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Short communication

Mechanism of chromium poisoning the conventional cathode material for solid oxide fuel cells

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HIGHLIGHTS

- A 3D model is used to evaluate temperature distribution in a solid oxide fuel cell.
- Traces of chromium diffusing into LSM degrade material conductivity.
- The porosity in pellet and applied pressure affect chromium poisoning materials.
- Chromium prefers to adsorb on the La(Sr)-O-terminated face.

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ABSTRACT

Chromium poisoning the $La_{0.875}Sr_{0.125}MnO_3$ (LSM) cathode for solid oxide fuel cells is a critical issue that can strongly affect the stability. In this study, we evaluate the temperature distribution in a SOFC based on a 3D model and then combine conductivity test and material computation to reveal the effects of chromium in SUS430 stainless steels on LSM conductivities. The starch concentration in LSM pellets and the applied pressure on the contact with interconnect materials show close relationships with the chromium poisoning behavior. The density functional theory (DFT) computing results indicate that chromium atoms preferably adsorb on the MnO_2-terminated and La (Sr)-O-terminated (001) surfaces. The resulting conclusions are expected to deeply understand mechanism of chromium deactivating conventional cathodes at some typical operational conditions, and offer crucial information to optimize the structure to avoid the poisoning effect.

1. Introduction

Solid oxide fuel cell is a promising power generator that can directly convert chemical energy to electrical energy via a series of electrochemical reactions [1]. Since the metallic interconnect serves as connection between cathode and anode of its neighboring cells and also acts as a sealing medium to avoid fuel and air meeting, it is thus indispensable to SOFC stacks [2]. The stability caused by the Cr-contained metallic interconnect is still an important issue, which can induce degradation of material properties and reduce power output.

Michael et al. confirmed the cell performance decrease due to the impact of Cr poisoning [3]and Taniguchi et al. reported that chromium escaped from the alloy into the cathode and then diffused to the cathode/electrolyte surface during the discharging process, which inhibited oxygen supply and reduced the reaction sites, leading to increase in cathodic polarization [4]. Jiang et al. reported that Cr species deposition such as Cr_2O_3 and $(Cr, Mn)_3O_4$-type spinal phase was more likely to happen at the cathode/electrolyte interface and formation of the $(Cr, Mn)_3O_4$-type spinal could be related to the presence of transition state Mn^{2+}, in which process electrical played an crucial role during the interaction between cathode and alloy [5,6].

Thermodynamic calculation indicated that chromium poisoning could be attributed to Cr substitution of the perovskite lattice, formation of $SrCrO_4$ in cathode containing less four valence ions (Fe^{4+}, Co^{4+}) and generation of Cr_2O_3 or $CrMn_2O_4$ at the triple phase boundaries (TPBs) [7]. Nevertheless, Hilpert et al. indicated that CrO_3(g) was the dominant species with the dry air and $CrO_2(OH)_2$(g) with wet air [8]. The Cr poisoning can be relieved by lowering the operational

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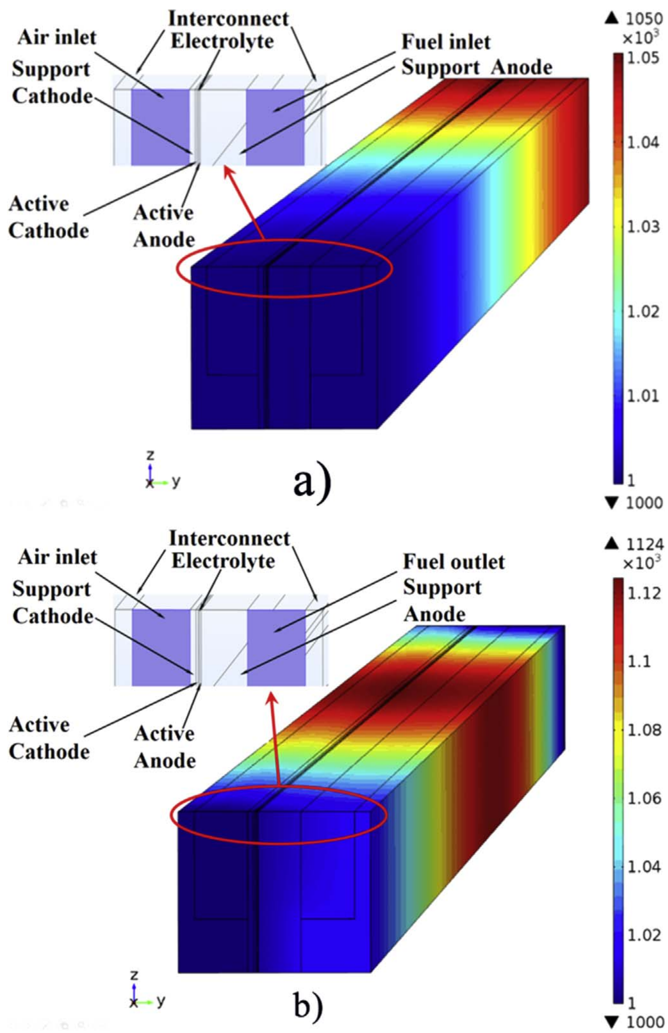

Fig. 1. Temperature distribution in a single cell: a) the co-flow pattern and b) counter flow pattern.

temperature, like using the Co/Cr-doped cathode material and the Mn free cathode (LNF) [9] and coating metallic interconnect [10]. In this study, we combined thermal modeling, material analysis and computation to reveal the possible effects of the two factors on Cr deactivating materials. The results can be helpful in improving the material design and optimizing structure to block Cr adsorption and diffusion in cathodes.

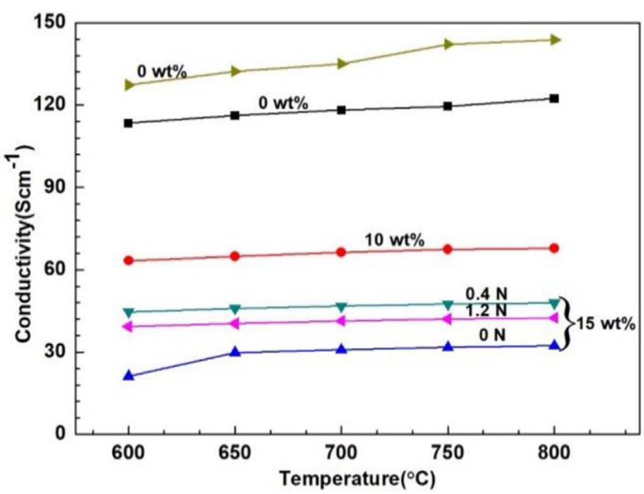

Fig. 3. Variation of LSM conductivities at the testing conditions.

2. Experimental

The starch with concentrations of 0 wt%, 10 wt% and 15 wt% mixed with the LSM using poly vinyl alcohol as binder were pressed to be pellets, which were then sintered at 1737 K for two hours. Thickness of LSM pellet was 0.72 mm after sintering. SUS430 stainless steel with the dimension of 20 mm × 20 mm and thickness of 0.5 mm was used to contact with the prepared LSM pellets. Therefore, LSM pellets contacting SUS430 with and without pressure were sintered at 1173 K for 100 h in air. The applied pressure was controlled at 0.4 N, 1.2 N, 1.8 N and 2.4 N. The weight of LSM was firstly measured after cleaning the surface and then the Van der Pauw four point method was used to measure the conductivity of LSM [11]. Four silver wires contacting with the rim of the pellet, which was then connected to an electrochemical working station (CHI660E) for the conductivity test.

3. Results and discussion

We have constructed a 3D bi-layer model for the anode-supported planar SOFC [12], where the fuel inlet is fed with mixed humid

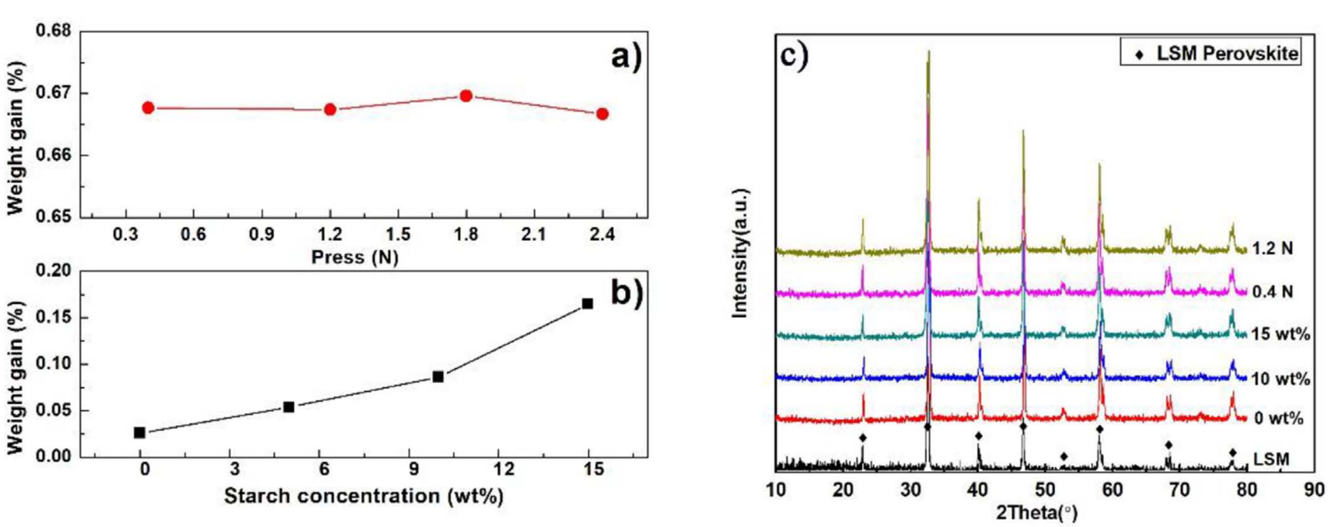

Fig. 2. Weight evolutions of LSM pellets after contacting with stainless steels at 1173 K for 100 h (a, b) and The XRD patterns for LSM pellets (c).