

Electronic Supplementary Material (ESI) for RSC Advances.
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Supplementary Information

Structure and Electrical Properties of Tetragonal Tungsten Bronze $\text{Ba}_2\text{CeFeNb}_4\text{O}_{15}$

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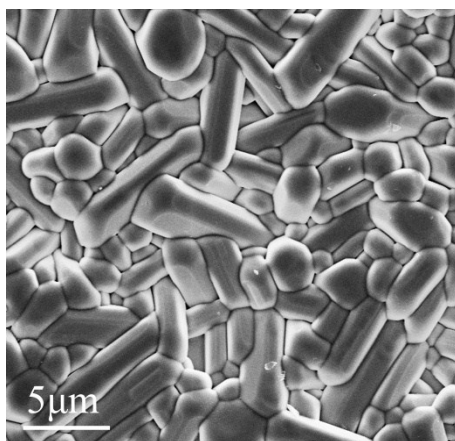


Fig. S1. SEM image of selected pellets surface for the as-synthesized BCFN.

The microstructure of BCFN ceramics was observed by scanning electron microscopy (SEM, Supra 55; Zeiss, Oberkochen, Germany). No impurity was observed.

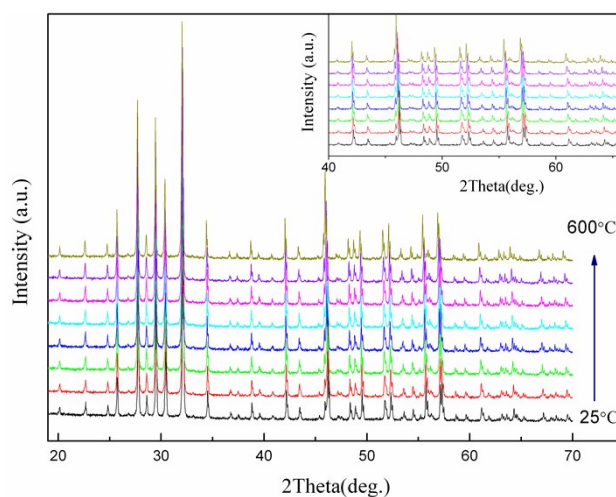


Fig. S2 XRD patterns of BCFN powder at different temperatures (25 – 600 °C). It shows that no phase transition occurs in the measured temperature.

The high-temperature powder X-ray diffraction patterns were collected on a laboratory diffractometer, (PANalytical X'Pert^{III}, Holland, Cu K α , $\lambda=1.5406$ Å) and an Anton Par HTK 1200 high-temperature attachment was used. Data were collected in 0.0131° steps. The heating rate was 10 °C/min, and the sample was held for 15 min at a specified temperature to reach heating equilibrium.

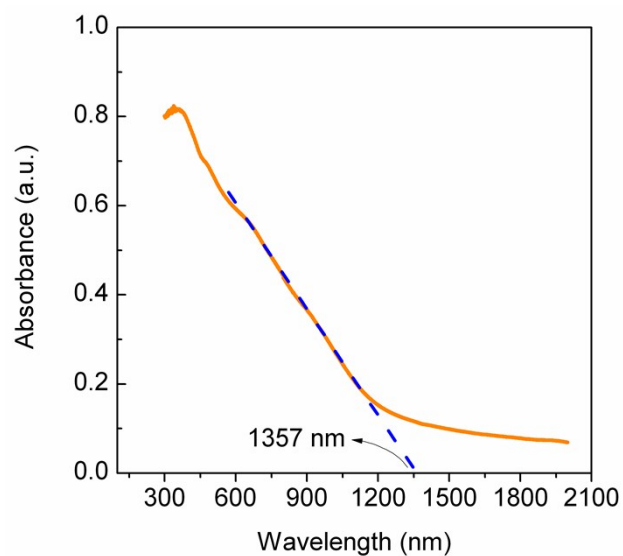


Fig. S3 UV-vis absorbance spectroscopy of as-sintered BCFN powders. Band gap estimated from the intercept of tangents to the plots was ~ 0.91 eV indicative of the existence of shallow energy levels due to oxygen vacancies.

UV-vis absorbance spectroscopy of the nanostructures was performed using a UV-vis spectrometer (VARIAN, Cary 5000) in a quartz cuvette.

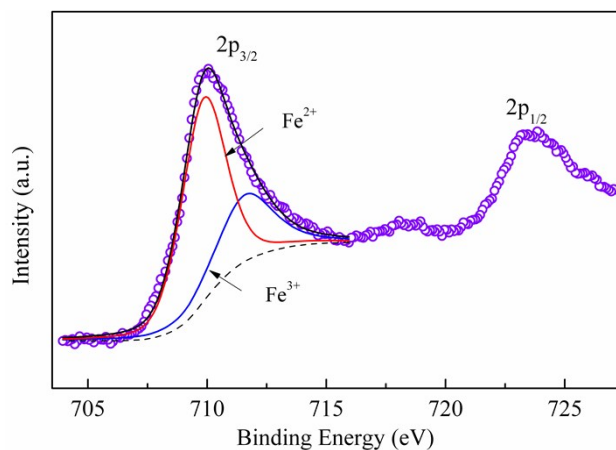


Fig. S4 X-ray photoelectron spectra of Fe2p for surface of as-sintered BCFN pellet. It suggests that the Fe^{3+} reduction to Fe^{2+} and oxygen loss in BCFN are significant in surface.

The surface properties of samples were characterized by X-ray photoelectron spectroscopy (XPS) on a ESCALAB 250 Xi (VG, UK) with Carbon (284.8 eV) as a marker.

Table S1 BVS Values Based on the Data Obtained from SPD Data

Atom	BVS	Atom	BVS
Ce	2.87(2)	O1	1.89(1)
Ba	2.02(1)	O2	2.06(2)
Fe1	3.31(3)	O3	1.95(1)
Nb1	5.10(4)	O4	2.22(3)
Fe2	3.31(3)	O5	1.98(3)
Nb2	5.10(4)		

Bond valence sums (BVS)¹ calculated from the refinements in Table S1 supports the validity of the structure and indicates the dominated existence of Fe³⁺ and Ce³⁺ instead of Fe²⁺ and Ce⁴⁺. Based on the XPS data in Fig. S4, defect concentration in surface are larger than that inside the grains.

¹ D. Brown, and D. Altermatt, *Acta Crystallogr.* 1985, **B41**, 244-247.