CHAPTER 1

INTRODUCTION

1.1 Overview

Oxide compounds are important inorganic substances due to their excellent mechanical, optical, electrical and magnetic properties, which prove them useful in numerous technological applications [1-3]. For example, mechanical oxides like Al_2O_3, CeO_2 and ZrO_2 have exceptional toughness, strength and hardness so they are extensively used in abrasives, heat engines, rocket nozzles, cutting tools, grinding wheels, and ceramic glazes. Optical oxides like SnO_2, TiO_2 and ZnO are photocatalytic materials which can be used in reflective optical coating for dielectric mirrors, dye-sensitized solar cells, invisible sunscreens, antifogging coatings, self-cleaning windows, and oxidizing agent for of organic pollutants. Electrical oxides like $BaTiO_3$, $Pb(Zr,Ti)O_3$ and $MZrO_3$ are ferroelectric materials which can be used as parts in capacitors, acoustic transducer, pyrodetectors, wave guide device, harmonic generation modulator, and actuators. Magnetic oxides like Fe_2O_3, Fe_3O_4 and $LnFeO_3$ are ferromagnetic materials which can be used in motors, transformers, sensors, data storage, and cancer detection and remediation. Further, to improve their efficiencies when used in applications, detailed understanding in these inorganic substances such as how to fabricate or control microscopic structure of oxide materials in relationships with their associated physical properties is very vital to design efficient devices.

The physical properties of perovskite oxide compounds vary with composition. For example, $LaNiO_3$ is a metallic oxide while $LaMnO_3$ is an antiferromagnetic insulating oxide. Further, most oxide materials do exist unusual but interesting properties owing to composition disordered. For instance, the partial substitution of other foreign atoms (doping atoms) into oxide material results in some remarkable phenomenon. For example, in $LaNiO_3$, a slight replacement of La ion by Sr, Ca, Ba, Pb ions, makes it metallic as well as ferromagnetic. In addition, $BaTiO_3$, commonly used in multilayer ceramic capacitors and positive-temperature coefficient thermistors (thermal sensitive variable resistor), is also expected to provide better-properties when being doped. Particularly, thin films of doped barium-based perovskites e.g. $(Ba_xSr_{1-x})TiO_3$ were found to have high permittivity, so they are being intensively studied as dielectrics in future generations of semiconductor-based dynamic random access memories. As can be seen the study of the microscopic structure surrounding doping atoms (local structure) in perovskite oxide materials are very important to understand their properties, while their structure properties relationships are of great importance in obtaining highly efficient applications [4]. Generally, local structure of perovskite oxide materials can be determined from x-ray interactions with the considered structures, which shall be given in details in the subsequent sections.

1.2 Purpose of the research

In this research, x-ray absorption spectroscopy experimental techniques will be applied to the various doped and undoped perovskite oxide materials to identify their local structures (oxidation state of absorbing atom, number and atomic distance of the neighboring atoms in each shell). The results will be useful to explain the better or poorer physical properties obtained from doping process. Additionally, this knowledge could be used as a guideline of how to improve the doping procedure in experiments. Further, with the local structure reported, it could supply important parameters for performing computer simulation such as ‘first principles electronic structure calculations’, molecular dynamics, Monte Carlo, and quantum Monte Carlo, to get deeper insight in the mechanism of the studied system.