ABSTRACT

This thesis investigates the properties of transition metal doped perovskite manganites from a theoretical and experimental point of view. Experimentally, we investigate the structural, surface morphological and dielectric properties of $Pr_{1-x}Zr_xMnO_3$ for x=0 and x=0.25 using XRD, FESEM, FTIR and LCR Meter, nanoparticles were synthesized by the sol-gel auto-combustion method. The XRD pattern revealed that structure of $PrMnO_3$ compound crystallized in perovskite orthorhombic with the space group Pbnm. Crystallite size decreased by the addition of 25% Zr. The unit cell volume was found to be increased by the substitution of 25% Zr. The FTIR spectra displayed the Mn-O-Mn bonds which are related to the MnO_6 octahedron and confirm the ABO_3 perovskite characteristic vibration. SEM results showed that with the addition of 25% Zr microstructures of prepared nanoparticles exhibit a bit agglomeration of very fine particles with smooth and round edges. EDX plot confirmed the existence of all the elements. LCR meter data revealed that by the substitution of Zr in $PrMnO_3$ dielectric constant and dielectric loss factor of samples increases. Impedance analysis disclosed that total impedance of the material decreases with the doping of Zr. The theoretical study also involves the investigation of structural properties as well as electronic properties using Density Functional Theory with PBE-sol approximation and mBJ method in Wien2k-code. Then we made a comparison between experimental & theoretical data. The theoretically calculated structural properties and lattice parameters were found in good agreement with our experimental results and other theoretical results.