Computational and Experimental Approach to La^{3+} Doping at the B-Site of $BiFeO_3$: Insights into $BiFe_{0.90}La_{0.10}O_3$ multiferroic

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Abstract

The structure and microstructure of $BiFeO_3$ and $BiFe_{0.90}La_{0.10}O_3$ ratify a successful synthesis of the perovskite material associated with the R3c space group. The structural parameters have been obtained by the Rietveld-refinement of XRD data followed by the DFT calculation. The computed band structure manifests the existence of the up-spin indirect band gap (E_g) in both samples, along with a reduced E_g for La doping in $BiFeO_3$ (2.73 eV). Apart from this, frequency-dependent dielectric properties of $BiFeO_3$ and $BiFe_{0.90}La_{0.10}O_3$ have been extensively studied theoretically as well as experimentally between 100 Hz to 100 MHz. Interestingly, the real part of the calculated dielectric function of the BFLO sample shifts from the larger positive values to the lower negative values with elevated frequency of the applied field. Therefore, experimental dielectric permittivity has been analyzed using the mathematical models of Logistic, Lorentz, and Polynomial functions. In addition, dynamic stability is reviewed by the phonon dispersion calculation that signifies entirely positive vibrational modes of both acoustic and optical phonons for $BiFeO_3$, while $BiFe_{0.90}La_{0.10}O_3$ exhibits two negative vibrational modes of acoustic phonons at -44.95 cm^{-1}. However, the calculated Debye temperature (θ_D) for BFLO is ~1214 K at 1000 K, which is ~2 times higher than it is for $BiFeO_3$ (~608K at 1000K). Consequently, $BiFeO_3$ and $BiFe_{0.90}La_{0.10}O_3$ samples are categorized as weak ferromagnetic based on magnetic saturation (M_s) of 6.49 and 0.13 emu/g, respectively. Finally, $BiFeO_3$ has been identified as ideal for energy storage electronic devices in higher frequency regions, while $BiFe_{0.90}La_{0.10}O_3$ is more suitable for lower frequency applications.

Keywords: La-doped BFO, Electronic Band Structure, Phonon PDOS, Negative Permittivity, Energy density.