Supplementary information

Tungsten Bronze Type Ceramics for Temperature-Stable Energy Storage Properties: A Feasibility Study

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S1. Structure of the tungsten bronze compounds

Figure S1a shows the general structure of tungsten bronze compounds with tetragonal and orthorhombic unit cells. Figure S2b shows that both pentagonal A1-sites and tetragonal A2-sites are occupied by Ba in BTN. The co-existence of pentagonal and tetragonal sites results in trigonal vacant c-sites.

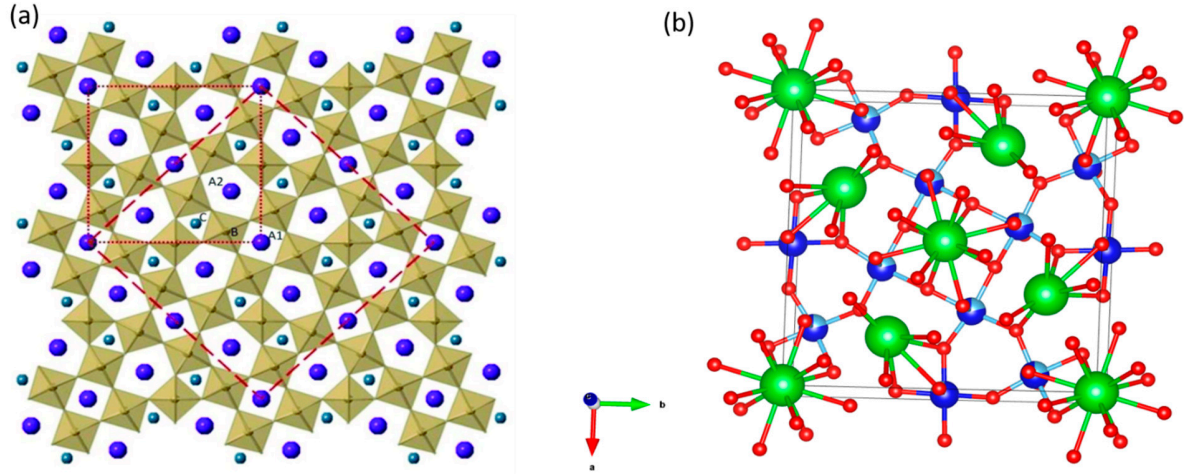

Figure S1. Tetragonal tungsten bronze (TTB) with tetragonal and orthorhombic unit cells indicated by dotted and dashed lines, respectively [1] (a); structure of BTN (green, Blue, red, black atoms indicate Ba, Nb, O, Ti respectively)

S2. Chemical Composition by Energy Dispersive Spectroscopy

Energy Dispersive Spectroscopy (EDS) (Quanta 200, FEI Co., USA) was conducted on polished BTN, BZN, STN and SZN samples to clarify the exact chemical composition. Three spots at different areas inside the samples were chosen for each sample and the average values were calculated. The result is shown in Table S1. It can be concluded that the correct composition was achieved in all sintered samples with homogenous compositions. The EDS spectra confirmed composition purity for all samples without extra elememts detected.

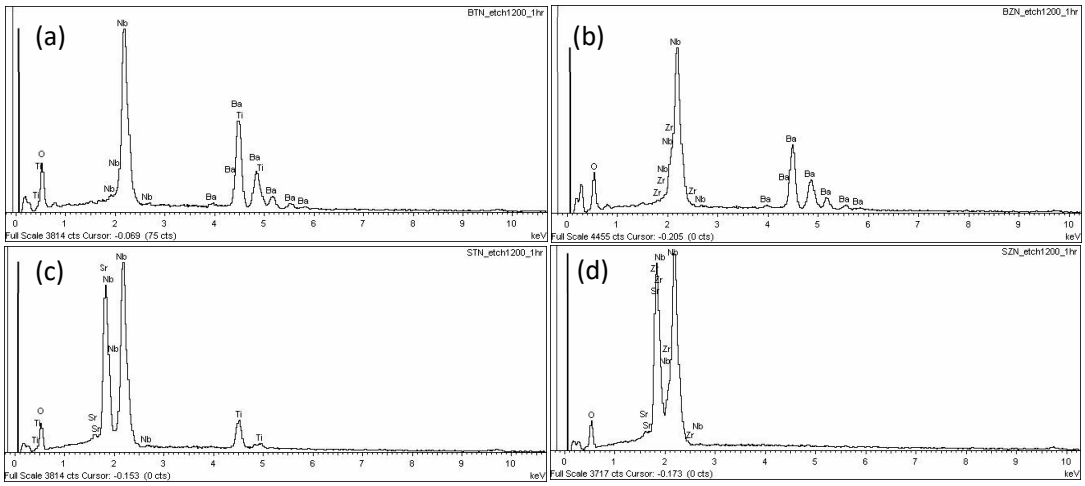

Figure S2 EDS Spectra of the four tungsten bronze samples, *i.e.,* BTN(a), BZN(b), STN(c) and SZN(d)

Table S1 EDS Result of the four tungsten bronze samples, *i.e.,* BTN, BZN, STN and SZN.

Sample	Atom percent (%)					
	Ba	Ti	Zr	Sr	Nb	O
$Ba_6Ti_2Nb_8O_{30}$	10.05	3.17			14.55	72.24
$Ba_6Zr_2Nb_8O_{30}$	10.83		4.61		15.14	69.42
$Sr_3TiNb_4O_{15}$		4.14		10.78	16.64	68.44
$Sr_3ZrNb_4O_{15}$			3.67	12.06	17.08	67.19

S3. XRD fitting

Figure S3 shows the plots generated by Rietveld refinement of BZN, STN and SZN samples where the raw data, calculated plot and the difference between the raw data and calculated are shown. BTN and SZN show a tetragonal structure with the space group *P*4*bm*. SZN and SZN both show orthorhombic structures with the space group $Pna2_1$. Based on the refinement, BTN and SZN samples are single phases without any secondary phases. In contrast, BZN shows 6% secondary phase $Ba_5Nb_4O_{15}$ (Space group $P\bar{3}m1$) and STN has an unidentified peak at 29.49°.

Supplementary information

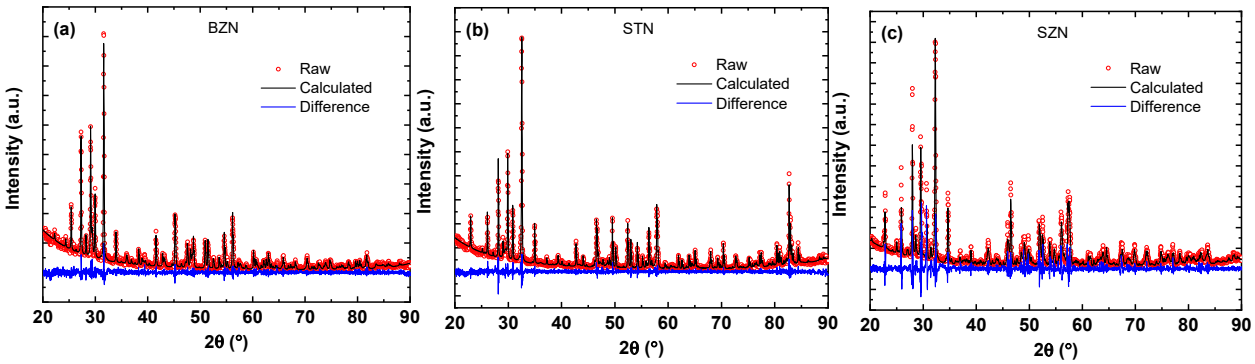

Figure S3. XRD raw data processed with Rietveld refinement of BZN (a), STN(b) and SZN (c) samples.

References

[1] J. Scott, Ferroelectric Relaxor Quantum Crystals, J Crystals 8(4) (2018) 180.