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Role of Gd-doping in conduction mechanism of BFO-PZO nanocrystalline composites: Experimental and first-principles studies

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Abstract

In this paper, in the conduction behaviour of Gd-doped $0.4BiGd_xFe_{(1-x)}O_3–0.6PbZrO_3$ (BFO-PZO) with x =0.0, 0.05, 0.10, 0.15, 0.20 composites, synthesized by solid-state reaction (mixed oxide) technique, was investigated. X-ray diffraction study with Rietveld refinement method revealed the formation of rhombohedral (*R*3*c*) phase. Dielectric constant and dielectric loss studies as a function of frequency reveal dispersion due to Maxwell-Wagner type of interfacial polarization while weak ferroelectric hysteresis loops have been recorded for all the samples. Complex impedance spectroscopy technique-based impedance, electrical modulus, and electrical conductivity of the composites revealed non-Debye type relaxation mechanism. Correlated barrier hopping (CBH) mechanism dominates in all the composites exhibiting high value of density of states (10^{23} eV^{-1} cm^{-1}) which increased further after doping with Gd. It was seen that doping of Gd affects the activation energy of these composites which was complemented by performing density functional theory calculations. Bader charge calculation was performed to understand the chemical environment and charge transfer upon doping. In addition, a small change in the bandgap was found which may cause the change in activation energy.

Keywords: Doping; ceramic composites; Rietveld refinement; DFT
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