**Enhancement of dielectric properties and conduction mechanism in BaTi0.85Sn0.15­O3 for energy storage application**

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**Abstract**

To achieve cost effective materials with improved dielectric properties, BaTiO3 and BaTi0.85Sn0.15O3 have been prepared by solid state reaction technique introducing a two step sintering method. The structure of the samples has been investigated by X-Ray diffraction (XRD) and Raman spectra at room temperature (RT~300 K). In addition, crystallographic microstructures and grain morphology have been evaluated by transmission electron microscopy (TEM) and scanning electron microscopy (SEM) respectively. Apart this, the band structure along with density of states (DOS) are evaluated using first principle calculations for BaTiO3 and BaTi0.85Sn0.15O3. The band structure depicts bandgap of 1.80 eV and 1.82 eV for BaTiO3 and BaTi0.85Sn0.15O3 respectively. The DOS calculation displays the increase in hybridization of Ba2+ (A site) and Ti4+ (B site) cations with oxygen octahedra resulting in off-center displacement of cations in Sn doped BaTiO3 sample. A disordered cubic phase is obtained in BaTi0.85Sn0.15O3 sample sintered at 1350 ℃ resulting in the highest dielectric constant $\left(ε\_{r}^{'}\right)$ with a minimum loss $\left(tanδ\right)$. The conduction mechanism has been analyzed from the temperature and frequency dependence of resistivity $\left(ρ\right)$. The overall forecasts indicate BaTi0.85Sn0.15O3 annealed at 1350 ℃ to be a potential candidate for energy storage capacitive devices in the electronic industry.

**Keywords:** Microstructure, Density of states, Orbital Hybridization, Off-center displacement, and Dielectric constant.