List of Figures

Fig. 1.1: Magnetic-field dependent resistivity in $(La,Ca)MnO_3$ (a) Resistivity versus temperature for x = 0.25 at different applied magnetic field (b) Magnetoresistance as a function of applied magnetic field for x = 0.33 [23].	2
Fig. 1.2: An ABO ₃ type of perovskite structure.	3
Fig. 1.3: Types of the Magnetoresistance.	4
Fig. 1.4: Energy levels and orbitals of Mn^{4+} and Mn^{3+} in a crystal field in octahedral symmetry and with axial elongation [49, 50].	10
Fig. 1.5: Schematic representation of Zener-Double diagram.	11
Fig. 1.6: Phase diagrams of (a) temperature versus concentration "x" and (b) temperature versus tolerance factor for $A_{0.7}A'_{0.3}MnO_3$ [53].	12
Fig. 1.7: Application of the Colossal Magnetoresistance manganite materials.	14
Fig. 1.8: Schematic diagram of the Tap recording [60].	15
Fig. 2.1: Schematic diagram of ball milling method [5].	28
Fig. 2.2: Magnetic Stirrer set-up.	29
Fig. 2.3: Schematic diagram depicting the Bragg's law of X-ray diffraction. The symbols used in the schematic have their usual meaning.	33
Fig. 2.4: Powder XRD apparatus set-up.	34
Fig. 2.5: SEM apparatus set-up.	37
Fig. 2.6: Schematic diagram depicting the working of a Scanning Electron Microscope.	38
Fig. 2.7: FE-SEM used for characterization of the samples.	40
Fig. 2.8: Schematic diagram representing working of TEM.	42

_____ viii)

Fig. 2.9: Schematic representation of EDAX.	43
Fig. 2.10: Schematic diagram depicting the working of Raman Spectra.	45
Fig. 2.11: Instrument set-up of Raman Spectroscopy.	45
Fig. 2.12: Schematic diagram depicting the working of VSM.	46
Fig. 2.13: PPMS Quantum Design set-up.	47
Fig. 2.14: XPS apparatus set-up.	48
Fig. 2.15: Set-up of Differential Scanning Calorimeter.	49
Fig. 2.16: Heat flux DSC cell cross section.	50
Fig. 2.17: Power Compensation DSC Cell Design.	51
Fig. 2.18: (a) Thermogravimetric Analyzer (TGA) and (b) Instrumental set-up of the TGA Analyzer.	53
Fig. 2.19: (a) The Differential Thermal Analyzer and (b) Instrumental set-up of DTA.	55
Fig. 3.1: Basic equations of the Kohn-Sham theory [5].	66
Fig. 3.2: Schematic representation of the pseudopotential method [5].	71
Fig. 4.1: Phase diagram of La _{1-x} Sr _x MnO ₃ manganite system [18].	77
Fig. 4.2: Crystal structure of ABO ₃ with MnO ₆ octahedral [19].	77
Fig. 4.3: Synthesis chart of Fe doped LSMO using ball milling method.	80
Fig. 4.4: The X-ray diffraction pattern of Fe doped LSMO manganite system.	82
Fig. 4.5: Rietveld refinement analysis of Fe doped LSMO with different doping concentration (0.15 to 0.35) at various calcination temperatures (800°C and 900°C).	85
Fig. 4.6: Rietveld refinement analysis of Fe doped LSMO with different doping concentration (0.15 to 0.35) at various calcination temperatures (1000°C and 1100°C).	86

_____ (ix)_____

Fig. 4.7: FE-SEM micrograph of the Fe doped LSMO samples prepared at different 90 calcination temperatures. The inset of figures displays concentration of Fe and calcination temperatures.

Fig. 4.8: FE-SEM micrograph of the Fe doped LSMO samples prepared at different 91 calcinations temperatures. The inset of figures displays concentration of Fe and calcination temperatures.

Fig. 4.9: TEM of Fe doped LSMO for x=0.15 at 800°C calcination temperature. 92

Fig. 4.10: EDAX spectra of LSMFO samples for different doping concentrations at various 93 temperatures. The inset of figures displays concentration of Fe and calcination temperatures.

Fig. 4.11: EDAX spectra of Fe doped LSMO samples for different doping concentrations 94 at various temperatures. The inset of figures displays concentration of Fe and calcination temperature.

Fig. 4.12: Raman spectra of the $La_{0.67}Sr_{0.33}Mn_{1-x}Fe_xO_3$ (x=0.15, 0.25 and 0.35) manganite 97 system at room temperature (300K).

Fig. 4.13: Raman spectra of the La_{0.67}Sr_{0.33}Mn_{1-x}Fe_xO₃ (x=0.15, 0.25 and 0.35) manganite 100 system at low temperature (80K).

Fig. 4.14: Magnetic field dependence of magnetization (M-H curve) at LT (3K) and RT 101 (300K) of LSMFO manganite materials.

Fig. 4.15: Temperature dependences of ZFC and FC magnetization of x = 0.15, 0.25 at 100 102 Oe.

Fig. 4.16: Formation energy of x = 0.15 at 800°C to 1100°C and x = 0.25 and 0.35 at 800°C. 106

Fig. 4.17: Lattice parameter optimization and convergence of energy using DFT 109 calculation.

х

Fig. 4.18: Electronic band structure and total density states of Fe doped LSMO samples (a) 110 0.15-800°C (b) 0.25-800°C (c) 0.35-800°C (d) 0.15-900°C (e) 0.15-1000°C (f) 0.15-1100°C.

Fig. 5.1: Application chart of the Sol-Gel method [5].

Fig. 5.2: Processing of nanoscale particle by sol-gel method [6].

Fig. 5.3: Flow chart of preparation of Fe doped LaSrMnO₃ by sol–gel technique. 121

Fig. 5.4: The X-ray diffraction pattern of Fe doped LaSrMnO₃ manganite system a) 124 x=0.15-800°C (b) 0.25-800°C (c) 0.35-800°C (d) 0.15-1000°C (e) 0.25-1000°C (f) 0.35-1000°C.

Fig. 5.5: Rietveld refinement X-ray diffraction pattern of Fe doped LaSrMnO₃ (a) x=0.15- 125 800°C (b) 0.25-800°C (c) 0.35-800°C (d) 0.15-1000°C (e) 0.25-1000°C (f) 0.35-1000°C.

Fig. 5.6: FE-SEM micrograph of the prepared LSMFO samples with different doping 129 composition at various calciantion temperatures (a) 0.15-800°C (b) 0.25-800°C (c) 0.35-800°C (d) 0.15-1000°C (e) 0.25-1000°C (f) 0.35-1000°C.

Fig. 5.7: The TEM analysis of LaSrMnFeO₃ prepared samples (a) 0.15-800°C (b) 0.25- 130 800°C (c) 0.35-800°C.

Fig. 5.8: EDAX analysis of prepared LSMFO samples (a) 0.15-800°C (b) 0.25-800°C (c) 132 0.35-800°C.

Fig. 5.9: EDAX analysis of prepared LSMFO samples (d) 0.15-1000°C (e) 0.25-1000°C (f) 133 0.35-1000°C.

Fig. 5.10: Raman spectra of the $La_{0.67}Sr_{0.33}Mn_{1-x}Fe_xO_3$ (x=0.15, 0.25 and 0.35) manganite 136 system at room temperature (300K).

Fig. 5.11: Lattice parameter optimization and convergence of energy using density 140 functional theory.

xi

Fig. 5.12: Electronic band structure and total density states of Fe doped LSMO samples (a) 141 0.15-800°C (b) 0.25-800°C (c) 0.35-800°C.

Fig. 5.13: Formation energy of x = 0.15, 0.25 and 0.35 at 800°C. 143

Fig. 6.1: Lattice parameters and unit cell volume of the different concentration of Fe doped 152 LSMO samples.