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УДК 538.9
doi:10.18.101/978-5-9793-0883-8-108-110

X-Ray Absorption Study of Magnetic Powder Materials $(La_XCe_{1-X})MnO_3$ AND $(Mg_XCu_{1-X})Fe_2O_4$

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Abstract

Perovskite type oxides with general formula ABO_3 may potentially replace noble metal catalysts due to their high activity, thermal stability and low costs [1]. The catalytic properties of ABO_3 basically depends on the nature of A and B ions. Therefore the electronic properties and catalytic activity of the perovskite-type oxides can be modified by substitution of other heterovalent ions into the A or B sites [2].

Cerium doped lanthanum cobaltite peroskites ($La_{1-x}Ce_xCoO_3$ with x=0, 0.2, 0.4) were prepared by the sol-gel method and characterized by X-ray diffraction (XRD), X-ray absorption (XAS), Energy dispersive X-ray spectroscopy (EDS). The results showed that the cerium doping promoted the structural transformation of $LaCoO_3$ from rhombohedral into cubic structure. High specific surface area and small crystallite size are achieved with x=0.2. The XAS results confirmed the formation of compound $La_{1-x}Ce_xCoO_3$. The structural parameters were determined by Rietveld analysis of the diffraction profiles. XAS measurements for Ce L_3, La L_3 and Co K– edges recorded at beam lines BL17C1 of National Synchrotron Center, Hsinchu, Taiwan. The data fitting was performed using the software package IFEFFIT.

Keywords powder materials, X-ray diffraction, IFEFFIT.

Синхротронное абсорбционное исследование магнитных порошковых материалов $(La_XCe_{1-X})MnO_3$ и $(Mg_XCu_{1-X})Fe_2O_4$

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Аннотация

Оксиды типа перовскита с общей формулой ABO_3 потенциально могут заменить катализаторы из благородных металлов благодаря их высокой активности, термической стабильности и низкой стоимости. В этой работе изучены структурные свойства ABO_3, связанные с особенностью взаимного расположения ионов гетеровалентных в узлах A и B.

Церия кобальтит, легированный лантаном ($La_{1-x}Ce_xCoO_3$ с x = 0, 0,2, 0,4) и медный феррит со структурой шпинели, легированный магнием $(Mg_xCu_{1-x})Fe_2O_4$ были исследованы методом поглощения синхротронных рентгеновских лучей (XAS). Измерения XAS для ($La_{1-x}Ce_xCoO_3$) выполнено на пучке BL17C1 Национального синхротронного центра, Синьчжу, Тайвань, а эксперименты XAS по $(Mg_xCu_{1-x})Fe_2O_4$ проводились на пучке 1W1B рентгеновского поглощения тонкой структуры в синхротронном центре Пекинского электрон-позитронного коллайдера (BEPC) в Китае. Обработка экспериментальных данных проводилась на пакетной программе IFEFFIT.

Ключевые слова: порошковые материалы, рентгеновские лучи, IFEFFIT

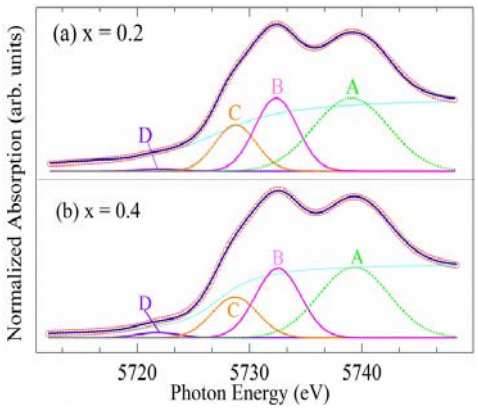

Fig. 1. CeL_3 XANES spectra of $La_{1-x}Ce_xCoO_3$ (x=0.2, 0.4) and results of least-squares-fit analysis (solid line through data open circles)

An integration of all these results obtained in the best performance of the sample when x = 0.2. XAS investigations have proved the actual incorporation of Ce ions, possibly in forms of Ce^{3+}, into the perovskyte. The results are in agreement with the increased lattice parameters and the evolution of the symmetry group in to pseudo-cubic demonstrated by the XRD. These observations are correlated with the enhanced La–O ionic bond and changes in ionic/covalent Co–O bonding properties with increasing Ce doping concentration.

Figure 1. shows normalized Ce L_3-edge X-ray absorption near edge structure (XANES) spectra of Ce-doped cobaltites together with the resultant fit. The characteristic double-peaked principal maximum is the signature of the intermediate valence nature arising from excited many body final states with different 4*f* occupancies [3].

A second part of the talk is devoted to XAFS study of $(Mg_xCu_{1-x})Fe_2O_4$ ferrite spinels. They are used in a broad range of applications due to their unusual magnetic properties, for example, for application the thermal coagulation therapy of cancer tumors [4].

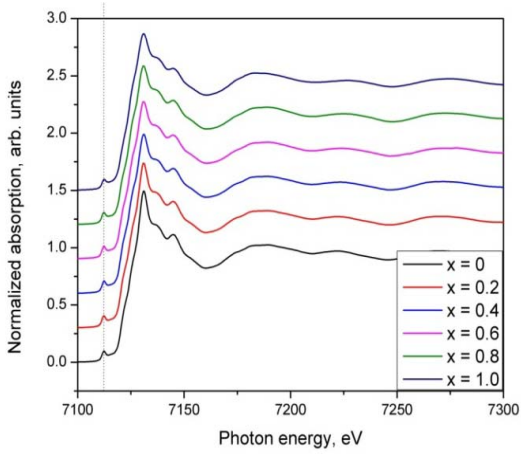

Fig. 2a. The site occupancy of Fe in $(Mg_xCu_{1-x})Fe_2O_4$

In our investigations, nano-scaled ferrite spinels $(Mg_xCu_{1-x})Fe_2O_4$ were synthesized by solid-state reactions. Performed transmission XAS experiments was carried out at beamline 1W1B-X-ray Absorption Fine Structure of the Beijing Synchrotron Radiation Facility at the Beijing Electron Positron Collider (BEPC) to determine the site occupancy of Fe and Cu -ions as well as the oxidation state of the irons. The measured spectra were processed using the above given programs IFEFFIT.

From the Fourier transformed EXAFS experiment data for (1s – 3d) transition we obtained that Fe3+ ions are occupied mainly at B site until x=0.4 (about 2.6 Å) and if above x=0.4, Fe ions are occupied mainly at A site (Fig.2a). But Cu2+ ions are occupied mainly at B site (Fig.2b).

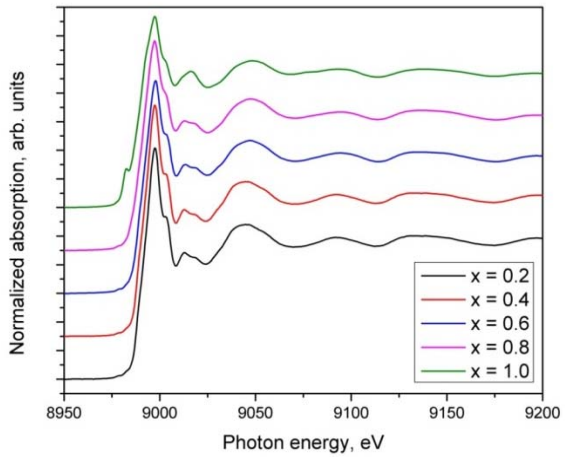

Fig. 2b. The site occupancy of Cu in $(Mg_xCu_{1-x})Fe_2O_4$

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УДК 536.7
doi:10.18.101/978-5-9793-0883-8-110-112

Exergy Analysis of a Pem Fuel Cell System at Various Loads

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Abstract

The energy systems (off-grid, hybrid and stand-alone system etc.) are have to meet the general requirements of the power system that provide the stability of system, continuously produce power and work efficiently. In this study, we determined the exergy and energy efficiencies of a 1.2 kW Nexa^{TM} PEM fuel cell stand-alone system used at various loads for stationary application. The fuel cell system was tested at loads from 25% to 75% of nominal power of module and non-constant pressure.

Keywords: exergy efficiency, energy efficiency, fuel cell

Анализ эксергии системы рем топливных элементов при различных нагрузках

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Аннотация

Энергитические системы (вне сети, гибридные и автономные системы и т. д.) должны соответствовать общим требованиям энергосистемы, которые обеспечивают стабильность системы и эффективно вырабатывать энергию. В данном исследовании мы определили эксергию и энергетическую эффективность системы из 1.2 кВт Nexa^{TM} PEM топливных элементов, используемых при различных нагрузках для стационарного применения. Систему топливных элементов испытывали при нагрузках от 25% до 75% от номинальной мощности модуля и непостоянном давлении.

Ключевые слова: энергетическая эффективность, эксергетическая эффективность, топливный элемент

Introduction

Fuel cell is an energy generator that experienced a quick development track, especially in the second half of 20th century. This technology converts chemical energy directly into electricity by combining oxygen from air with hydrogen gas without combustion. The hydrogen can be defined as alternative fuel which have non-toxic in asset, have high power production, is environmentally friendly and is one of the major candidates nowadays world.

Energy analysis is based on first law of thermodynamics, whereas exergy analysis is based on both the first and second laws of thermodynamics, that it seeks to find out the true potential of thermal systems. In fuel cell system the exergy efficiency is the ratio of the electrical output power and maximum possible work output [1].

Sevjidsuren et al. [2] performed exergy analysis of 1.2 kW Nexa^{TM} fuel cell module at variable operating temperatures, pressures, cell voltages, mass flow rates and air stoichiometrics. In this literature, the external loads were changed from 2A to 10 A with step of 2 A in every 5 min. The exergy flow and exergy efficiency of the distributed energy system using small-scale fuel cell is investigated in Shin'ya et al. [3]. They were determined the exergy flow and difference in efficiency at variable environmental temperatures and load factors.

Differing from the literature, the purpose of this study is to determine the exergy and energy efficiency of the stand-alone PEM fuel cell system, which has moderate capacity, is environmentally friendly and is used for partially supply a daily load of power users.

Experimental part

We used the Nexa^{TM} 1.2 kW PEM fuel cell system in this work, the Nexa^{TM} 1.2 kW power module is a fully integrated system that produces unregulated DC power from a supply of pure hydrogen and oxygen (from ambient air). And with the use of an external fuel supply, operation is continuous, limited only by the amount of fuel storage [4].