Preface

The discovery of manganite compounds which possess perovskite type structure have exciting properties from both the basic research as well as from technological point of view. Furthermore, the divalent alkali metal doped rare earth manganites have attracted the attention of researchers in recent time due to their novel properties such as insulator to metal transition and large magnetoresistance (MR). To understand the properties of materials existing from earlier times or the newly developed, useful for the device technology both theoretical and experimental methods have been intensively used. As most of the technology pursued using this material requires proper film growth, extensive efforts are made on material synthesis, structural and physical characterization and finally the device fabrication. Novel properties exhibited by manganites depend on tolerance factor, A and B site substitutions, grain boundary and external or internal pressure. The mixed valence perovskite manganites $R_{1-x}A_xMnO_3$ possessing CMR property are strongly correlated electron systems with strong interplays among the charge, spin, orbital, and lattice degrees of freedom that leads to complex structural, electronic, phonon and magnetic phase diagrams. In the family of perovskite materials some of the commonly observed features are colossal magnetoresistance, ferroelectricity, superconductivity, charge ordering, spin dependent transport, high thermo power and the interplay of structural and magnetic properties. The physics involved in manganites include double exchange (DE) mechanism, Jahn-Teller distortion, size variance and fascinating metallic behavior making them one of the prominent topics in the field of condensed matter physics. The CMR further influences the metal-to-insulator (MIT) transition, the nature of electronic transport, charge-ordering, magnetism etc.

The colossal magnetoresistance materials give fascinating effect such as the transition from a paramagnetic insulator at high temperatures to a ferromagnetic metal at low temperature due to Zener double exchange. Zener proposed a transport mechanism between Mn^{3+} and Mn^{4+} ions, where one e- is transferred from Mn ions to neighbouring Mn ions. Furthermore, the Jahn-Teller distortion is a parameter that largely influences the magnetic properties of manganites.

The solid sample perovskites can be synthesized in variety of shapes and sizes depending upon their single crystals, amorphous solids, thin films, polycrystalline powder etc. In the current research work, we used planetary ball milling and sol-gel methods to obtain the nano sized manganites. These samples have been characterized for its different behavior by various experimental techniques such as XRD, FE-SEM, Raman spectroscopy, EDAX and magnetic properties (VSM). FE-SEM images are taken at Sprint testing solution, Mumbai. The facility of Raman spectroscopy present at UGC-DAE CSR, Indore is used to study the vibrational properties at room as well as low temperature while magnetic measurements under field cooled and zero fields cooled at UGC-DAE CSR, Mumbai.

The interesting part of the present work is to understand the formation and properties at atomistic level by density functional theory (DFT) calculation of the experimentally obtained LSMFO samples and find most favorable condition and method of preparation of the class of materials. We have performed structural, electronic, magnetic and phonon properties of some selected Fe doped $La_{0.67}Sr_{0.33}MnO_3$ samples using first principle calculation based on Density functional theory (DFT) using VASP simulation package. Based on the comparative study of the results obtained from various characterization tools, the process parameters as well as synthesis method are identified for the doped manganites.