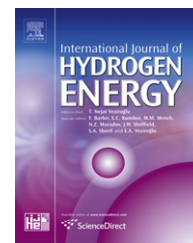


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# Multi-scale design simulation of a novel intermediate-temperature micro solid oxide fuel cell stack system

S.F. Lee, C.W. Hong\*

Department of Power Mechanical Engineering, National Tsing Hua University, Hsinchu 30013, Taiwan

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## ABSTRACT

This paper presents a multi-scale simulation technique for designing a novel intermediate-temperature planar-type micro solid oxide fuel cell (mSOFC) stack system. This multi-scale technique integrates the fundamentals of molecular dynamics (MD) and computational fluid dynamics (CFD). MD simulations are carried out to determine the optimal composition of a potential electrolyte that is capable of operation in the intermediate-temperature region without sacrifice in performance. A commercial CFD package plus a self-written computational electrochemistry code are employed to design the fuel and air flow systems in a planar five-cell stack, including the preheating manifold. Different samarium-doped ceria (SDC) electrolyte compositions and operating temperatures from 673 K to 1023 K are investigated to identify the maximum ionic conductivity. The electrochemical performance simulation using an available 5-cell yttria-stabilized-zirconia (YSZ) mSOFC stack shows good agreement with our experimental results. The same stack design is used to predict a novel SDC-mSOFC performance. Feasibility studies of this intermediate-temperature stack are presented using this multi-scale technique.

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## 1. Introduction

Fuel cells are one of the most promising technologies for the next generation of green hydrogen applications. They are suitable for many kinds of power plants, ranging from small auxiliary power units to distributed heat and power cogeneration systems. High temperature solid oxide fuel cells (SOFCs) are used with a wide variety of hydrocarbon fuels, including pure hydrogen, from various sources. They are influenced less by fuel impurities than other kinds of low temperature fuel cells, such as polymer-membrane fuel cells. The high operating temperature also promotes the fuel reaction rate without the requirement for expensive platinum catalysts. However, high temperature operations incur two major problems: the first is thermal stress fatigue and the second is slow startup from cold conditions. Recent targets to

reduce the operating temperature require new solid electrolytes with high conductivities at intermediate/low temperature regions (400–800 °C) [1]. This study uses molecular simulation techniques to identify the optimized solid oxide electrolyte composition to achieve the target.

The solid oxide electrolyte acts as a conductor of oxygen ions between the cathode and anode of a high temperature fuel cell. Material characteristics such as mechanical strength, electrical conductivity and thermal stability can be measured experimentally. However, the optimized solid electrolyte composition is expensive and tedious to determine using experimental trial-and-error. Molecular dynamic simulation is a convenient technique to predict these material characteristics in a more efficiency way, provided that the molecular structure is setup correctly. Detailed oxygen ion transport phenomena inside the electrolyte molecular structure can be

\* Corresponding author. Tel.: +886 3 5742591; fax: +886 3 5722840.

E-mail address: [cwhong@pme.nthu.edu.tw](mailto:cwhong@pme.nthu.edu.tw) (C.W. Hong).

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visualized using this technique. Molecular simulations of the baseline electrolyte, yttria-stabilized zirconia (YSZ), and some new materials, e.g. yttria-doped ceria (YDC), have been carried out in the past [2–5]. Among many new substituted ceria ceramics, samarium-doped ceria (SDC) was reported to be effective in intermediate/low temperature regions [6–10]. However, none of the scaled up stack performance was reported. The SDC is chosen in this paper as the anode supported electrolyte for designing a novel fuel cell single cell as well as a multi-cell stack system. In addition to the composition effect, the solid electrolyte temperature field is also an important issue in overall SOFC performance [11]. A non-uniform temperature distribution easily causes many technical problems, such as thermal cracks and seal leakage, that reduce the overall efficiency or even damage the cells [12,13]. A three-dimensional (3-D) numerical simulation technique is employed in this study to investigate the SOFC performance under different configuration designs.

This study first simulated the transport dynamics of the oxygen ions in the potential solid electrolyte and further extended the nano-scopic ionic conductivity to macro-scopic performance prediction. The simulation technique integrates the fundamentals of molecular dynamics and computational fluid dynamics. The former is a self-written code and the latter employs a commercial package. The variations in ionic conductivity and diffusion coefficient due to the composition and thermal effects are predicted. The optimal composition with the maximum ionic conductivity can be determined. In the computational fluid dynamics simulations, 3-D pressure, temperature and current fields in an actual size multi-cell stack design can be emulated. The baseline example is a commercially available 5-cell YSZ-SOFC stack, simulated and later examined using our experimental results. This was performed to validate the prediction performance of this tool. The example case study aims at the novel SDC-mSOFC performance using the same stack design. The multi-scale simulation is performed to evaluate the feasibility of future intermediate/low temperature mSOFC designs.

## 2. Simulations models

### 2.1. Molecular dynamics for solid electrolytes

Qualified electrolytes for SOFCs require rapid ionic transport, negligible electronic conduction and acceptable thermodynamic stability over a wide range of temperatures. Current ceramic material options can be categorized into three types: zirconia fluorites for those operated above 800 °C; lanthanum manganite-based perovskites for intermediate-temperature SOFCs (600–800 °C); and ceria fluorites suitable for low temperature (400–600 °C) range. The zirconia electrolyte has been the most popular choice for current commercially available SOFCs. We chose the samarium-doped ceria (SDC) for future low temperature applications and compared the performance against the commercial zirconium design. Fig. 1 shows the molecular structure of the SDC which is based on a face centered cubic (FCC)  $\text{Ce}^{+4}$  cations, packed with oxygen ions surrounded by ceria tetrahedrons. The dopant in this SDC

is  $\text{Sm}_2\text{O}_3$ . The dissolution of samaria into the fluorite phase of the  $\text{Ce}-\text{O}_2$  causes an extra charge of +1. To maintain the electrical neutrality, every two substitutions of  $\text{Sm}^{+3}$  will form an oxygen vacancy.

The potential function between these charged ions can be expressed using the Born-Meyer-Buckingham two-body function [14], which is

$$u(r_{ij}) = -\frac{A_{ij}}{r_{ij}^6} + B_{ij} \exp(-r_{ij}/\rho_{ij}) + \frac{q_i q_j}{4\pi\epsilon_0 r_{ij}} \quad (1)$$

where  $r_{ij}$  is the distance between two ions;  $A_{ij}$ ,  $B_{ij}$  and  $\rho_{ij}$  are empirical constants (see Table 1 which is obtained from [15]);  $\epsilon_0$  is the dielectric constant;  $q_i$  and  $q_j$  denote the charge of ions  $i$  and  $j$ . The first term on the right hand side represents the attraction between the atoms and the second term represents the repulsive force. Both terms account only for the short range force. The third term is the electrostatic force which takes into account the coulomb interaction between charges at a longer distance. Our simulation system defines a cubic box consisting of  $5 \times 5 \times 5$  crystallographic unit cells, shown in Fig. 1. There are 1500 ions contained in the whole simulation system. The unit cell volume varies with temperature because of the thermal expansion effect. The relation between the side length and the operating temperature is expressed by [16]:

$$L(T) = U_c \times L_0 [1 + \alpha(T - 298)] \quad (2)$$

where  $L(T)$  is the system side length at temperature  $T$ ;  $U_c$  is the number of unit cells in each side;  $L_0$  is the lattice constant which varies with the dopant ( $\text{Sm}_2\text{O}_3$ ) concentration (listed in Table 2 which is abstracted from [17]);  $\alpha$  is the thermal expansion coefficient, which is  $1.1 \times 10^{-5} \text{ K}^{-1}$  for the SDC. Three-dimensional periodic boundary conditions are assigned to the simulation system. The Coulomb effect is induced by the charged ions and solved using the Ewald summation technique [18]. All Newtonian equations of the ionic motion are integrated using Gear's predictor-corrector algorithm [19] with a time step of 2.0 fs. The simulation was carried out under the NVT (constant number of molecules, volume and temperature) ensemble. The final equilibration criterion was monitored using the temperature variation and the fluctuation in the total system energy.

From the equilibrated results, we can analyze the trajectory of all ions and calculate their mean square displacement (MSD) and diffusion coefficient ( $D$ ) in time period  $t$  using:

$$\text{MSD}(t) = \frac{1}{N} \sum_{n=1}^N \langle [\vec{r}_n(t_0 + t) - \vec{r}_n(t_0)]^2 \rangle = B + 6D(t) \quad (3)$$

where  $N$  is the total number of ions;  $B$  is a constant;  $\vec{r}_n$  denotes the position vector;  $t_0$  is the initial time step and the angle brackets  $\langle \rangle$  represent the time average. The oxygen ionic conductivity can be evaluated from the Nernst–Einstein relation as below:

$$\sigma_{\text{O}_2} = \frac{Nq^2D}{k_B T H_R} \quad (4)$$

where  $\sigma_{\text{O}_2}$  is the oxygen ionic conductivity;  $N$  is the number density of the oxygen ions;  $q$  is the mobile ion charge;  $D$  is the diffusion coefficient evaluated from Eq. (3);  $k_B$  is the Boltzmann

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