Supplementary data

Effect of Fe-doping on structure and magnetoelectric properties of $(Ba_{0.85}Ca_{0.15})(Ti_{0.9}Zr_{0.1})O_3$ synthesized by chemical route

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Rietveld Refinement procedure

The starting atomic parameters for the tetragonal and rhombohedral phases, described in the space group (SG) *P*4*mm*, and *R*3m, respectively, were taken from Kwei *et al*. [1]. In the Rietveld refinements, were refined the following parameters: scale-factors and zero-point; the

background profile was modelled using a 10th order shifted Chebyshev polynomial function; unit cell parameters and profile coefficients − one Gaussian (G_W), an angle-independent term and two Lorentzian terms L_X and L_Y − peak correction for asymmetry, and sample displacement effects. Furthermore, atomic positions and isotropic displacement parameters (U_{iso}) were also refined; occupancies of Ba and Ca were constrained to be 0.85 and 0.15, respectively, in all the refinements, according to the stoichiometry of the synthesis. Furthermore, the same atomic positions and U_{iso} were given to these two atoms, and restrained to be identical. Similarly, following the stoichiometry of the synthesis, the occupancies of the BO_6 octahedral site were constrained to be 0.9 and 0.1 for Ti and Zr in BCTZO sample (restraining their atomic position and U_{iso} to be the same); likewise, in samples were iron was present, the occupancies were also constrained to be the same as those of the synthesis, *i.e.* 0.88, 0.02, and 0.1 for Ti, Fe, and Zr, respectively, in case of Fe-2 (with Ti, Zr, and Fe having restrained the same atomic positions and U_{iso}).

Once the bond lengths and bond angles were calculated from the listing of distances and bond angles from GSAS, they were used to obtain a 3D rendering of the tetragonal phase, by means of the VESTA software package [2]. Also, the distortion index (D) and quadratic elongation (QE) of the BO_6 octahedral site in the tetragonal phase were calculated, according to the formalisms of Baur [3], and Robinson *et al.* [4], respectively.

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