

Supporting Information

Enhanced antiferroelectric phase stability in La-doped AgNbO_3 : perspectives from the microstructure to energy storage property

Fig. S1 Rietveld refinement of neutron diffraction pattern of (a) ANL0, (b) ANL1, (c) ANL2, (d) ANL3, (e) ANL4, showing experimental data (points), calculated data (line) and difference (lower line) profiles.

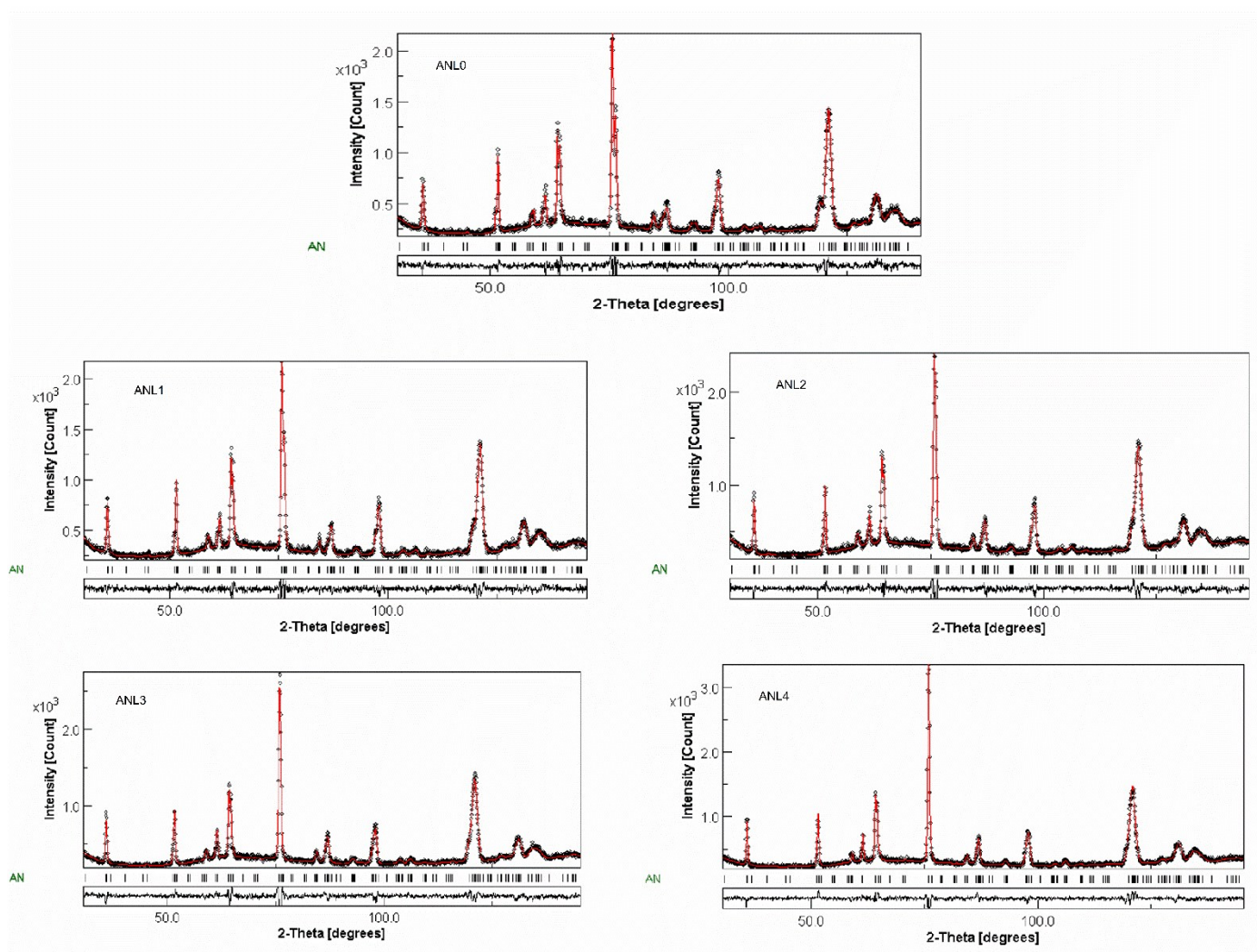


Table. S1 Cell parameters, calculated density and R-factors for ANLX ceramics at 25 °C.

Composition	a	b	c	Density	Rwp	Rexp
ANL0	5.5526(3)	5.6066(3)	15.6656(7)	6.7763	0.0604	0.0553
ANL1	5.5500(3)	5.6026(3)	15.6827(8)	6.7854	0.0542	0.0528
ANL2	5.5476(3)	5.5965(4)	15.6966(9)	6.7981	0.05593	0.0512
ANL3	5.5437(3)	5.5932(4)	15.7022(9)	6.8129	0.0651	0.0546
ANL4	5.5431(3)	5.5872(3)	15.7186(9)	6.8204	0.0579	0.0543

Table. S2 Refined results of atomic coordinates for pure AgNbO₃ at room temperature.

Atom	x	y	z	B _{eq} (Å ²)
Ag1	0.757(3)	0.252(3)	0.75	0.36(9)
Ag2	0.75	0.25	0.5	=B _{eq} (Ag1)
Nb	0.740(3)	0.728(1)	0.625	0.13(1)
O1	0.804(1)	0.760(3)	0.75	0.39(9)
O2	0.695(1)	0.75	0.5	=B _{eq} (O1)
O3	0.467(5)	0.532(5)	0.637(2)	=B _{eq} (O1)
O4	-0.032(5)	0.467(5)	0.612(2)	=B _{eq} (O1)