Ferroelectricity driven by 'A' and 'B' site off-centered displacements in cubic phase with *Pm*-3*m* space group

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The present work is based on the development of a new lead-free perovskite system $(Ba_{1-x}Ca_x)(Sn_{0.11}Zr_{0.05}Ti_{0.84})O_3$ (BCSZTx); $0 \leq x \leq 0.20$, exhibiting ferroelectricity in an average cubic structure [1]. The x-ray diffraction measurements have shown a simple cubic phase with Pm-3m space group for all the compositions. Despite having a centrosymmetric cubic phase, a slim hysteresis loop has been observed via PE loop measurements. Raman spectroscopic measurements have revealed the presence of local ordering in the macroscopically cubic matrix, corresponding to 'A' and 'B' sites. The cooperative behaviour of 'A' and 'B' site off-centered (local) atoms leading to microscopic polar symmetry in the macroscopically cubic matrix is held responsible for the observed ferroelectricity [2-4]. Owing to the aforementioned contrapositive behaviour, these ceramics have shown a diffuse dielectric phase transition with relaxor nature and thus exhibit a high value of dielectric constant. Eventually, we have clearly observed a decisive role of Ca^{2+} dopant at 'A' site in BCSZTx ceramic system leading to the enhancement in the ferroelectric and dielectric properties. The presence of a slim hysteresis loop along with broad and diffuse dielectric nature makes these ceramics a potential candidate for energy storage applications.

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