Effect of ionic radii on the Curie temperature in Ba_{1-x-y}Sr_xCa_yTiO₃ compounds

A. Berenov,^a F. Le Goupil^a and N. Alford^a

^a Department of Materials, Imperial College London, London, SW7 2AZ, UK.



Supplementary Figure S1. XRD pattern of $Ba_{0.65}Sr_{0.35}TiO_{3.}$ The inset shows tetragonal splitting of (200) peak in series A compounds.



Supplementary Figure S2. SEM images of $Ba_{0.65}Sr_{0.35}TiO_3$ (a) and $Ba_{0.78}Ca_{0.22}TiO_3$ (b) pellets thermally etched at 1400 $^\circ C$ for 0.5 hrs



Supplementary Figure S3. Temperature dependences of DSC signal for compounds from series A.

Supplementary Ta	able S4 ICP and	l DSC results of	f studied BSCT	samples.
------------------	-----------------	------------------	----------------	----------

Intended composition	Analysed composition	<i>Т</i> _{R-О} /К	Т _{О-Т} /К	<i>Т</i> _С /К
Series A				
$Ba_{0.65}Sr_{0.35}TiO_3$	$Ba_{0.655(2)}Sr_{0.349(1)}TiO_{3}$	171	218	291
$Ba_{0.69}Sr_{0.24}Ca_{0.07}TiO_{3}\\$	$Ba_{0.704(2)}Sr_{0.237(1)}Ca_{0.076(1)}TiO_{3}$	145	206	325
$Ba_{0.74}Sr_{0.12}Ca_{0.15}TiO_{3}\\$	$Ba_{0.742(14)}Sr_{0.120(2)}Ca_{0.144(1)}TiO_3$	NA	163	358
$Ba_{0.78}Ca_{0.22}TiO_3$	$Ba_{0.798(9)}Ca_{0.206(1)}TiO_3$	NA	NA	394
Series B				
$Ba_{0.8}Sr_{0.2}TiO_3$	$Ba_{0.796(3)}Sr_{0.197(1)}TiO_3$	187	251	341
$Ba_{0.6}Sr_{0.2}Ca_{0.2}TiO_3$	$Ba_{0.607(6)}Sr_{0.202(3)}Ca_{0.198(1)}TiO_{3}$	NA	NA	320
Ba _{0.9} Ca _{0.1} TiO ₃	Ba _{0.887(1)} Ca _{0.113(2)} TiO ₃	139	224	402
$Ba_{0.85}Sr_{0.1}Ca_{0.05}TiO_3$	$Ba_{0.854(2)}Sr_{0.100(1)}Ca_{0.046(1)}TiO_3$	173	248	376
$Ba_{0.78}Sr_{0.1}Ca_{0.12}TiO_3$	$Ba_{0.794(2)}Sr_{0.103(1)}Ca_{0.103(1)}TiO_3$	NA	NA	369
$Ba_{0.75}Sr_{0.1}Ca_{0.15}TiO_{3}\\$	$Ba_{0.754(2)}Sr_{0.101(1)}Ca_{0.145(1)}TiO_3$	NA	NA	363
$Ba_{0.7}Sr_{0.1}Ca_{0.2}TiO_3$	$Ba_{0.704(1)}Sr_{0.102(1)}Ca_{0.195(1)}TiO_3$	NA	NA	357
Series C				
$Ba_{0.68}Sr_{0.32}TiO_3$	$Ba_{0.692(3)}Sr_{0.321(6)}TiO_3$	176	227	302
$Ba_{0.62}Sr_{0.28}Ca_{0.1}TiO_3$	$Ba_{0.625(3)}Sr_{0.283(4)}Ca_{0.098(1)}TiO_{3}$	NA	180	307



Supplementary Figure S5. T_C as a function of c/a for the studied compounds.



Supplementary Figure S6. T_c as a function of $\sigma^2 + (\langle r_{A-site} \rangle - r_{A-site}^0)^2$ for samples studied in this work.



Supplementary Figure S7. T_C as a function of $\sigma^2 + \left(\frac{r_{A-site}^0}{\langle r_{A-site} \rangle}\right)^2 \left(\langle r_{A-site} \rangle - r_{A-site}^0\right)^2$ for titanates with isoelectronic (Ba_{1-x-y}S_xCa_yTiO₃ this work) and non-isoelectronic (Pb_{1-x}Ba_xTiO₃⁻¹, Ba_{1-x}La_xTiO₃⁻²) doping on the A site.

¹ T. Ikeda, J. Phys. Soc. Jap. **14** 1286 (1959)

² L. Ben and D. C. Sinclair, Appl. Phys. Lett., **98** 092907 (2011)