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

Supporting information

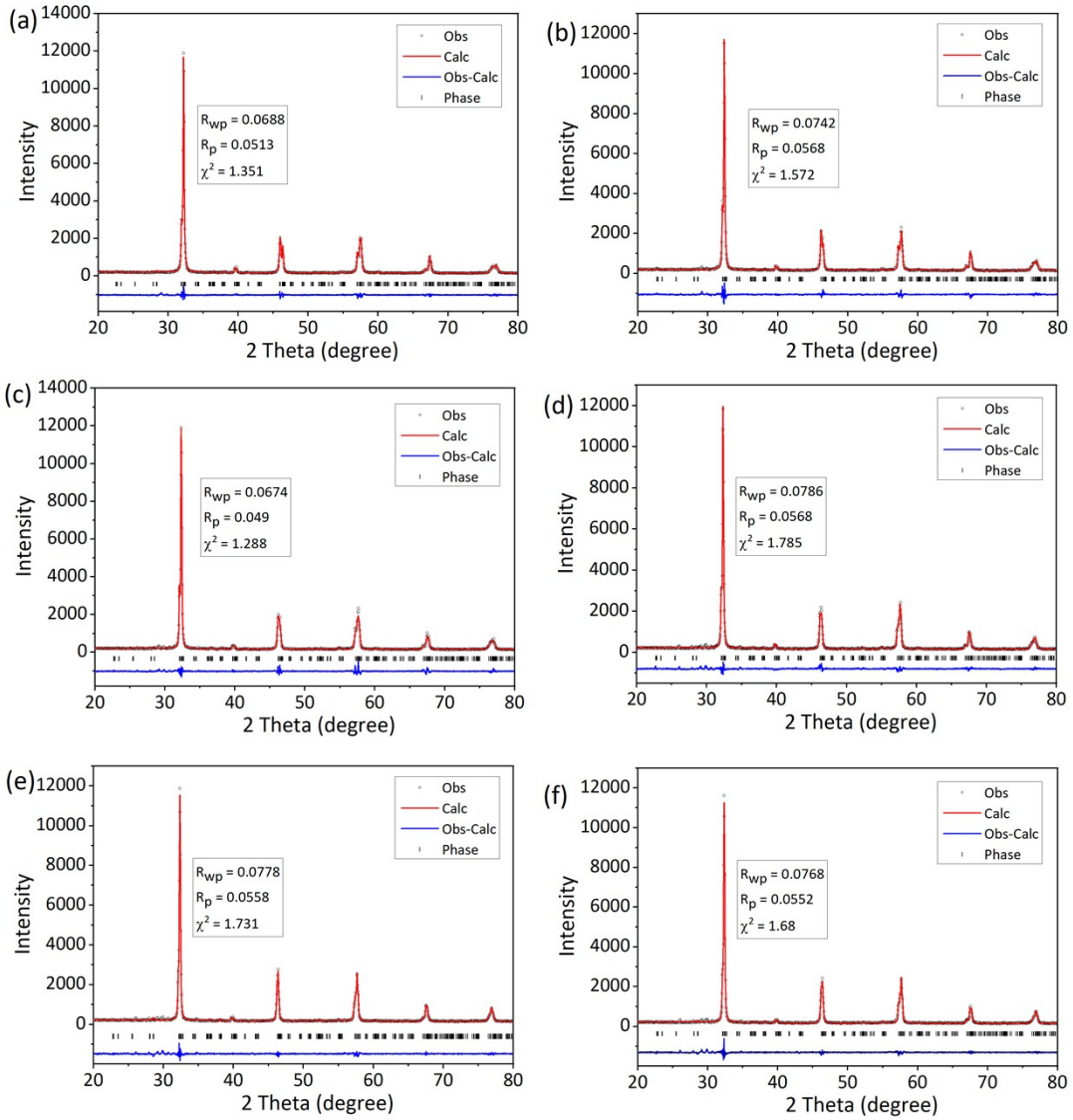

Fig. S1 Fitted X-ray powder diffraction profiles based on *Pbcm** for (a)AN, (b)ANT10, (c)SANT1, (d)SANT2, (e)SANT3 and (f)SANT4 ceramics, showing observed (points), fitted (line) and difference (lower) profiles.

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* It cannot distinguish between *Pbcm* and $Pb2_1m$ space group, *Pbcm* model may provide a better description of the crystallographic structure.[1]

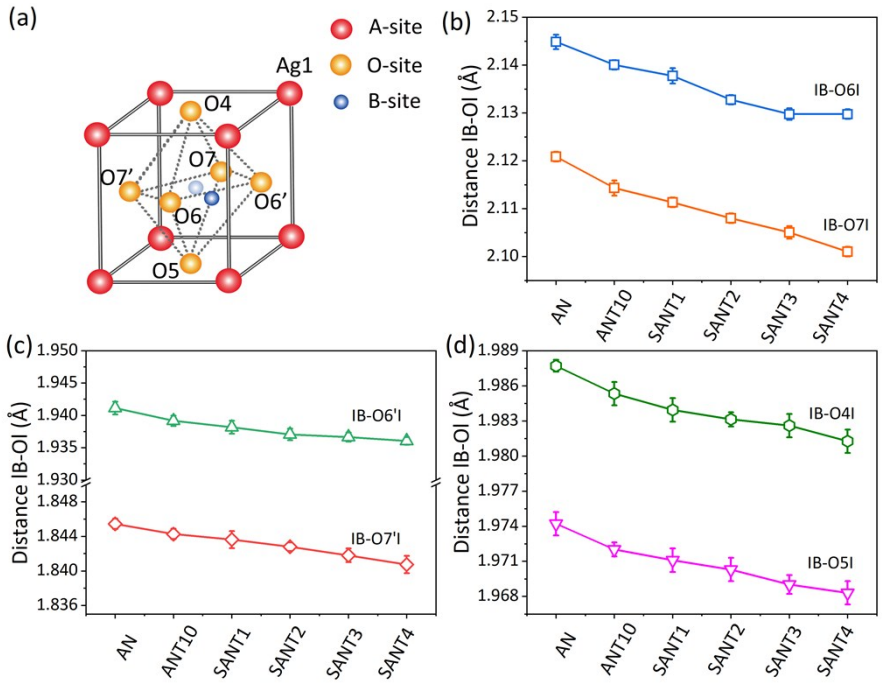

Fig. S2 (a) general structural characteristics of AN system, the average distance of (b) |B-O6|, |B-O7|, (c) |B-O6'|, |B-O7'|, and (d) |B-O4|, |B-O5|.

Fig. 2(a) displays some main structural characteristics, including the displacement of Ag1 and B-site cations, as well as the locations of O4, O5, O6, O7, O6' and O7' in [BO6] octahedron. The |B-O6|, |B-O7|, |B-O6'| and |B-O7'| [Fig. S2(b) and (c)] in the horizontal plane decrease after Ta and Sm modification due to suppressed cell volume, which is consistent with decreased lattice parameters a and b. A similar tendency is also observed for |B-O4| and |B-O5| in the vertical axis, as shown in Fig. 2(d), which is associated with the decreased B-site displacement. Although the calculated lattice parameter c increases after Sm modification, the decreased B-site displacement from the center of [BO_6] octahedron shortens the distance between B and O in the vertical axis, which is further verified by enhanced O4-B-O5 angle degree Fig. S3. The stronger B-O band will constrain oxygen in [BO_6] octahedron and inhibit octahedral rotation.[2-4]

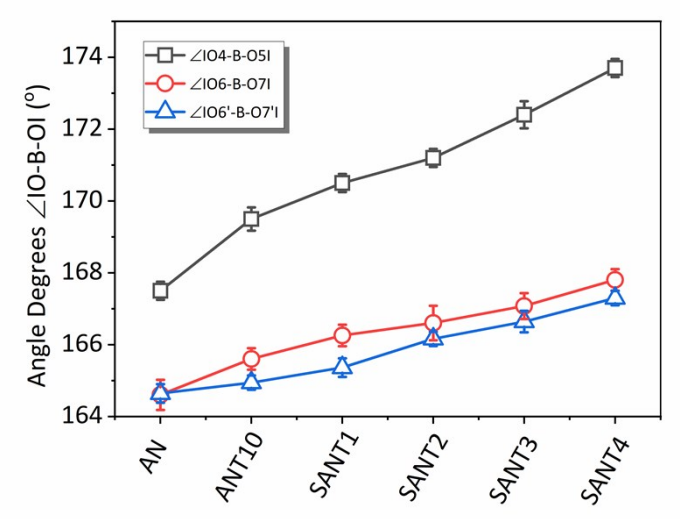

Fig. S3 the angle degrees of O4-B-O5, O6-B-O7 and O6'-B-O7'.

Fig. S3 shows the angle degrees, i.e. ∠|O6-B-O7|, ∠|O6'-B-O7'| in the horizontal axis and ∠|O4-B-O5| in the vertical axis. All angles are found to increase, related to the weakened B-site ion displacement. The enhanced angle degrees indicates that [BO_6] octahedron exhibits lower distortion after Sm and Ta modification.[2] In addition, the enhancement of ∠|O4-B-O5| is more significant compared with ∠|O6-B-O7| and ∠|O6'-B-O7'|, indicating that decreased B-site ion displacement can make a greater impact on B-O band in the vertical axis than ones in the horizontal axis.

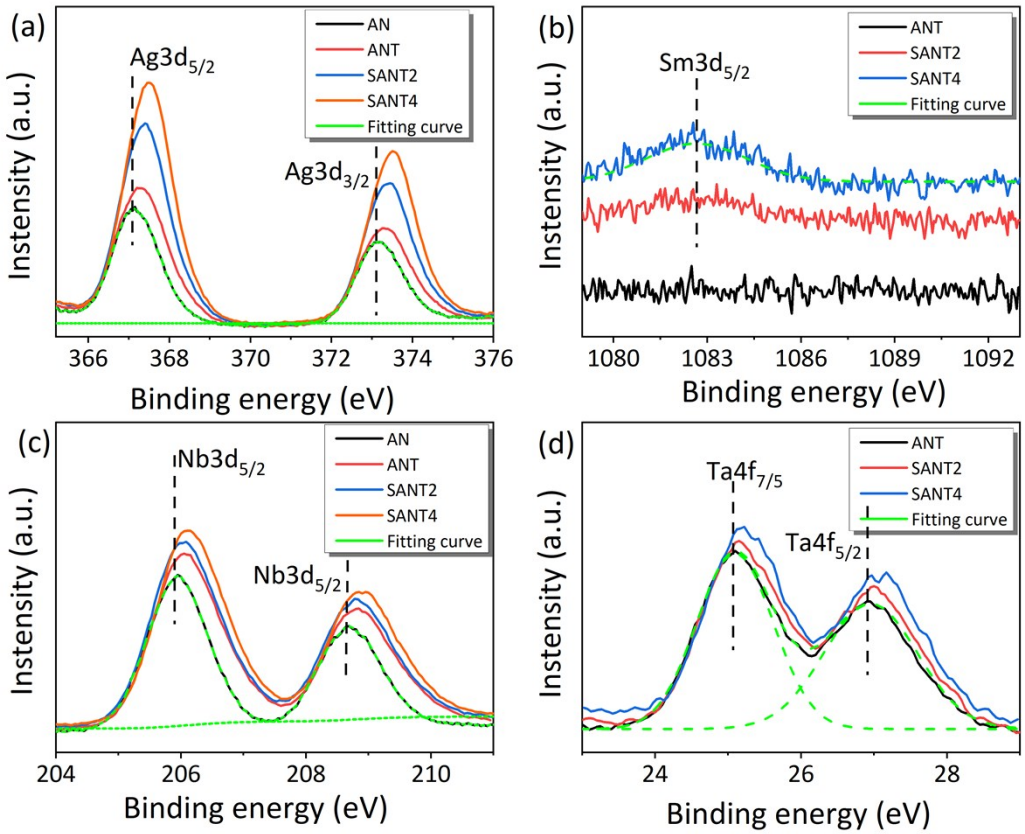

Fig. S4 XPS spectra of (a) Ag3d, (b) Sm3d, (c)Nb3d and (d) Ta4f core level for the SANT*x* ceramics with selected compositions.

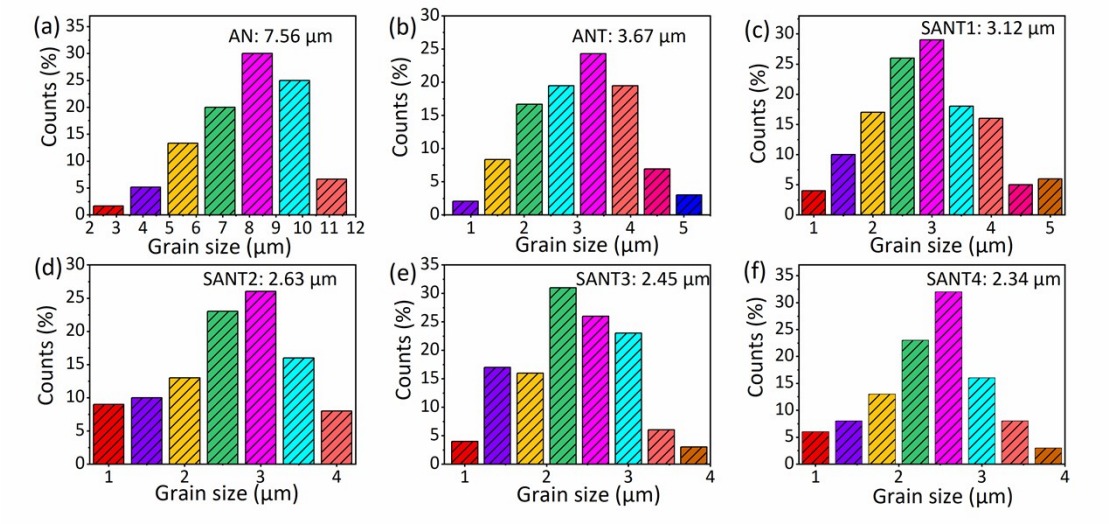

Fig. S5 Estimated grain size distribution for (a)AN, (b)ANT10, (C)SANT1, (d)SANT2, (e)SANT3 and (f)SANT4 ceramics.

Table S1 Crystal and refined parameters for the as-prepared samples

Specimens	AN	ANT10	SANT1	SANT2	SANT3	SANT4
Space group	*Pbcm*	*Pbcm*	*Pbcm*	*Pbcm*	*Pbcm*	*Pbcm*
Unit cell	a= 5.5605(1) Å	a= 5.5475(2) Å	a= 5.5466(1) Å	a= 5.5442 (1) Å	a= 5.5436(1) Å	a= 5.539(1) Å
dimensions	b=5.6141(2) Å	b=5.6013(2) Å	b=5.6004(1) Å	b=5.599(2) Å	b=5.596(1) Å	b=5.5893(2) Å
	c=15.6696(5) Å	c=15.6729(5) Å	c=15.6804(4) Å	c=15.685(5) Å	c=15.6867(5) Å	c=15.689(4) Å
Volume	489.16(2) $Å^3$	487.41(1) $Å^3$	487.085(3) $Å^3$	486.863(3) $Å^3$	486.634(3) $Å^3$	485.785(2) $Å^3$
Density (fitted)	6.767 g/cm^3	6.879 g/cm^3	6.866 g/cm^3	6.861 g/cm^3	6.855 g/cm^3	6.843 g/cm^3
Refining	R_{wp}=0.0688	R_{wp}=0.0742	R_{wp}=0.0674	R_{wp}=0.0786	R_{wp}=0.0778	R_{wp}=0.0768
parameters	*R*p=0.0513	*R*p=0.0568	*R*p=0.049	*R*p=0.0568	*R*p=0.0558	*R*p=0.0552
	χ^2=1.351	χ^2=1.572	χ^2=1.288	χ^2=1.785	χ^2=1.731	χ^2=1.68

Table S2 Refined results of atomic coordinates for (a) AN, (b) ANT10 and (c) SANT2 ceramics based on *Pbcm* space group

(a)

Atom	Site	*x*	*y*	*z*	Occ.	U_{ios} (Å^2)
Ag1	4*d*	0.7546(3)	0.23634(1)	0.75	1	0.0226(5)
Ag2	4*c*	0.7492(3)	0.25	0.5	1	0.0226(5)
Nb	8*e*	0.7484(1)	0.729(1)	0.6254(2)	1	0.0118(0)
O1	4*d*	0.719(08)	0.77	0.75	1	0.037(3)
O2	4*c*	0.796(1)	0.75	0.5	1	0.037(3)
O3	8*e*	0.454(1)	0.547(2)	0.612(3)	1	0.037(3)
O4	8*e*	0.992(2)	0.509(3)	0.639(1)	1	0.037(3)

(b)

Atom	Site	*x*	*y*	*z*	Occ.	U_{ios} (Å^2)
Ag1	4*d*	0.7464(4)	0.2389(1)	0.75	1	0.047(3)
Ag2	4*c*	0.7398(03)	0.25	0.5	1	0.047(3)
Nb/Ta	8*e*	0.75374(2)	0.73(01)	0.6267(2)	1	0.0408(2)
O1	4*d*	0.7174(02)	0.7444(1)	0.75	1	0.053(5)
O2	4*c*	0.804(03)	0.75	0.5	1	0.053(5)
O3	8*e*	0.4725(4)	0.4632(2)	0.6093(3)	1	0.053(5)
O4	8*e*	1.001(2)	0.4441(5)	0.6493(5)	1	0.053(5)

(c)

Atom	Site	*x*	*y*	*z*	Occ.	U_{ios} (Å^2)
Ag/Sm1	4*d*	0.7516(2)	0.2439(4)	0.75	1	0.086(2)
Ag2	4*c*	0.7426(4)	0.25	0.5	1	0.086(2)
Nb/Ta	8*e*	0.747(04)	0.7359(05)	0.624(4)	1	0.036(2)
O1	4*d*	0.7227(2)	0.746(1)	0.75	1	0.033(2)
O2	4*c*	0.83(03)	0.75	0.5	1	0.033(2)
O3	8*e*	0.517(1)	0.539(3)	0.586(2)	1	0.033(2)
O4	8*e*	1.0568(4)	0.446(06)	0.6178(5)	1	0.033(2)

References

1. Y. Tian, L. Jin, H. F. Zhang, Z. Xu, X. Y. Wei, G. Viola, I. Abrahams and H. X. Yan, *J. Mater. Chem. A*, 2017, **5**, 17525-17531.
2. I. Levin, V. Krayzman, J. C. Woicik, J. Karapetrova, T. Proffen, M. G. Tucker and I. M. Reaney, *Physi. Rev. B*, 2009, **79**, 104113.
3. J. Frantti, S. Ivanov, S. Eriksson, H. Rundlo¨f, V. Lantto, J. Lappalainen, and M. Kakihana, Phys. Rev. B, 2002, 66, 064108.
4. I. Levin, J. C. Woicik, A. Llobet, M. G. Tucker, V. Krayzman, J. Pokorny and I. M. Reaney, *Chem. Mater.*, 2010, **22**, 4987-4995.