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14. ABSTRACT

Multiple student research abstracts are included for summer 2011. All students presented their research results as posters or orals in the Undergraduate Research Summer Institute at Benedict College. Arianna Gladney won the second prize in oral competition and Barbara Fleming won the seond price in the poster section.

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Report Title

2011 Summer Student Research

ABSTRACT

Multiple student research abstracts are included for summer 2011. All students presented their research results as posters or orals in the Undergraduate Research Summer Institute at Benedict College. Arianna Gladney won the second prize in oral competition and Barbara Fleming won the seond price in the poster section.

Title: Oxygen Reduction Reaction (ORR) of Solid Oxide Fuel Cells

Author: Arianna Gladney, Senior, Biology

Mentor: Prof. Changyong Qin

Abstract:

In this project, the oxygen reduction reaction (ORR) of solid oxide fuel cells (SOFCs) was studied in order to understand the enhancement of adding a molten carbonate on the strontium-doped lanthanum manganese (LSM)/ yttria-stabilized zirconia (YSZ) cathode at low temperatures in SOFCs in order to lower cost and increase lifetime of the cell. By combining stable oxygen species such as molecular oxygen (O_2), superoxide (O_2^-), peroxide (O_2^{2-}) and atomic oxygen ion (O^{2-}) with carbonate (CO_3^{2-}) it was found that individual oxygen shows a strong interaction with carbonate. Stable complex structures (CO_5^{2-}) & (CO_4^{2-}) were also produced by interacting carbonate with oxygen. In addition, molten carbonates $(Li_2CO_3)_4$, $(K_2CO_3)_4$ and $(LiKCO_3)_4$ were built and optimized in order to study the different compositions of carbonate and to look at bond distance and charge. Our studies show that a new ORR mechanism is likely by adding a molten carbonate to LSM/YSZ cathode of SOFCs.

Title: Investigation on new anode materials for SOFC application

Author: Jacob Deputy, Freshman, Environmental Health Science

Mentors: Prof. Changyong Qin, and Kevin Huang

Abstract:

Solid oxide fuel cells (SOFCs) convert the chemical energy of a fuel directly into electricity. Although the SOFCs operate at a high temperature, they have several significant applications due to more cleaner, more efficient energy conversion than either a conventional power plant or lower temperature polymer-based fuel cells. The requirements for SOFC anode materials are good chemical and mechanical stability under SOFC operating conditions, high ionic and electronic conductivity over a wide range of P_{O2}, good chemical and thermal compatibility with electrolyte and interconnect materials, high surface oxygen exchange kinetics and good catalytic properties for the anode reactions and so on. Among the reported materials systems from previous publications, materials with perovskite structure are promising are promising particularly where two ions with complimentary function are present on the B-site at high concentration. Our current research focuses on the synthesis of Sr_2GaVO_6 and Sr_2ScVO_6 double perovskite anode material using solid reaction method for SOFC application. The start materials are Sr_2CO_3, Ga_2O_3,V_2O_5 and Sc_2O_3. The powders were mixed proportionally according to the chemical reaction equation (1) and (2) as below:

$4SrCO_3 + V_2O_5 + Ga_2O_3 = 2\ Sr_2GaVO_6 + 4CO_2$ (1)
$4SrCO_3 + V_2O_5 + Sc_2O_3 = 2\ Sr_2ScVO_6 + 4CO_2$ (2)

Then, the powders were homogenized using agate mortar and pestle with acetone as medium and PVB as binder. We pressed them into pellet (diameter of about 20 mm, thickness of about 3 mm) uniaxially at 9 MPa and heated in air and H_2 reduction atmosphere in alumina crucible to 1500 ^{O}C, respectively.

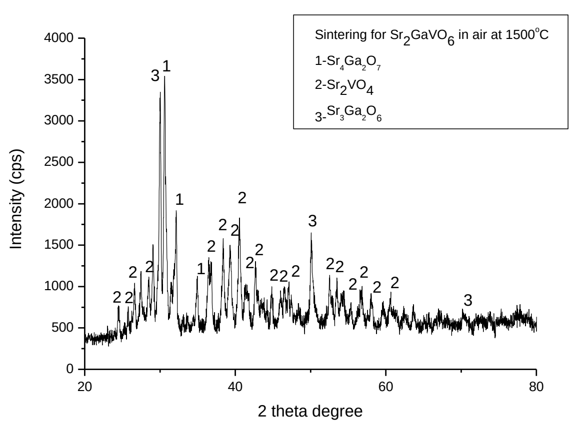

Fig.1 the XRD patterns of compound for Sr_2GaVO_6 in air

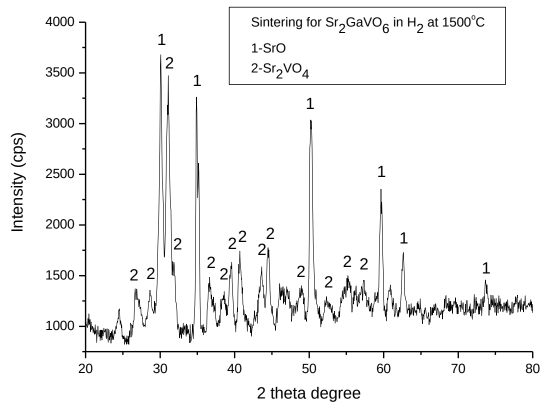

Fig.2 the XRD patterns of compound for Sr_2GaVO_6 in H_2 reduction atmosphere

Fig.1 and Fig.2 are the XRD patterns of the compound in air and H_2 reduction atmosphere using Sr_2CO_3, Ga_2O_3 and V_2O_5 as starting materials, respectively. The main composition of the compound in air is $Sr_4Ga_2O_7$, Sr_2VO_4 and $Sr_3Ga_2O_6$. The main composition of the compound in H_2 reduction atmosphere is SrO and Sr_2VO_4. Unfortunately, we did not obtain the goal of Sr_2GaVO_6 perovskite anode material. Further investigation needs to be done in the future.

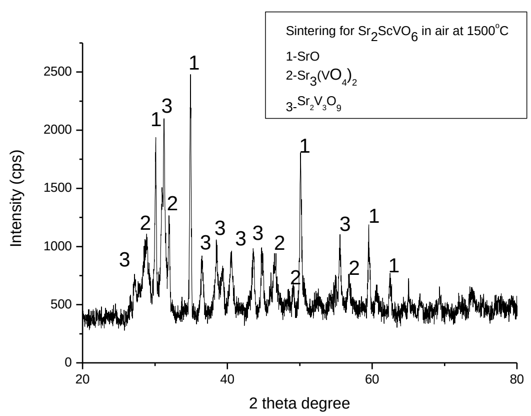

Fig.3 the XRD patterns of compound for Sr_2ScVO_6 in air

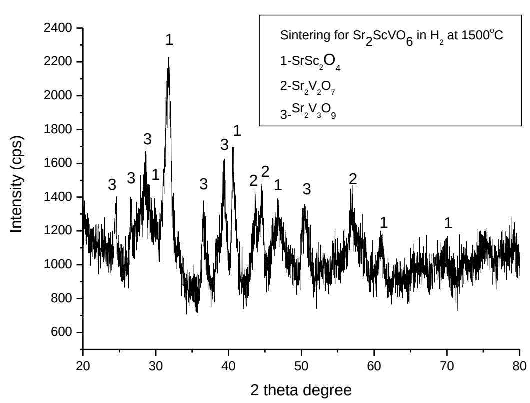

Fig.4 the XRD patterns of compound for Sr_2ScVO_6 in H_2 reduction atmosphere

Fig.3 and Fig.4 are the XRD patterns of the compound in air and H_2 reduction atmosphere using Sr_2CO_3, Sc_2O_3 and V_2O_5 as starting materials, respectively. The main composition of the compound in air is SrO, $Sr_3(VO_4)_2$ and $Sr_2V_2O_9$. The main composition of the compound in H_2 reduction atmosphere is $SrSc_2O_4$, $Sr_2V_2O_7$ and $Sr_2V_3O_9$. Unfortunately, we did not obtain the goal of Sr_2ScVO_6 perovskite anode material. Further investigation needs to be done in the future.

Title: Study of High Conductivity Electrolyte Ba- and Mg-doped $LaGaO_3$

Author: Alisha Lucas, Senior, Biology

Mentor: Prof. Changyong Qin

Abstract:

Fast-ion conductors play a critical role in the performance of solid oxide electrochemical cells (SOECs). Sr- and Mg-doped LaGaO3 (LSGM) is one family of perovskite-structured fast-ion conductors discovered in 1990s; it exhibits much higher oxide-ion conductivity than ZrO2-based ones, rendering it to be a promising solid electrolyte for intermediate temperature SOECs. Replacing Sr with Ba in LSGM could potentially lead to enhanced proton conductivity at lower temperature as a result of increased size of A-cation. In this study, we report synthesis and characterizations of a Ba- and Mg-doped LaGaO3 (LBGM). The LBGM was prepared by solid state reaction of constituent oxides/carbonates at 1450oC for 5 hours. XRD results indicated a single-phase perovskite structure while SEM revealed a dense microstructure. AC impedance spectroscopy measurements yielded an oxide-ion conductivity of 0.002 - 0.099 S/cm from 500oC to 800oC. These preliminary results suggest that LBGM be further investigated for proton conductivity study in the near future.

Title: The Synthesis of Colbaltocenium Containing Polymers via living ATRP

Author: Barbara Fleming, Senior, Chemistry

Mentors: Prof. Changyong Qin, Benedict College
Dr. Chuanbing Tang, and Dr. Lixia Ren, University of South Carolina

Abstract:

Among metallopolymers, metallocene-containing polymers have attracted significant attention since they have great potential in catalytic, optical, magnetic and biological applications due to their unique geometries and physicochemical properties of metallocenes. However, a largely missing part from current efforts is to develop side-chain cobaltocenium-containing polymers. Significantly different from widely studied non-ionic hydrophobic ferrocene (18-e)-containing polymers, isoelectronic-cobaltocenium (18-e) polymers are a class of cationic polyelectrolytes. Given the potential electrostatic interactions, high stability (both thermally and chemically), unique solubility (e.g. water soluble) coupled with high redox potentials of cobaltocenium cations; cobaltocenium-containing polymers are expected to exhibit intriguing properties. This class of organometallic polymers may find new applications in the areas of biosensors, anticancer drugs, and use as precursors for advanced materials.

This project focused on the synthesis and characterization of polymers with cobaltocenium located in the middle of polymer chains. We tried to synthesize cobaltocenium derivatives from cobaltocenium acid via esterification, and obtained the cobaltocenium-containing initiators, which were used for atom transfer radical polymerization (ATRP). The polymerization of different type of monomers like *tert*-butyl acrylate (tBA) and styrene (St) initiated by these initiators was successful and confirmed from proton Nuclear Magnetic Resonance (HNMR) and Gel Permeation Chromatography (GPC) analyses. All polymers exhibited low polydispersity indexes and controlled molecular weight. The cobaltocenium-containing polymers showed reversible redox properties, which might be used as redox-based biosensors. Thermal properties of this type of polymers were also characterized.