Synthesis, Crystal Structure, and Electrochemical Properties of Layered SBSC as Cathode for IT-SOFC

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Abstract: IT-SOFC cathode materials such as the double perovskite SmBa0.6Sr0.4Co2O5+ (SBSC) are being studied as possible cathode materials. SBSC are the subject of this investigation, which focuses on their crystal structure, electrochemical characteristics, single cell performance, and microstructure characterization. A tetragonal structure with P4/mmm space group and lattice parameter of 3.866 a, 3.866 b, c, and v = 113.40 is determined by the Rietveld refinement. The P4/mmm space group and lattice parameter of 3.866 are determined by the P4/mmm refinement. Precise polarization resistance (Rp) values of a half cell specimen on the SDC electrolyte were found to be 1.8 (600oC), 0.42 (700oC), and 0.13 (800oC) cm2 at 600, 700, and 800oC, respectively, while the peak power density of single cell Ni-SDC|SDC|SBSC was found to be 302 mW/cm2 at 700oC. All of the findings indicated that SBSC64 cathode is a more promising prospective cathode material for IT-SOFC than other cathode materials.

Keyword: SOFC, cathode, crystal structure, electrochemical, cell performance

1. Introduction

Renewable energy has risen to become a great source of energy since it promises to emit the least amount of pollution; this has piqued the interest and attention of researchers over the last several decades, who have worked to create fuel cells. Solid oxide fuel cells (SOFCs) have the potential to be the most efficient and flexible fuels when compared to all other kinds of fuel cells [1-3]. Solid oxide fuel cells are a type of fuel cell that uses solid oxide as a fuel. Carbon solid gasification (e.g., municipal solid waste and biomass) is one of the fuels available from SOFC, which ranges from hydrogen through natural gas, coal gas, and carbon solid gasification [4,5]. One of the most important issues in SOFC applications is that the cathode electrochemical activity reduced substantially as a result of the temperature reduction. The cathode, which is a component of the SOFC, plays an essential role in determining the overall performance of the cell. The discovery of novel cathode materials with high electrocatalytic activity performance is now attracting a great deal of interest for use in intermediate temperature solid oxide fuel cells (IT-SOFCs) [6,7].

It has been widely shown that double perovskite shows outstanding electrochemical performance, and the structure has been extensively investigated for use in IT-SOFC systems operating in the temperature range of 600-800oC. Because of its high concentration of oxygen vacancies, high electrical conductivity, and catalytic activity [8,] the double perovskite structure, in which rare-earth ions (RE) occupy site A, barium site A, and cobalt site B, has been extensively described in the past few decades. In order to better understand the characteristics

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of double-layered perovskites with the chemical formula LnBaCo2++ (lanthanide-selected lanthanide), research has been conducted [9-11] to examine their structure and composition. Several researchers, including Subardi et al., have shown that the double perovskite oxides composed of SmBa0.5Sr0.5Co2O5+ [12] and LaBa0.5Sr0.5Co2O5+ [13] have very high electrocatalytic activity when compared to other cathode materials.

As a possible cathode material for IT-SOFCs, many research groups have studied the electrochemical characteristics of a novel kind of mixed ionic and electronic conducting (MIEC) oxide, cation ordered LnBaCo2O5+ (Ln = La, Pr, Sm, Gd, Y), which has been ordered by cation order [14-16]. In cathodes material, cobalt is advantageous for the activation of oxygen reduction and, as a result, the activation polarization loss is reduced compared to other materials [17,18]. The substitution of Sr for Ba in LnBaCo2O5+ layered perovskite has been shown to increase electrical conductivity while simultaneously improving the electrochemical characteristics of the cathode. Chemical stability between the cathode and electrolyte was enhanced by substituting Sr for Ba in GdBaCo2O5+[19], and oxygen transport was increased due to the replacement of Sr for Ba in GdBaCo2O5+. When Sr is substituted for Ba in YBaCo2O5+, Mckinlay and colleagues discovered that the structure changes from orthorhombic to tetragonal, with an increase in electrical conductivity [20]. [21] In addition, Meng et al. discovered that Sr doping in YBaCo2O5++ enhanced electrical conductivity owing to a larger number of electronic holes originating from the increased interstitial oxygen [21] that was seen.

Using SmBa0.6Sr0.4Co2O5+ (SBSC) oxide as a cathode for a solid oxide fuel cell (SOFC) operating at intermediate temperatures, we evaluated the oxide's structural characteristics, electrochemical performance, power density, and microstructure in order to determine its suitability for this application.

2. Experimental

Prepare the anode and cathode using a solid state reaction technique, with reference to prior publications [22,23] for more information. The stoichiometry technique was used to determine the composition of the cathode material, which consisted of Sm2O3, BaCO3, CoO, and SrCO3 ions. An uniform combination of cathode powder material is obtained by grinding it with alumina balls, which is subsequently dried at 65 degrees Celsius. Prior to being crushed using a mortar and pestle, the cathode material is calcined at 1000oC for 4 hours and then allowed to cool to room temperature in the open air for a further 24 hours. Carbon, NiO, and Sm2O3 are combined together in an alcohol solution to form the anode material. In a series of steps, drying, grinding, and granulating with PVA are followed by a final step of anode preparation (60 mesh). Manufacturing specimens in half-cell and single-cell configurations utilizing hydraulic press machines Using screen printing methods, the half cell specimen arrangement is SBSC (90 percent)+SDC (10 percent)|SDC|SBSC(90 percent)+SDC(10 percent)|SDC|SBSC(90 percent)+SDC(10 percent). Meanwhile, the sol-gel technique is being utilized to produce Ce0.8Sm0.2O1.9 (SDC) electrolyte powder. The procedure begins with the addition of Ce(NO3)3.6H2O and Sm(NO3)3.6H2O to the starting ingredients.

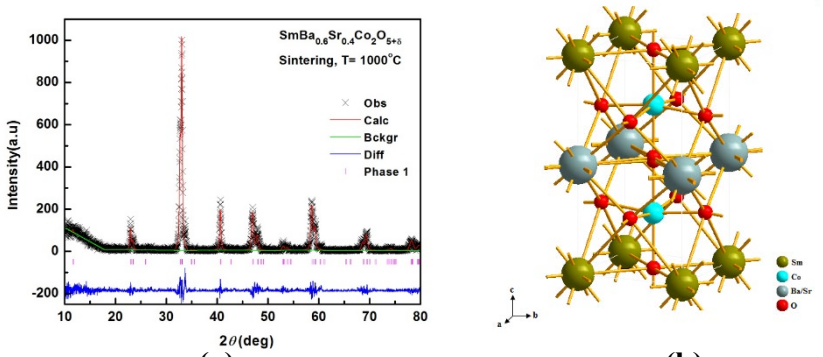
The SBSC cathode paste was applied to both sides of the SDC electrolyte discs in a circle that was 1 mm thick and 13 mm in diameter, with the paste being applied in a circular pattern. After the cathode material is sprayed on the surface of the electrolyte using a screen printing method, it is sintered at a temperature of 1000oC for 4 hours in the open air. A working electrode (WE) with a surface area of 0.385 cm2 was painted onto the cathode paste on one hand, and a cathode paste was painted onto the other. The Ag (RE) reference electrode is positioned about

0.3-0.4 cm away from the WE. It is necessary to put the CE on the opposite side of the SDC disc [24-26] to ensure that the CE is active. Anode-supported fuel cells are used to construct a single cell, which is configured as Ni-SDC|SDC|SBSC in nature. For further information on the manufacturing of single cells, please see our group's publications published elsewhere [27]. Evaluations of the samples used in this research include XRD, electrochemical characteristics, microstructure, and I-V, which is used to estimate the power density for single cell performance.

3. Result and Discussion

3.1. Crystal Structure

Figure 1(a) depicts the XRD pattern of SBSC powder after it was calcined at 1000oC for 4 hours, during which time the XRD peaks typical of double perovskite oxide were found. The preparation of the sample powder was excellent, and there were no peaks produced by contaminants in the SBSC structure could be found. The SBSC structure may be indexed to the space group of a tetragonal P/mmm based on Reitveld refinement data, and their structure data is given in Table 1 based on Reitveld refinement data. A = 3.866, b = 3.866, c =7.589, and v = 113.40 are the lattice parameters of the SBSC cathode structure, and reliability factors Rwp = 0.29 and Rp = 0.20 are obtained. The good match between the predicted profiles and the actual data demonstrates that cations are well ordered between Sm3+ and Ba2+/Sr2+ ions in the ordered perovskite lattice, which is consistent with previous findings.[28].



In Fig. 1 (a), the XRD profiles for SBSC calcined at 1000oC were calculated (solid line) and observed (crosses) with their respective differences (bottom line) shown on a graph. (b) The crystal structure of SBSC at room temperature, in which the Ba2+/Sr2+ ions were arranged in an ordered perovskite lattice structure.

Refinement data has led to the placement of the Sm atoms in the first of the three sites, the Ba and Sr atoms in the second of the three sites, and the Co atoms in the third of the three locations (0.5,0.5,0). There are three different types of oxygen atom sites: O1 at the 4i (0,0.5,z) site, O2 at the 1c (0.5,0.5,0) site, and O3 at the 2h (0,0.5,z) site (0.5,0.5,z). Figure 1 depicts a picture of the crystal structure of the specimen while it is at room temperature (b). Furthermore, the SBSC cathode exhibited excellent structural stability; when the specimens were calcined at temperatures ranging from 1000 to 1100oC, the structure did not change, and both samples were classified as belonging to the tetragonal space group [23].

Table 1. Crystallographic information for SBSC from NPD data at room temperature, cell parameters obtained by the Rietveld refinement

Atom	Wyckoff position	x	y	z	Uiso	Occ
Sm	1a (0 0 0)	0	0	0	0.0059	0.8230
Co	2h (½ ½ z)	1/2	1/2	0.25173	0.0001	0.9211
Ba	1b (0 0 ½)	0	0	0.5	0.0393	0.6000
Sr	1b (0 0 ½)	0	0	1/2	0.0073	0.4000
O1	4i (0 ½ z)	0	1/2	0.27880	0.0080	0.8561
O2	1c (½ ½ 0)	1/2	1/2	0	0.0214	0.8427
O3	2h (½ ½ z)	1/2	1/2	0.50785	0.1560	0.4820

3.2 Electrochemical Properties

A measure of overall cathodic characteristics related with gas-phase oxygen reduction, bulk diffusion/oxygen surface, and oxygen reduction is the polarization resistance. A half cell arrangement was used to analyze the electrochemical impedance spectra (EIS) of the SBSC(90 percent)+SDC(10 percent) cathode combination. Fig. 2 shows a typical EIS of the SBSC(90 percent)+SDC(10 percent) cathode on SDC electrolyte when tested at different temperatures ranging from 600 to 850 degrees Celsius. The impedance spectrum is fitted to an analogous circuit with the help of the Z-view program. The Rp values of SBSC(90 percent)+SDC(10 percent) cathode are 1.8, 0.42, and 0.13 cm2 at 600, 700, and 800oC, respectively, which are much lower than the values of SLBF cathode, which are 2.60, 0.49, and 0.22 cm2 at 600, 700, and 800oC, respectively [29]. Furthermore, as shown in Table 2, the Rp values of the SBSC(90 percent)+SDC(10 percent) cathode at 600oC are compared to those previously published, as previously stated. When compared to the other cathodes, the SBSC(90 percent)+SDC(10 percent) cathode exhibits the greatest electrocatalytic activity toward the oxygen reduction process (ORR).

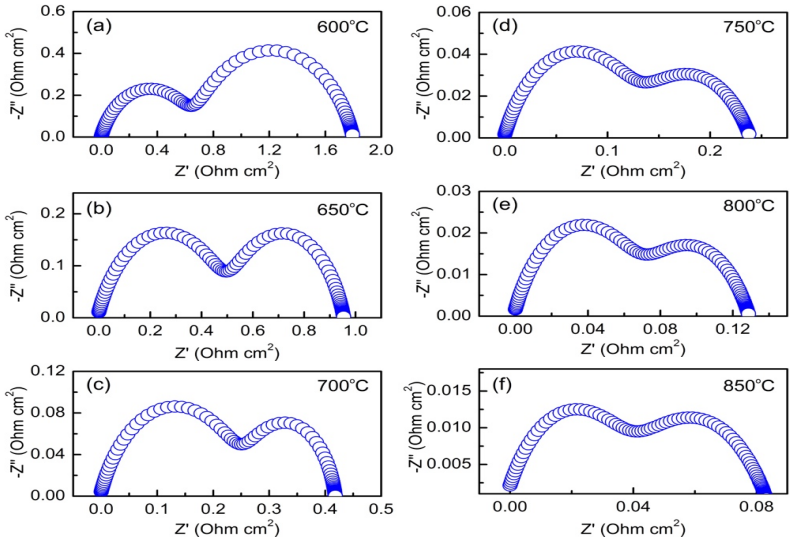


Fig. 2. Impedance spectra of SBSC(90%)+SDC(10%) cathode on SDC half cell at various temperatures from 600-850°C.

Cell performance may be improved by employing electrolyte-based materials such as SDC to modify the cathode surface. This is a proven way of increasing cell performance. Consider the polarization resistance (Rp) values of the pure SBSC55 cathode (i.e., without infiltration) at 600oC, 700oC, and 800oC. These values are 4.17, 0.95, and 0.36 cm2 at 600, 700, and 800oC. Rp values are significantly reduced when the SDC electrolyte is infiltrated at a pure SBSC55 cathode, demonstrating that particles active in both electrochemical processes (i.e, electrochemical reactions at the electrode-electrolyte interface and oxygen diffusion adsorption at the gas cathode surface interface) are simultaneously enhanced by particles active in both electrochemical processes at the electrode-electrolyte interface (nano SDC). When 0.39 mg cm-2 SDC was added to the porous SBSC55 cathode, the Rp values progressively dropped substantially to 2.95, 0.73, and 0.15 cm2 at 600, 700, and 800oC, respectively, indicating a considerable reduction in the cathode resistance. Afterwards, when the amount of SDC infiltrated into the cathode was raised to 0.65 mg cm-2, the Rp values dropped significantly to 1.28, 0.32, and 0.11 cm2 at 600 oC, 700 oC, and 800 oC, respectively [30]. The Rp values were 1.28, 0.32, and 0.11 cm2 at 600 oC, 700 oC, and 800oC, respectively. As a result, the infiltration technique has the potential to be very successful in increasing the electrochemical activity of cells.

Table 2. Comparison of polarization resistance (Rp) values at 600°C based on double perovskite cathode structure

Composition	Rp(Ω/cm^2)	Reference
$PrBaCoFeO_{5+\delta}$	2.76	[31]
$PrBa_{0.5}Sr_{0.5}Co_{1.9}Ni_{0.1}O_{5+\delta}$	8.56	[32]
$NdBa_{0.5}Sr_{0.5}CoCuO_{5+\delta}$	3.77	[33]
$NdBa_{0.5}Sr_{0.5}Co_{0.5}Fe_{1.5}O_{5+\delta}$	3.66	[34]
$SmBa_{0.5}Sr_{0.5}Co_{1.5}Fe_{0.5}O_{5+\delta}$	32.2	[35]
$GdBaCo_2O_{5+\delta}$	2.11	[36]
$YBaCo_2O_{5+\delta}$	4.59	[37]
$YBa_{0.6}Sr_{0.4}Co_2O_{5+\delta}$	2.24	[22]
SBSC(90%)+SDC(10%)	1.80	This work

3.3 Single Performance

Figure 3(a) depicts the voltage and cell performance of a Ni-SDC|SDC|SBSC cell as a function of current density when H2 is used as the fuel and air as the oxidant at different temperatures ranging from 500 to 800 degrees Celsius. At 600, 700, and 800 degrees Celsius, the power densities achieved by the cell with SBSC cathode are 104, 302, 5, and 289.4 mWcm-2, respectively, indicating that the cell is capable of producing high power densities. When compared to other cathodes operating under comparable circumstances, the SBSC cathode demonstrated a greater power density. Example: At 700oC, the power density of SmBaCoCuO5+ [38], GdBaFeNiO5+ [39], and PrBa1-xFe2O5+ [40] cathodes achieves 253, 1.82, and 183 mWcm-2, respectively, whereas other cathodes obtain 253, 1.82, and 183 mWcm-2.

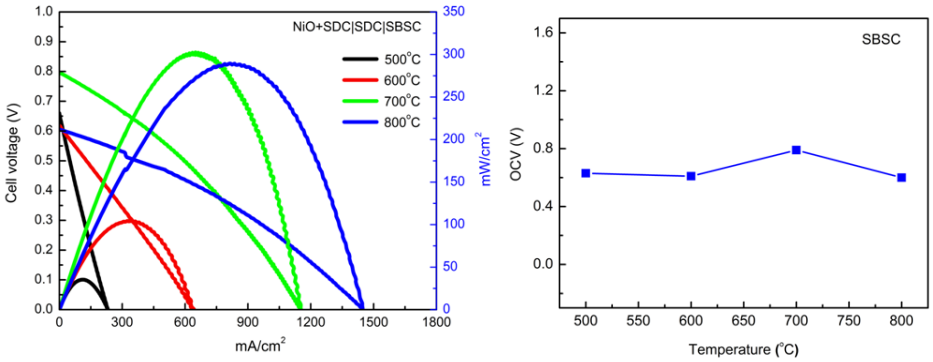
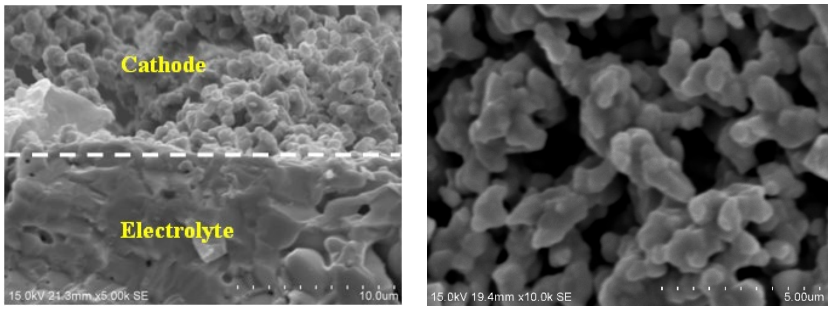


Fig. 3 (a) The single cell performance of Ni-SDC|SDC|SBSC at a temperature between 500-800ºC, and (b) OCV values during cell test.

The open circuit voltages (OCVs) shown in Fig.3(b) are 0.61, 0.79, and 0.6 at 600, 700, and 800oC, respectively, which are lower than the theoretical values. A number of reasons contribute to the OCV loss in general, including an internal short-circuit caused by electronic conduction, the oxidation of the ceria from Ce4+ to Ce3+, a structural flaw caused by the electrolyte layer, and oxygen penetration caused by electronic conduction. The alteration of the cathode surface using electrolyte-based materials such as SDC, as part of the infiltration technique, may improve the performance of the cell and enhance its efficiency. As previously reported, SDC nanoparticles impregnated on the porous surface of the SBSC55 cathode resulted in a substantial increase in the power density values [30] when the cathode was used. [31] In one example, the SBSC55 cathode power density was 470 mWcm-2 at 700oC when no SDC solution was infiltrated into the cathode; however when 0.13, 0.39 and 0.65 mg cm-2 of SDC solution were infiltrated into the cathode, the power density values increased significantly, reaching 485, 620, and 755 mWcm-2, respectively, at 700oC. These findings suggest that surface modification by infiltration with an electrolyte material such as SDC, along with a single cell's electrochemical performance, may enhance the electrochemical performance of the cell.

3.4 SEM Image

The structure of the cathode has a significant impact on electron and oxygen transport. In the fuel cell, the cathode structure has characteristics that influence the performance of the fuel cell, including the kinetics of the reaction, charge transport, and mass transportation preprocesses [42,43]. (a) SEM picture of a cross-sectional for the half cell specimen, which was produced at 1000oC for 2 hours in air, and (b) top view of the SBSC cathode, both shown in Figure 4(a). The adhesion between the cathode and the electrolyte is shown to be very excellent in Fig. 4(a), as shown. The grain size of the SBSC cathode was evenly distributed in the region of 2-3 m and was porous in composition. In SOFC operations, good shape is very beneficial in ensuring fast oxygen diffusion, as well as in reducing polarization resistance and increasing current..



(a) (b)

Fig. 4 (a) SEM image of cross-sectional for the half cell specimen fabricated at 1000°C for 2 h in air, and (b) top view of the SBSC cathode.

4 Conclusions

On the basis of the SDC electrolyte, the SBSC cathode was studied as a possible cathode material for an intermediate temperature solid oxide fuel cell (IT-SOFC) using the SBSC cathode. Using the SBSC cathode structure as an example, we can see that it is indexed to a tetragonal (P/mmm) with lattice parameters of a = 3.866, b = 3.866, c =7.589, and v = 113.4. The polarization (Rp) values of the half cell samples range from 1.8 to 0.13 cm2 at temperatures ranging from 600 to 800 degrees Celsius. At 700 degrees Celsius, the single cell achieved a maximum power density of 302 mWcm-2. Due to its superior performance, the SBSC cathode offers more potential for use in intermediate temperature solid oxide fuel cells..

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