Supplementary Information

# Crystal Structure, Chemical Bond, and Microwave Dielectric Properties of $Ba_{1-x}Sr_x(Zn_{1/3}Nb_{2/3})O_3$ Solid Solution Ceramics

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## Results and discussion

Table S1. A detailed list of the abbreviations

| Acronym | Full name explanation |
|---|---|
| BZN | $Ba(Zn_{1/3}Nb_{2/3})O_3$ |
| BSZN | $Ba_{1-x}Sr_x(Zn_{1/3}Nb_{2/3})O_3$ |
| XRD | X-ray diffraction |
| XPS | X-ray photoelectron spectroscopy |
| FWHM | full width at half-maximum |
| JCPDS | Joint Committee on Powder Diffraction Standards |
| DAM | defect activated mode |
| SEM | Scanning electron microscopy |
| $\Delta_{octahedral}$ | octahedral distortion |
| AG | average grain size |
| $\varepsilon_r$ | dielectric constant |
| $Q\times f$ | quality factor |
| $\tau_f$ | temperature coefficient of resonant frequency |
| $E_b$ | bond energy |
| $U_b$ | lattice energy |
| SZN | $Sr(Zn_{1/3}Nb_{2/3})O_3$ |
| $A_mB_n$ | binary bond subtype of the multivariate crystals |
| $f_i$ | bond ionicity |
| n | refractive index |
| $C^\mu$ | heteropole part |
| $f_i^\mu$ | ionic values of the $\mu$-bond |
| $f_c^\mu$ | covalent values of the $\mu$-bond |
| $E_g^\mu$ | average energy band |
| $E_h^\mu$ | isotropic polarization |
| $b^\mu$ | correction factor |
| $(Z_A^\mu)^*$,$(Z_B^\mu)^*$ | the effective valence electron number |
| $exp(-\kappa_s^\mu r_0^\mu$ | Thomas-Fermi shielding factor |
| $d^\mu$ | length of the u bond |
| m,n | number of anions and cations in $A_mB_n$ |
| $r_0^\mu$ | ionic radius of the $\mu$-bond |
| $\alpha_B$ | Bohr radius of a constant |
| $k_F^\mu$ | fermi wave vector |
| $(n_\mu)^*$ | price of electronic number |
| $v_b^\mu$ | bond volume |
| $N_{cA}^\mu$, $N_{cB}^\mu$ | coordination numbers of A and B atoms attached to $\mu$ bonds in a cell |
| $N_b^v$ | bond density of $\mu$-bonds (number of $\mu$ bonds in 1cm$^3$) |
| $E_{A-A}$, $E_{B-B}$ | homonuclear bond energies |
| $t_c$ | covalent co-mixing factors |
| $t_i$ | ionic co-mixing factors |
| $S_A$, $S_B$ | electronegativity of A and B ions |

| | |
|---|---|
| $\Delta S_B$ | change in electronegativity |
| Ei | energies contributed by the ionic bonds |
| Ec | energies contributed by the covalent bonds |
| $U_{bi}^{\mu}$ | lattice energy of the ionic part |
| $U_{bc}^{\mu}$ | lattice energy of covalent part |
| $Z_{+}^{\mu}$ | cationic valence states |
| $Z_{-}^{\mu}$ | anionic valence states |
| $\alpha_{theo}$ | theoretical dielectric polarizability |
| $\alpha_{obs}$ | observed dielectric polarizability |
| $V_m$ | molar volume ($V_{cell}/Z$) |
| b' | constant ($4\pi/3$) |
| $\Delta$ | deviation |
| $R_i$ | individual bond length of oxygen octahedron |
| $\overline{R}$ | average bond length of oxygen octahedron |
| $V_{ij}$ | sum of all of the valences from a given atom i |
| $R_{ij}$ | bond valence parameter |
| $d_{ij}$ | length of a bond between atoms i and j |

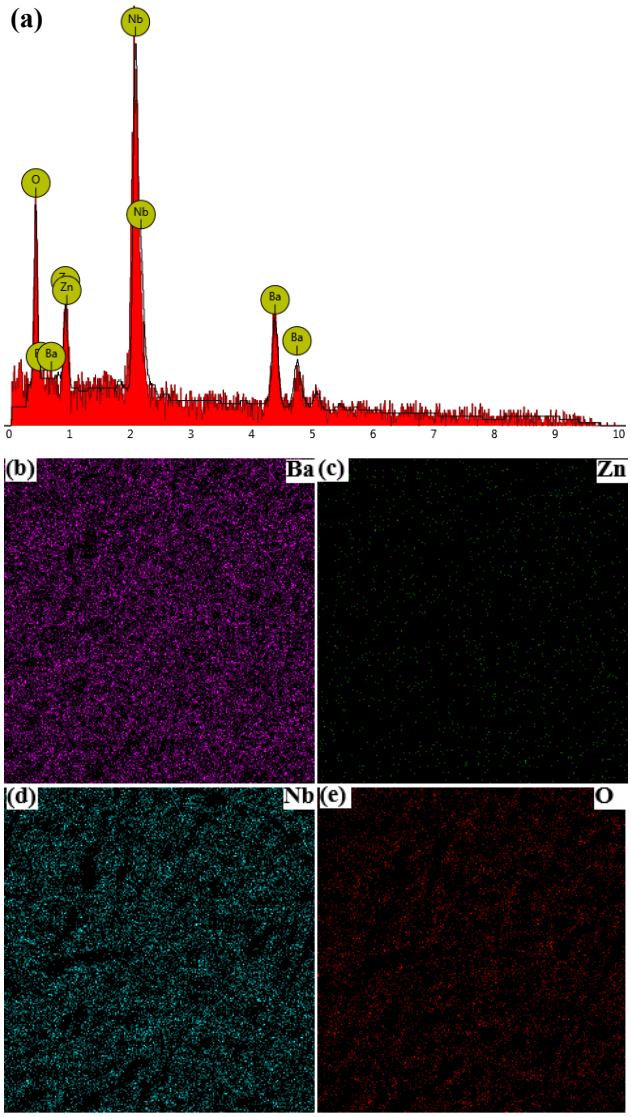


Figure S1. The EDS mapping and corresponding spectrum for the sample with $x = 0$

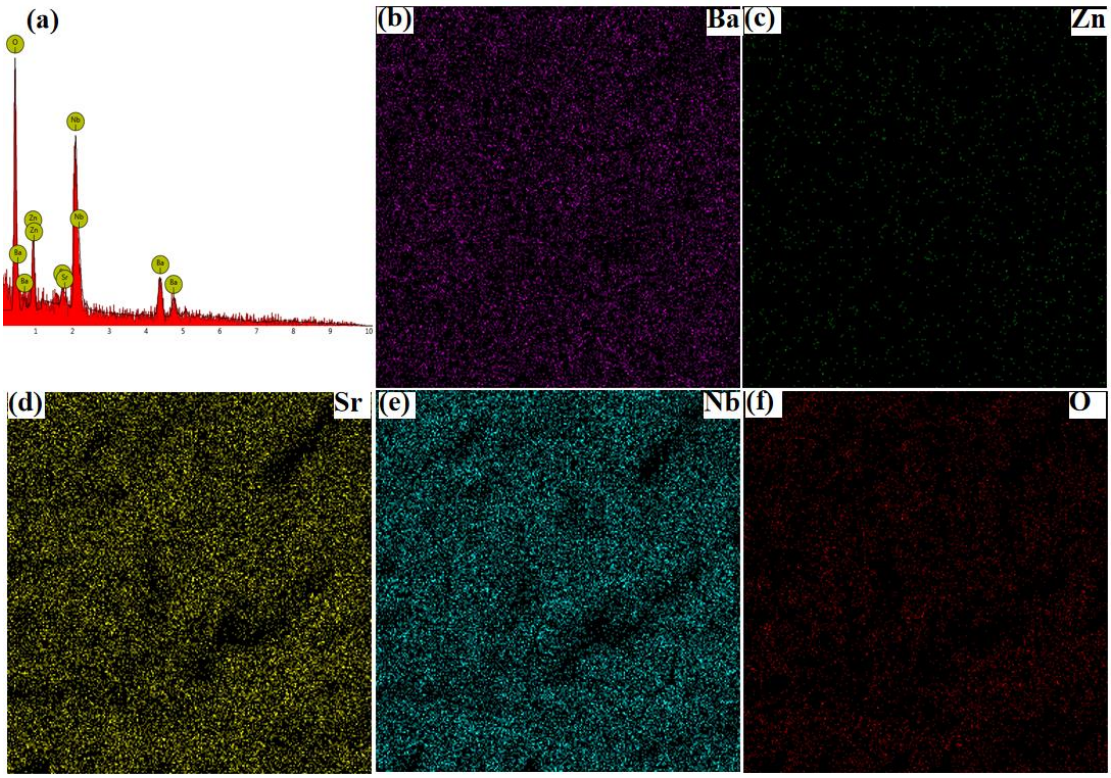


Figure S2. The EDS mapping and corresponding spectrum for the sample with $x$ = 0.1

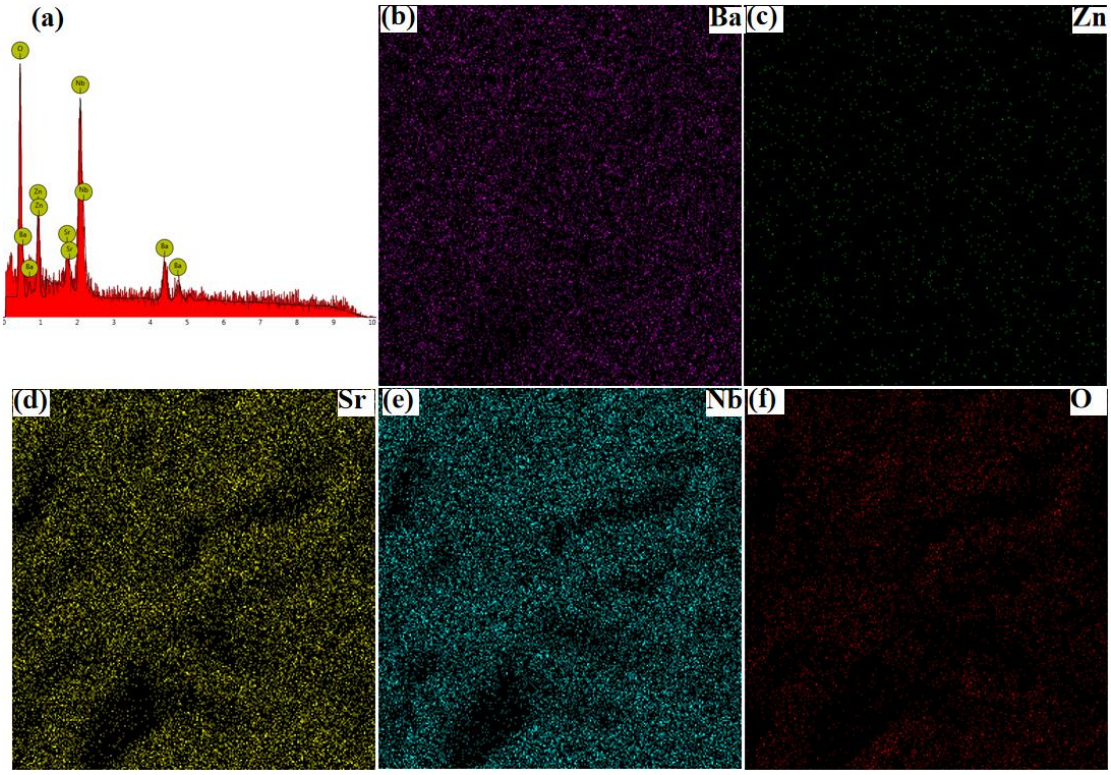


Figure S3. The EDS mapping and corresponding spectrum for the sample with $x$ = 0.2

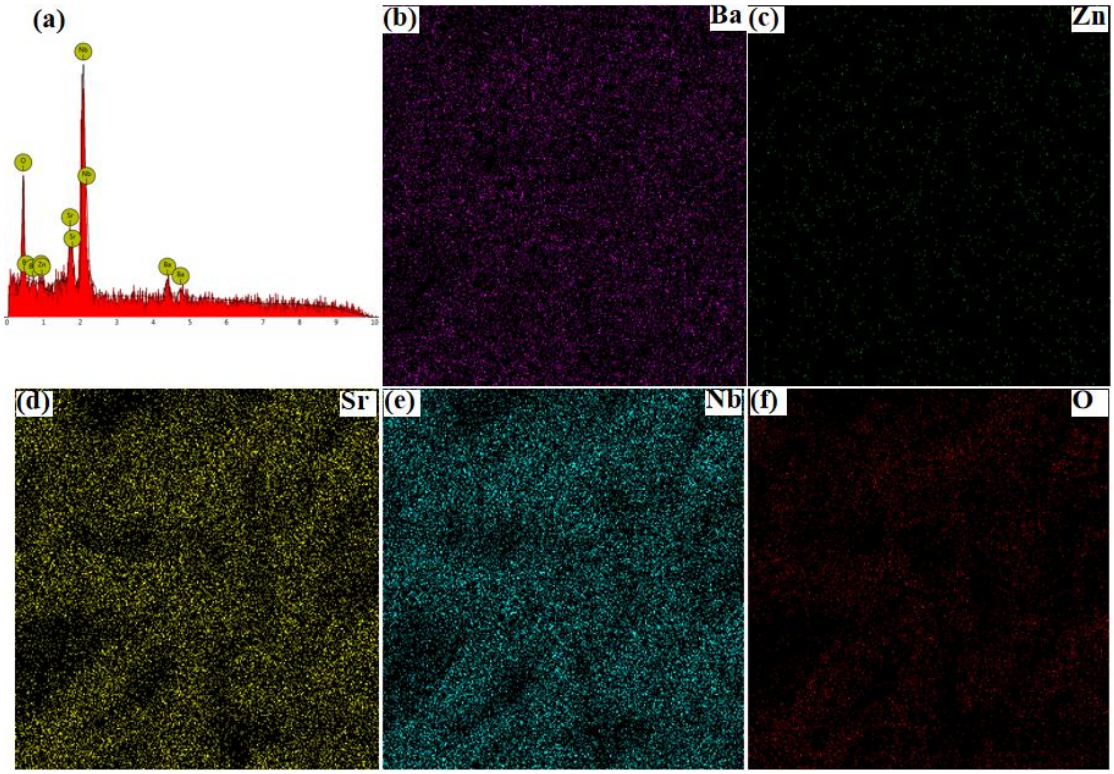


Figure S4. The EDS mapping and corresponding spectrum for the sample with $x$ = 0.4

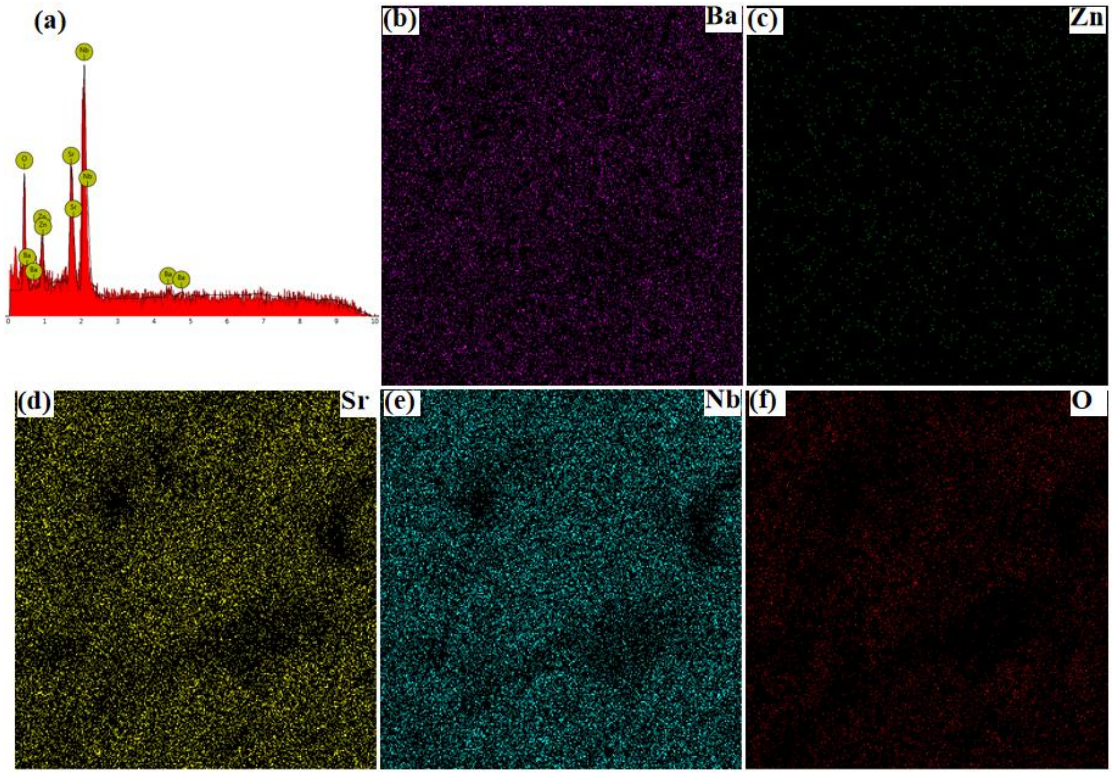


Figure S5. The EDS mapping and corresponding spectrum for the sample with $x$ = 0.6

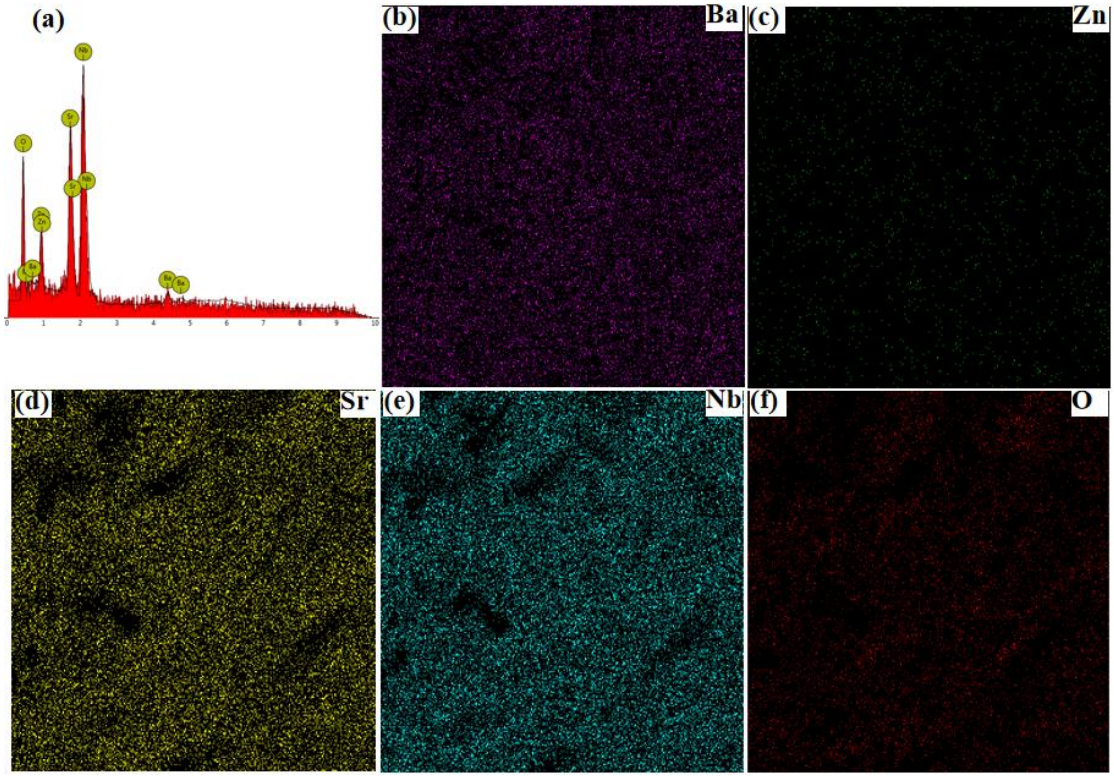


Figure S6. The EDS mapping and corresponding spectrum for the sample with $x$ = 0.8