Density Functional Theory Study of Colossal Magnetoresistance Material $La_{0.67}Sr_{0.33}Mn_{1-x}Fe_xO_3$ Prepared Using Two Different Routes

Summary

Thesis

Submitted to

The M. S. University of Baroda, Vadodara, India

For the Degree of

Doctor of Philosophy

in Science

in the subject of Physics

By

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2019

Summary

The mixed-valence manganese oxide perovskites also known as manganites are still considered as the modern materials and receive tremendous attention not only from the field of basic science but also from the current cutting-edge technology. Out of many interesting properties of manganites, the most fascinating property is the Colossal Magnetoresistance (CMR) which is currently being explored by a sizable fraction of the condensed matter community and its popularity is reaching almost the same level that of the one-time popular high temperature superconducting cuprates. The CMR is an intrinsic property of manganese based perovskite oxides that displays changes in resistance with significant orders of magnitude under the influence of an external magnetic field. The perovskite manganites 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 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 advent of excellent and upto date technology, various prototypes are manufactured using various synthesis processes. The manganites also have potential applications in the solid electrolytes, catalysts, sensors, solid state memories and magnetic microwave devices. Some of the other important applications of manganites are magnetic refrigeration, advanced hard disk read heads, recording devices, bottom electrode in the fabrication of ferroelectric memories. The CMR effect further influences the metal-to-insulator (MIT) transition, the nature of electronic transport, charge-ordering, magnetism etc. The MIT coincides with the ferromagnetic to paramagnetic transition. In mixed valent manganites, the Zener Double Exchange (ZDE) and Jahn-Teller effect is very important to study the CMR behavior and conduction process between two Mn ions. This mechanism gives

the concept of simultaneous transfer of an electron from the Mn^{3+} to the oxygen and from the oxygen to the neighbouring Mn^{4+}. Figure shows the temperature and magnetic field variations of resistivity for a $La_{0.75}Ca_{0.25}MnO_3$ and magnetoresistance percentage (MR%) as a function of applied magnetic field.

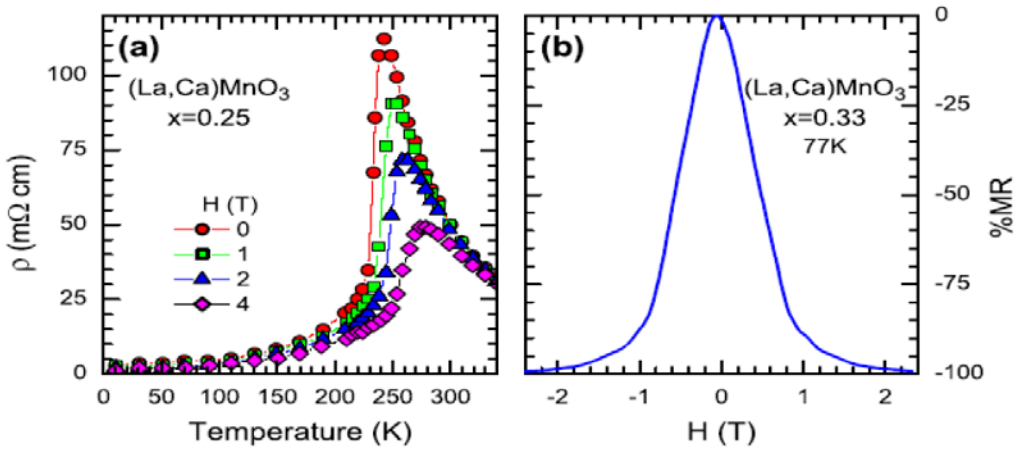

Fig. 1: Magnetic-field dependent resistivity in $(La,Ca)MnO_3$ (a) Resistivity versus temperature for x = 0.25 at different applied magnetic field (b) Magnetoresistance as a function of applied magnetic field for x = 0.33.

The present work is a blend of investigations of various physical properties aimed both at the understanding of the physics involved and the analysis of an important class of compounds called as manganites revived great deal of attention from application point of view. During the present work, we have synthesized the trivalent earth element Fe^{3+} doped manganites using the two important methods namely the planetary ball milling and sol-gel routes for wide range of temperature and doping concentration. The present work is mainly aimed towards understanding and detecting the best synthesis route for fabricating the nanoscale polycrystalline manganite systems out of the selected two methods; the ball milling and sol-gel routes in terms of time duration, low reaction time, annealing temperature and cost-effectiveness with the help of state-of-the density functional theory (DFT) based first principles calculations. The manganite system

investigated during the present work is $La_{0.67}Sr_{0.33}Mn_{1-x}Fe_xO_3$ (x=0.15, 0.25 and 0.35). The Fe doped $La_{0.67}Sr_{0.33}MnO_3$ (LSMO) manganite systems have revealed several interesting results on the structural, electronic, magnetic and vibrational properties. Looking to the importance of structure – property relation a systematic study and analysis of the bond length and bond angle dependent structural, magnetic and vibrational properties using XRD is performed. In addition, the effect of grain size and grain morphology on various properties of nanostructured $La_{0.67}Sr_{0.33}Mn_{1-x}Fe_xO_3$ (x=0.15, 0.25 and 0.35) manganites synthesized using both routes have been carried out. Furthermore, interesting part of the thesis work is to the understand the manganite properties with the clear insight into the responsible mechanism achieved by performing the atomistic high-throughput calculations under the framework of the *state-of-the-art* density functional theory. The good agreement between the experimentally synthesized and characterized manganite systems with the first-principles based DFT results once again prove the reliability of DFT based *ab initio* calculations and also significantly contributes to the theoretical database by adding up the missing details on the considered manganites. The DFT calculations clearly able to bring out the possibility of formation of the manganite through formation energy calculation. The calculated structural, electronic and vibrational properties help in understanding the reason of preferred methods of synthesis for manganites. The specific motivation of the present work is as follows:

1. Synthesis of manganite samples using two synthesis routes: Ball milling and Sol-gel.
2. Effect of doping of Fe at Mn site on properties of manganites.
3. Using DFT studies identify the best route out of two above mentioned synthesis routes of manganites. For this structure property relation together with the formation energy analysis analyzed using their own experimental parameter.

Summary

The present thesis comprises of the research findings and briefly explained in the following chapters.

In **chapter 1**, a brief introduction of the manganite materials and colossal magnetoresisatnce (CMR) material includes the basic concepts, important applications and various factors affecting CMR materials. It gives a brief introduction to its classification of magnetoresistance. Moreover, a brief explanation of the manganite systems chosen for this study is also provided.

Chapter 2 deals with the various experimental tools and methods to discuss the synthesis and characterization techniques to determine the properties of the Fe doped LSMO such as structural, elemental, magnetic, vibrational etc. This chapter also discusses the details about the methodology for preparing the polycrystalline doped manganite compounds using sol-gel and ball milling methods. Various characterization methods to understand the structural relation with the properties of LSMO manganites have been discussed. The working and operation of the X-ray diffraction for structural analysis, PPMS Quantum Design magnetometer to study the magnetic properties, Field emission electron microscope (FE-SEM) to study the surface morphology and Raman spectroscopy for vibrational properties are also presented.

Chapter 3 presents the brief description of the density functional theory starting with the history and need for its development. Original construction of Hohenberg and Kohn is discussed. The chapter also introduces a methodology to treat the calculation of ground state properties of the system based on Kohn-Sham formulation of DFT, which is based on the approximations for the exchange energy term. A brief layout of Vienna Ab-initio Simulation Package (VASP) utilized for computing the proposed properties of the systems is also presented.

Fourth chapter deals with the real research problem and efforts to resolve some issues in the related field. The structural, surface morphological, vibrational and magnetic properties of

$La_{0.67}Sr_{0.33}Mn_{1-x}FexO_3$ (x=0.15, 0.25, 0.35) synthesized using ball milling method are presented. The comparison of the results with the available outcome of the material is analyzed on the basis of different concentrations and temperature employed on the samples. The density functional theory calculations for the formation energy, electronic and vibrational properties are discussed and correlated with the experimental results.

In **chapter 5**, the structural, surface morphological, vibrational and magnetic properties of $La_{0.67}Sr_{0.33}Mn_{1-x}Fe_xO_3$ (x=0.15, 0.25, 0.35) synthesized using sol-gel method is discussed. The comparison of results with different composition as well as temperature employed to the samples is thoroughly discussed. Thus, here we present the results of experimental study to understand the relationship of small amount of Fe doping with the various properties. We make the attempt to compare the results of samples obtained from planetary ball milling and sol- gel route together with the DFT calculations to find the simple, easiest way to synthesize the polycrystalline CMR materials.

Chapter 6 presents the conclusion based on the comparative study of manganite samples $La_{0.67}Sr_{0.33}Mn_{1-x}Fe_xO_3$ (LSMFO) prepared using two experimental techniques ball milling and sol-gel for different concentrations of iron and calcination temperatures. We have used density functional theory based high throughput calculations to draw a significant conclusion to understand the formation of LSMFO prepared using two different methods. We have considered same concentration of iron doping and calcination temperatures for understanding the technique dependent synthesis and relevant properties. The structure property relation obtained through different characterization techniques has been analyzed and understood at atomic level. The electronic band structures and phonon modes obtained using density functional theory have been used to interpret the valence band spectra, magnetization and Raman spectra obtained from

various corresponding experimental techniques. An analysis in the conclusion chapter is put forward to justify the differences in the properties of manganite samples prepared using mentioned techniques.

The specific conclusions based on the present study are listed below:

1) The Fe doped LSMO samples are prepared using two methods ball milling and sol-gel by varying Fe concentration and calcination temperature.
2) Samples are characterized using XRD, FE-SEM, EDAX, VSM and Raman spectroscopy.
3) The spin-polarized density functional theory is performed to corroborate the experimental findings and to understand the formation of these samples at atomistic level.
4) The XRD pattern shows that the LSMFO samples synthesized using ball-milling and sol-gel methods exhibit the rhombohedral (R-3c) structure.
5) The Fe concentration modifies the frequencies of A_{1g} and E_g Raman modes. However, the changes are more significant in the case of sol-gel prepared samples.
6) The reduction in the intensity of the peaks and increase in broadening with increase in Fe concentration and calcination temperature is observed which arises from the change in bond angle and bond length of Mn-O-Mn causing the MnO_6 octahedron distortion.
7) E_g and A_{1g} modes which soften with the concentration hardens with calcination temperature.
8) The spin-polarized calculations show metallic behavior without any intimation of antiferromagnetism for these systems.
9) The formation energy calculations indicate that the combination of lower concentration of Fe and higher calcination temperature may be suitable condition for the formation of Fe doped LSMO samples. Based on formation energy, the ball mill method shows better

thermodynamic stability of the samples. This may be due to the fact that the ball milling method involves atomic level mixing while forming a solid compound in which metals of the final product are present in proper stoichiometry.

List of Publications

PUBLICATIONS INCLUDED IN THE THESIS

- "Temperature effect on Raman Spectroscopic Study of the Fe doped $La_{0.67}Sr_{0.33}MnO_3$Prepared Using Ball Milling Method",
  Nidhi M Astik, Prafulla K. Jha and Vasant Sathe
  Physics of the Solid State, **61**, 1-8 (2019).
- "Influence of Fe Substitution on Structure and Raman Spectra of $La_{0.67}Sr_{0.33}MnO_3$: Experimental and density functional studies,
  Nidhi M Astik, H. Soni, P. K. Jha and Vasant Sathe
  Physica B: Condensed Matter, **541**, 103-110 (2018).
- "Structural, Morphological and Thermal Properties of Ball Milled Fe Doped Nanoscale $La_{0.67}Sr_{0.33}MnO_3$",
  Nidhi Astik, Prafulla K. Jha and Arun Pratap
  J. of Electronic Materials **47** (3), 1937-1943 (2018).
- "Synthesis and Characteristic of Nanocrystalline $La_{0.7}Sr_{0.3}MnO_3$Manganites by Solid State Reaction Route"
  Nidhi Astik, Swapnilkumar Patil, Parag Bhargava and Prafulla K Jha
  AIP Conference Proceedings **1728**, 020467 (2016).

Papers Presented In International / National Conferences and School Program

- Poster Presentation on Experimental and Density Functional Studies on Vibrational Properties of $La_{0.67}Sr_{0.33}Mn_{1-x}Fe_xO_3$ (x=0.15, 0.25 and 0.35), **Nidhi Astik,** Prafulla K. Jha and Vasant Sathe " National Conference on Recent Trends in Material Science (RTMS-2018)", at M. S. University of Baroda, Vadodara (24^{th} -25^{th} March, 2018)
- Poster Presentation on Structural and Vibrational Properties of $La_{0.67}Sr_{0.33}Mn_{1-x}Fe_xO_3$ (x=0.25) Manganite System: Experimental and Density Functional Studies, **Nidhi Astik**

and Prafulla K. Jha "International Winter School-2018", "Frontiers in Materials Science" at JNCASR Bangalore (3^{rd} - 7^{th} December, 2018).

- ✍ Poster Presentation on Synthesis and Structural Properties of Fe Doped $La_{0.67}Sr_{0.33}MnO_3$ Composite System, **Nidhi Astik** and Prafulla K. Jha "International Crystallographic Computing school", at IISc Bangalore (15^{th} -20^{th} August, 2017).
- ✍ Poster Presentation on Influence of Fe Substitution on Raman Spectra of $La_{0.67}Sr_{0.33}MnO_3$, **Nidhi Astik** and Prafulla K. Jha "International conference on Perspectives in Vibrational Spectroscopy" at University of Lucknow, Lucknow (5^{th} -8^{th} Nov. 2016).
- ☞ Poster Presentation on Effect of Fe doping on a thermal properties of $La_{0.67}Sr_{0.33}MnO_3$ Manganite'' **Nidhi Astik**, Prafulla K. Jha and Arun Pratap **"**National conference on Recent Trends in Science of Materials", 2015 (NCSM-2K15)'' at M. S. University of Baroda, Vadodara (28-30 Dec. 2015).
- ✍ Poster Presentation on Investigation of Structural and Morphological Properties of Fe doped at Mn site in$La_{0.67}Sr_{0.33}MnO_3$ Manganite System'' **Nidhi Astik** and Prafulla K. Jha "National conference on Recent Materials Characterization (NCMC-16)'' at M. S. University of Baroda, Vadodara (18-19 March 2016).
- ✍ Poster Presentation on "Synthesis and Characteristic of Nanocrystalline $La_{0.7}Sr_{0.3}MnO_3$Manganites by Solid State Reaction Route" **Nidhi Astik**, Swapnilkumar Patil, Parag Bhargava and Prafulla K Jha "International Conference on Condensed Matter Physics and Applied Physics (ICC-15)" at Govt. Engg. College, Bikaner, Rajasthan (30-31 October 2015).

December 26, 2018 20:02 1st draft
Физика твердого тела, 2019, том 61, вып. 4

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Temperature effect on Raman Spectroscopic Study of the Fe doped $La_{0.67}Sr_{0.33}MnO_3$ Prepared Using Ball Milling Method

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(Recevied June 21, 2018;
Revised October 15, 2018;
Acćepted October 30, 2018)

Polycrystalline samples of $La_{0.67}Sr_{0.33}Mn_{0.65}Fe_{0.35}O_3$ (LSMFO) were synthesized using the standard ball mill method with different calcination temperatures ranging from 800°C to 1100°C for 7 h. The phase purity of these samples was confirmed using X-ray diffraction (XRD) patterns. All samples were found to have rhombohedral crystal structure with $R\bar{3}c$ space group. The lattice parameters, cell volume, bond angle and bond length have been obtained using the Rietveld refined by FullProf software. The average crystallite size calculated using the Debye-Scherrer formula was to be found between 27 and 60 nm. Surface morphology of the prepared samples has been examined using a scanning electron microscope (SEM). SEM images show the formation of well-arranged grain sizes distributed from 240 to 400 nm, much larger than one estimated using the Scherrer formula. All tiny particles are highly agglomerated with the increasing temperature and porosity decrease with increasing temperature. An analysis of the frequencies and peak broadening of Raman modes as a function of temperature clearly shows the significant temperature effect on the A_{1g} and E_g modes of LSMFO. The shifts and broadening of the A_{1g} and E_g modes are discussed in light of the oxygen sublattice distortion. Our study shows the reduction in distortion with increasing the calcination temperature, which suggests a decrease in the JT effect.

DOI: 10.21883/0000000000

1. Introduction

For many years, extensive studies have been performed to understand the nature of the bulk as well as thin film samples of perovskite manganese oxides of the form $R_{1-x}A_xMnO_3$ (where R is a rare earth ion and A is a divalent alkali earth ion) particularly after the discovery of colossal magnetoresistance (CMR) in them [1–8]. In this regard, $La_{1-x}Sr_xMnO_3$ (LSMO) has attracted most attention due to its excellent catalytic, thermal, electrical and magnetic properties useful for potential applications in magnetic sensors, reading heads for magnetic memories and as a cathode in solid oxide fuel cells [9–13]. Furthermore, these manganites exhibit puzzling properties arising from the coupling of spin, lattice, charge and structural degrees of freedom and are governed by several factors such as method of preparation, percentage and size of divalent ions. Several methods such as the coprecipitation or precipitation, sol–gel, ball milling and the combustion conventional ceramic are often used to prepare these materials. The mechanical ball milling method is an efficient technique to synthesize many unique materials such as nanostructured crystalline, amorphous alloys and nanoparticles from powder oxides due to high flexibility, simple control of process parameters and ability to produce a wide range of materials [14]. A number of consideration such as double exchange (DE) and superexchange (SE) interactions, Jahn–Teller distortions with electron-phonon interactions and polaron formation, phase separation and site disorder have been used to explain the CMR, one of the most exciting phenomena of manganites [15]. However, a disagreement on the theoretical explanation of CMR behaviour suggests inclusion of something beyond these due to involved complexities [16].

It is established that the properties of manganites are highly influenced by the degree of compositional flexibility such as A-site and B-site doping [17–20]. The A (rare-earth) site doping is the doping of another ion A' with a valence different from A is partially substituted for A, while B (manganese) site doping is the partial substitution of B ions by another ion B' of different valence. The electronic structure of manganitesshows a core spin of 3/2 for Mn ions and an extra e_g electron with its spin aligned to the core electron due to strong exchangefor a dopant dependent fraction $(1-x)$ [21]. These electrons may coherently hop of such electrons to the adjacent sites by mens of polarization conserving process. One of the two most successful theories to explain the CMR and related properties is the double exchange theory which considers the magnetic coupling between Mn^{3+} and Mn^{4+} ions [22]. The amount of the pairs of Mn^{3+} and Mn^{4+} depends on the doping level of the perovskite or its oxygen stoichiometry. However, this doping results in a distortion of the perovskite structure with direct influence on the Mn–O bond length and Mn^{3+}–O–Mn^{4+} bond angle [22]. It is noteworthy that the ferromagnetic (FM) coupling and

Physica B: Condensed Matter
Volume 541, 15 July 2018, Pages 103-110

Influence of Fe substitution on structure and Raman spectra of $La_{0.67}Sr_{0.33}MnO_3$: Experimental and density functional studies

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https://doi.org/10.1016/j.physb.2018.04.038

Highlights

- The Fe Doped $La_{0.67}Sr_{0.3}MnO_3$ is synthesized using ball mill method.
- The structural and morphological characterization is done using XRD, EDAX and SEM.
- Effect of Fe doping on Vibrational spectra is analyzed using Raman Spectroscopy.
- To support the experimental results density functional theory calculations are also performed.

Abstract

We present experimental and theoretical studies on the effect of Fe doping at Mn site, on the structural, morphological, electronic and vibrational properties of $La_{0.67}Sr_{0.3}MnO_3$ nanoparticle. The samples of $La_{0.67}Sr_{0.3}MnO_3$ and $La_{0.67}Sr_{0.33}Mn_{1-x}Fe_xO_3$ (x = 0.15, 0.25 and 0.35) have been prepared by ball milling route. The phase purity of these samples has been confirmed using X-ray diffraction, while compositional analysis is done using EDAX. The morphological analysis done using scanning microscope indicates the agglomeration. The vibrational analysis which is done using Raman scattering and density functional theory (DFT) calculations show a substantial shift in A_{1g} and E_g modes with Fe doping. The E_g modes become broader with Fe doping. The UV–visible spectra were measured in the energy range of 1–5 eV and compared with DFT results. The spin polarized density functional calculations show an increase in density of states at Fermi level due to MnO_6octahedra modification and significant magnetism on Fe doping. The total magnetic moment is found

Journal of ELECTRONIC MATERIALS, Vol. 47, No. 3, 2018
https://doi.org/10.1007/s11664-017-5994-7

Structural, Morphological, Differential Scanning Calorimetric and Thermogravimetric Studies of Ball Milled Fe Doped Nanoscale $La_{0.67}Sr_{0.33}MnO_3$ Manganite

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The ball milling route has been used to produce the $La_{0.67}Sr_{0.33}Mn_{0.85}Fe_{0.15}O_3$ (LSMFO) nanocrystalline sample from oxide precursors. The sample was characterized using x-ray diffraction (XRD), a scanning electron microscope (SEM), energy dispersive x-ray spectroscopy (EDAX), differential scanning calorimetry (DSC) and thermogravimetric (TGA) measurements. The x-ray diffraction confirms the phase purity of sample and shows that the sample crystallizes in the rhombohedral perovskite structure with a R-3c space group. The scanning electron micrograph shows the presence of well-faceted crystallites of LSMFO. The EDAX spectrum demonstrates the molar ratio of different elements of nanocrystalline LSMFO. Furthermore, the crystallite size using the Debye–Scherrer formula and William-Hall analysis has been found as 24 nm and 29 nm, respectively. Our results support the idea that a good quality nanocrystalline LSMFO sample can be obtained using the ball milling route. We also discuss the DSC and TGA curves and analyse the results in terms of phase transition, calcination temperature and activation barrier energies.

Key words: Manganites, ball-milling, calcinations, XRD, SEM-EDAX, DSC, TGA

INTRODUCTION

There has been continuing interest in the study of doped rare-earth manganite perovskites with general formula $Ln_{1-x}A_xMnO_3$, (where Ln = La, Nd, Sm… rare earth ions and A = Ba, Sr, Pb and Ca; divalent alkaline earth ions) due to their peculiar physical properties arising from the strong coupling between spin, charge, orbit and lattice degrees of freedom and observed colossal magnetoresistance (MR) effect in them.[1–9] These doped manganites exist in a verity of phases of perovskite structure and have their potential applications in transducer and sensor, catalysis, permanent magnets, high temperature superconducting, novel electronic materials and solid oxide fuel cells.[10–17] It is a widely recognized fact that the pairs of Mn^{3+} and Mn^{4+} ions play a major role in double exchange (DE) interaction for the ferromagnetic and metallic properties in these manganese oxides. The DE effect arises due to the exchange of electrons from neighbouring Mn^{3+} to Mn^{4+} ions through oxygen when their core spins are parallel and hopping is not favoured for anti-parallel spins.[18] Furthermore, an additional mechanism, Jahn–Teller distortion (JT), has also been found responsible for the transport properties in these compounds. The JT effect causes further degeneracy of the e_g orbital of the Mn^{3+} in MnO_6 octahedral and results in electrical transport via hopping.[19–21] There are several methods, such as the solid state reaction, sol–gel and ball milling for the preparation of homogeneous samples of these materials required in various industrial applications.[22–24] It is found that the substitution of

(Received July 8, 2017; accepted November 22, 2017; published online December 5, 2017)

Synthesis and Characteristic of Nanocrystalline $La_{0.7}Sr_{0.3}MnO_3$ Manganites by Solid State Reaction Route

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Abstract. Nanocrystalline stoichiometric $La_{0.7}Sr_{0.3}MnO_3$ (x=0.3) manganites have been synthesized through solid-state reaction by ball milling mechanical method at two different sintering temperatures 1250°C and 1350°C. The synthesized samples were characterized using X-ray diffraction (XRD) and found to have rhombohedral crystal structure (R-3c). The calcined samples exhibited a pure single phase perovskite, had a crystallite size of about 47-51 nm. The morphology of the prepared nanocrystalline manganites were recorded by the field emission gun-scanning electron microscope (FEG-SEM) and EDAX.

INTRODUCTION

The perovskite manganites of type $R_{1-X}A_XMnO_3$ where R is La^{3+}, Pr^{3+}, Nd^{3+} and A is Ca^{2+}, Sr^{2+}; received great deal of attention in last decades due to their unusual magnetic and transport properties, especially the colossal magnetoresistance (CMR) [1-3]. The strontium doped perovskite – type manganites $La_{1-X}Sr_XMnO_3$ (LSMO) have attracted remarkable interest due to their various potential applications such as magnetic sensors, reading heads for magnetic memories and as a cathode in solid oxide fuel cells due to its excellent catalytic, thermal, electrical, phonon and magnetic properties [4-8]. The properties of these materials are governed by several factors such as method of preparation, doping percentage and size of divalent ions [9-11]. In addition, these manganites have attracted much attention in recent time due to colossal magnetoresistance effect [12] and their intriguing physics. The colossal magnetoresistance in a strongly correlated electron system arises due to strong interactions among the charge, spin, orbital and lattice degree of freedom, such as double-exchange interaction, super-exchange interaction, Jahn-Teller type electron-lattice distortion, Hund's coupling etc., leading to complex structural, magnetic and electronic phase diagrams. Furthermore, the $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) amongst several other manganites is of particular interest due to its high T_c of 380 K, a large magnetic moment at room temperature and highest magnetoresistance (MR) near the room temperature [13-15]. Several preparation techniques to synthesize these materials such as mechanochemical, sol-gel, co-precipitation and solid state reaction have been developed. However, the solid state route has been recognized as a powerful method for the production of novel, high performance as well as low cost materials such as ferrites, intermetallic etc [16-18].

In this work, an effort has been made to synthesize Sr doped $LaMnO_3$ system in nano regime i.e. $La_{1-X}Sr_XMnO_3$ (x=0.3) nanoparticles by solid state reaction method. We also present the effect of sintering temperature on structure of these nanocrystalline $La_{0.7}Sr_{0.3}MnO_3$ manganites.

EXPERIMENTAL PROCEDURE

Magnetic nanoparticles of $La_{1-x}Sr_xMnO_3$ (LSMO) x = 0.3 were prepared via conventional solid state reaction method by mechanical ball milling method using ingredients La_2O_3 (99.9%), SrO_2 (99.9%) and MnO_3. Stoichiometric amounts of starting compounds are mixing for 3h and sintering at 1250 and 1350°C for several hours with intermediate grinding steps using 250 rpm. The powder was subjected to the mechanical milling process in air

International Conference on Condensed Matter and Applied Physics (ICC 2015)
AIP Conf. Proc. 1728, 020467-1–020467-4; doi: 10.1063/1.4946518
Published by AIP Publishing. 978-0-7354-1375-7/$30.00