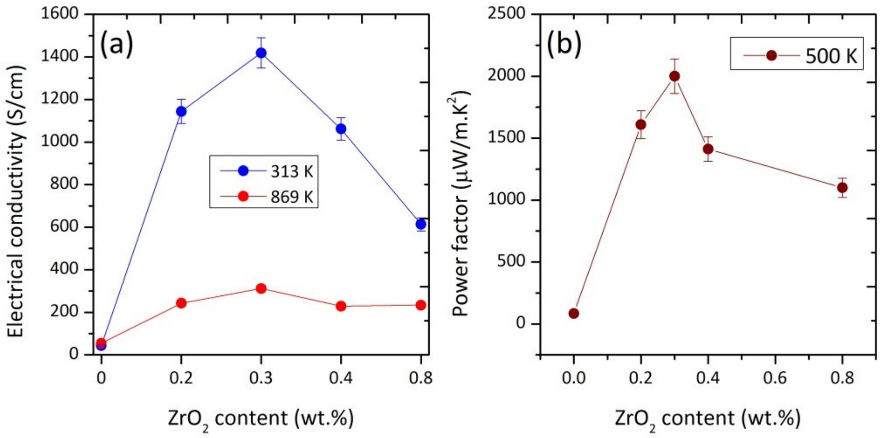

Figure S.9 (a) *Electrical conductivity at 313 and 869 K, and* ***(b)*** *power factor at 500 K with respect to ZrO_2 content.*

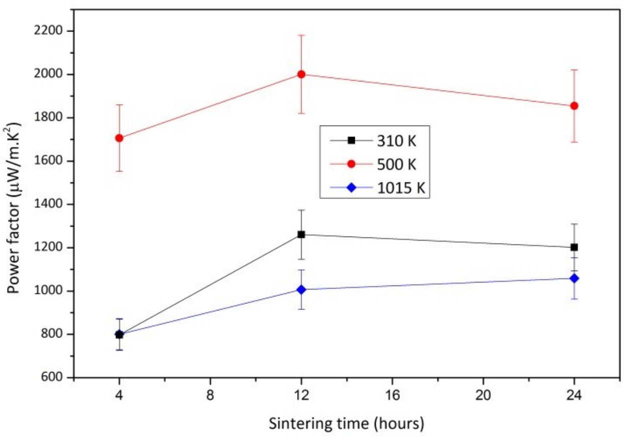

Figure S.10 *Measurement temperature (310, 500 and 1015 K) and sintering time dependence of power factor for 3Z-12 samples*

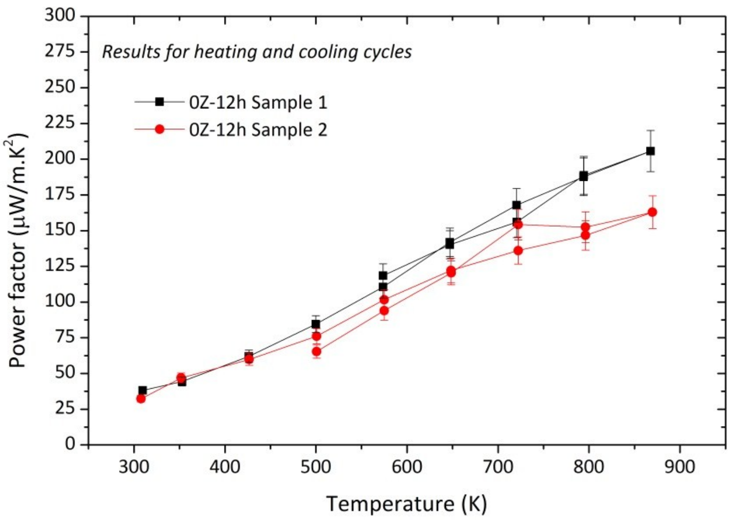

Figure S. 11 *Thermoelectric power factor for two different 02-12h samples during heating and cooling cycles of measurement*

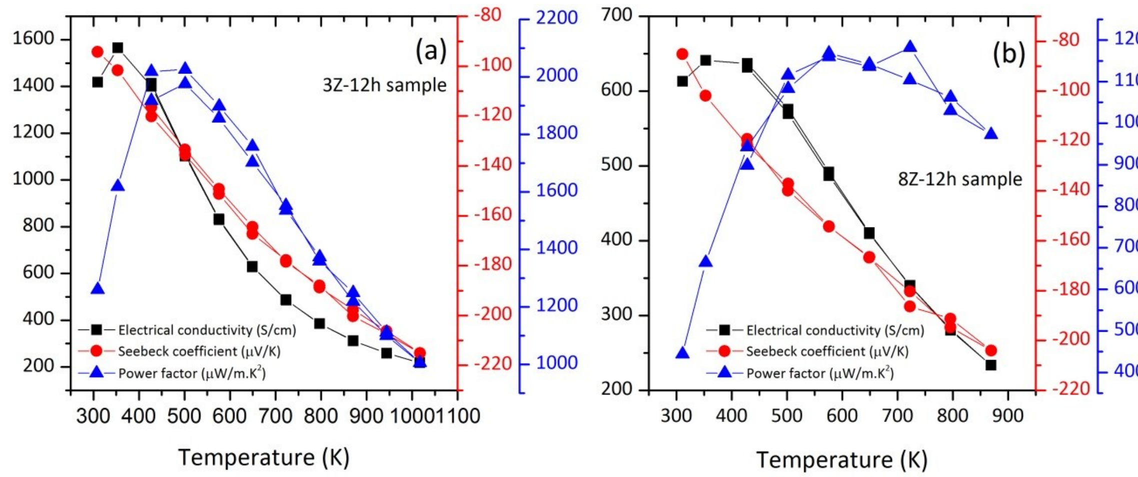

Figure S.12 *Heating and cooling cycle data for electrical conductivity, the Seebeck coefficients and power factor data for 3Z-12h and 8Z-12h samples*

Table S.1 *Structural parameters and Ti-O bond lengths for $Sr_{0.9}Nd_{0.1}TiO_3$ samples co-doped with 0.5 wt.% B_2O_3 and x different amounts of ZrO_2 from SXPD data (λ=0.825939(10) Å).*

ZrO_2 content (wt.%)	**0**	**0.3**	**0.8**
Space Group	*I4/mcm*	*I4/mcm*	*I4/mcm*
R_{wp}/GOF	12.84/1.45	4.85/3.18	13.69/1.67
Lattice Parameters			
a (Å)	5.518449(2)	5.518705(3)	5.521464(2)
c (Å)	7.820044(5)	7.820201(7)	7.823195(5)
V (Å^3)	238.1460(3)	238.1729(4)	238.5024(2)
Sr/Nd			
X / Y / Z	0 / 0.5 / 0.25	0 / 0.5 / 0.25	0 / 0.5 / 0.25
b_{eq}	0.003(2)	0.079(3)	0.090(2)
Occupancy	0.9/0.1	0.9/0.1	0.9/0.1
Ti			
X / Y / Z	0 / 0 / 0	0 / 0 / 0	0 / 0 / 0
b_{eq}	0.224(2)	0.073(4)	0.172(3)
Occupancy	1	1	1
O1			
X / Y / Z	0 / 0 / 0.25	0 / 0 / 0.25	0 / 0 / 0.25
b_{eq}	0.248(17)	0.200(30)	0.400(20)
Occupancy	1	1	1
O2			
X	0.23330(12)	0.23147(19)	0.23379(13)
Y	0.73330(12)	0.73147(19)	0.73379(13)
Z	0	0	0
b_{eq}	0.179(11)	0.300(20)	0.335(16)
Occupancy	1	1	1
Bond lengths			
Ti-O1	1.95501	1.95505	1.95579
Ti-O2	1.95584	1.95469	1.95626

Table S.2 *Thermoelectric Power factors for $SrTiO_3$ based thermoelectric oxides*

Composition	**Sample characteristics**	**PF_{max} ($\mu W/m.K^2$)**	**Temperature (K)**	**Reference**
A-site doping				
$Sr_{1-x}La_xTiO_3$	Single-crystal	3600	300	19
$Sr_{0.9}Nd_{0.1}TiO_3$	Polycrystalline	1690	423	2
$Sr_{0.9}Pr_{0.1}TiO_3$	Polycrystalline	1400	670	15
$Sr_{0.9}Nd_{0.1}TiO_{3-\delta}$	Polycrystalline	1550	440	9
$Sr_{0.85}Pr_{0.15}TiO_3$	Polycrystalline	1320	773	20
$Sr_{0.9}Gd_{0.1}TiO_{3-\delta}$	Polycrystalline	1600	570	5
$Sr_{0.91}La_{0.09}TiO_{3-\delta}$	Polycrystalline	1352	500	21
$Sr_{0.94}Y_{0.04}TiO_{3-\delta}$	Polycrystalline	1164	423	16
$Sr_{0.9}Nd_{0.1}TiO_{3\pm\delta}$ + 0.5 wt% B_2O_3 + 0.3 wt% ZrO_2	Polycrystalline	2000	500	* This study
B-site doping				
$SrTi_{0.9}Ta_{0.1}O_{3-\delta}$	Polycrystalline	1420	470	22
$SrTi_{0.9}Nb_{0.1}O_3$	Polycrystalline	1450	523	23
Dual doping				
$Sr_{0.83}La_{0.10}Dy_{0.07}TiO_3$	Polycrystalline	1237	700	4
$Sr_{0.95}La_{0.05}Ti_{0.95}Nb_{0.05}O_3$	Polycrystalline	2370	473	24
$Sr_{0.80}La_{0.13}Ti_{0.95}Nb_{0.05}O_3$	Polycrystalline	1300	525	13
$Sr_{0.85}La_{0.075}Sm_{0.075}TiO_{3-\delta}$	Polycrystalline	1400	573	25
$Sr_{0.9}La_{0.1}Ti_{0.9}Nb_{0.1}O_3$	Polycrystalline	1700	623	26
A-site deficient				
$Sr_{0.94}Ti_{0.80}Nb_{0.2}O_3$	Polycrystalline	1625	450	12
$Sr_{0.775}La_{0.15}TiO_{3-\delta}$	Polycrystalline	1400	473	6
$Sr_{0.95}Ti_{0.9}Nb_{0.1}O_{3-\delta}$	Polycrystalline	1600	450	8
$Sr_{0.75}La_{0.1}Dy_{0.1}TiO_3$	Polycrystalline	1216	373	27
Inclusion/Additive				
$SrTi_{0.85}Nb_{0.15}O_3$ + 3wt% YSZ	Polycrystalline	720	400	28
$Sr_{0.9}La_{0.1}TiO_3$ + 0.6wt% Graphene	Polycrystalline	2500	330	29

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