



Shape deformation analysis of anode-supported solid oxide fuel cell by electro-chemo-mechanical simulation



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ABSTRACT

In this study, the analysis of a solid oxide fuel cell (SOFC) is conducted, starting at a high temperature under the assumption of a stress-free during cell sintering at that temperature level. The deformation during the temperature decrease after sintering is reflected not only in the initial shape of the cell at a low temperature, but also in the deformation behavior during operation. The time variation of the cell shape is clarified in terms of thermal, chemical, and creep strains. In these simulations, we use our previously developed analysis method for electrochemical and mechanical coupling phenomena by incorporating general-purpose finite element analysis software and its pre-/post-processing functions.

1. Introduction

Components of solid oxide fuel cells (SOFCs) are exposed to high temperatures and gas pressures under operation [1–3]. Subjected to the starting and stopping control, the performance of SOFCs is gradually degraded [4,5]. One of the degradation factors can be thermal expansive deformation due to temperature change [6,7], while the expansive deformation under a reducing environment is a characteristic of SOFCs [8,9]. These deformations inevitably invoke an unexpectedly large stress owing to the mutual constraints of the components, which causes mechanical deterioration. In addition, creep plays a primary role in long-term operation at high temperatures. Various studies on numerical calculations have been conducted to analyze the electrochemical and mechanical deformations of SOFCs under operation [10–18].

To enable the prediction of such mechanical degradation of SOFCs during operation, we previously developed an analysis system for electrochemical and mechanical coupling phenomena [19,20] by incorporating general-purpose finite element analysis software and its pre-/post-processing functions. We also conducted validation analyses to examine its ability to quantitatively reproduce measured data [20,21]. Through numerical examples, the mathematical model implemented in the developed system was validated. The dependences of material properties on the temperature and the chemical potential of

oxygen are empirically obtained and stored in separate spreadsheets then introduced into the system so that the actual operation environment can be realized. After the potential simulations, deformation problems are then solved. The temperature-induced strain and reduction or oxidation-induced strain calculated in the transient analysis for the potentials, which are also stored in spreadsheets beforehand and used in the stress analyses for the quantitative evaluation of creep deformation. However, stress-free distributions of SOFCs have not been considered in our previous simulations, although several studies pointed out the residual stress distributions in SOFCs [22,23].

In this study, we perform simulations whose start points of simulations are set at a high temperature under the assumption of a stress-free distribution during cell sintering. The deformation during the temperature decrease after sintering is reflected not only in the initial shape of the cell at room temperature, but also in the deformation behavior during operation. The time variation of the cell shape is clarified in terms of thermal, chemical, and creep strains. In this study as well as [10], the thermal strain and creep strain during temperature change are calculated. On the other hand, we do not investigate any effect of reduction strain relating to Ni-NiO [24]. It is noted that the stress free-state is indicated a condition at which the cell is sintered. In the simulation method proposed by the authors in the previous works, the stress-free condition is specified as the initial condition and we postulated that the cell is under the stress-free condition in the room

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temperature. This assumption is not necessarily correct since it suggests that there is no effect concerning the thermal shrinkage due to temperature decrease, which motivated us to investigate the shape deformation when a stress-free state at high temperature is considered.

2. Mathematical model for evolution of SOFC

2.1. Electrochemical model

The SOFC system is described by the motion of oxygen ions and electrons. The relationship between the electrochemical potentials of oxygen ions $\eta_{O^{2-}}$ and electrons η_{e^-} is expressed by the following equation of the local equilibrium:

$$\mu_O = \eta_{O^{2-}} - 2\eta_{e^-}, \quad (1)$$

where μ_O is the chemical potential of oxygen.

The local transport of the chemical potential of oxygen μ_O is governed by the following unsteady diffusion equations:

$$-\frac{c^i}{2F}\dot{\mu}_O = -\nabla \cdot \mathbf{i}_{O^{2-}} + j_{O^{2-}}, \quad (2)$$

$$-\frac{c^i}{2F}(-\dot{\mu}_O) = -\nabla \cdot \mathbf{i}_{e^-} + j_{e^-}, \quad (3)$$

where F is Faraday's constant and the capacitance of material i , $c^i = (-4F^2/V_m^i)\partial\mu_O/\partial\delta^i$, is assumed to depend on the concentration of oxygen vacancies δ^i and the molar volume V_m^i . The current densities of oxygen ions and electrons are denoted by $\mathbf{i}_{O^{2-}}$ and \mathbf{i}_{e^-} , and $j_{O^{2-}}$ and j_{e^-} are the reaction current densities of oxygen ions and electrons, respectively, which are generated in porous electrodes. $\mathbf{i}_{O^{2-}}$ and \mathbf{i}_{e^-} are defined as follows:

$$\mathbf{i}_{O^{2-}} = -(\sigma_{O^{2-}}^i/-2F)\nabla(\eta_{O^{2-}}), \quad (4)$$

$$\mathbf{i}_{e^-} = -(\sigma_{e^-}^i/-2F)\nabla(2\eta_{e^-}), \quad (5)$$

where $\sigma_{O^{2-}}^i$ and $\sigma_{e^-}^i$ are the ionic and electronic conductivities of material i , respectively, both of which are expressed as functions of temperature θ and the partial pressure of oxygen p_{O_2} , which is calculated by the following equation:

$$\mu_O = \mu_O^\circ + \frac{1}{2}R\theta \ln p_{O_2}, \quad (6)$$

where $\mu_O^\circ = 0$ is the oxygen potential under the standard condition and R is the gas constant. Substituting Eqs. (4) and (5) into Eqs. (2) and (3), respectively, and considering Eq. (1), the governing equations of potentials of the oxygen ions and electrons are obtained as follows [19–21]:

$$\frac{c^i}{2F}(2\dot{\eta}_{e^-} - \dot{\eta}_{O^{2-}}) = -\nabla^2\eta_{O^{2-}} + j_{O^{2-}}^i, \quad (7)$$

$$\frac{c^i}{2F}(\dot{\eta}_{O^{2-}} - 2\dot{\eta}_{e^-}) = -\nabla^2(2\eta_{e^-}) + j_{e^-}^i. \quad (8)$$

The reaction current densities are calculated using the following equations [21]:

$$j_{O^{2-}}^{\text{Anode}} = j_0^{\text{Anode}} p_{H_2}^{-0.03} p_{H_2O}^{0.4} \exp(-18400/\theta) \left\{ \exp \frac{2(1-\alpha)F\Delta E}{R\theta} - \exp \frac{-2\alpha F\Delta E}{R\theta} \right\}, \quad (9)$$

$$j_{O^{2-}}^{\text{Cathode}} = j_0^{\text{Cathode}} p_{O_2}^{0.2} \exp(-85859/\theta) \left\{ \exp \frac{2(1-\alpha)F\Delta E}{R\theta} - \exp \frac{-2\alpha F\Delta E}{R\theta} \right\}, \quad (10)$$

where j_0^{Cathode} and j_0^{Anode} are the exchange current densities, α is a constant, and $\Delta E = (\mu_{O^{\text{Gas}}} - \mu_{O^{\text{Solid}}})/2F$ is the difference in voltage, where $\mu_{O^{\text{Gas}}}$ and $\mu_{O^{\text{Solid}}}$ are the chemical potentials of oxygen in gas and solid phases, respectively.

2.2. Mechanical model

The governing equations of the deformation problem are written in the following forms [19,20]:

$$\nabla \cdot \mathbf{T} + \rho \mathbf{b} = 0, \quad (11)$$

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^c + \boldsymbol{\varepsilon}^r + \boldsymbol{\varepsilon}^\theta, \quad (12)$$

$$\mathbf{T} = \mathbf{C} : \boldsymbol{\varepsilon}^e, \quad (13)$$

$$\dot{\boldsymbol{\varepsilon}}^c = \dot{\gamma} \mathbf{T}' / \|\mathbf{T}'\|, \quad \dot{\gamma} = C_1 \|\mathbf{T}_{\text{eq}}\|^{C_2} \exp(-C_3/\theta), \quad (14)$$

$$\boldsymbol{\varepsilon}^\theta = \alpha \Delta \theta \mathbf{1}, \quad (15)$$

$$\boldsymbol{\varepsilon}^r = \beta \Delta \delta \mathbf{1}, \quad (16)$$

where \mathbf{T} is the Cauchy stress, ρ is the mass density, \mathbf{b} is the body force, $\boldsymbol{\varepsilon}$ is the total strain, $\boldsymbol{\varepsilon}^e$ is the elastic strain, $\boldsymbol{\varepsilon}^c$ is the creep strain, $\boldsymbol{\varepsilon}^r$ is the chemical strain, $\boldsymbol{\varepsilon}^\theta$ is the thermal strain, \mathbf{C} is the elastic constant tensor, \mathbf{T}' is the deviatoric stress, \mathbf{T}_{eq} is the equivalent stress, and C_1, C_2, C_3 are material parameters. The reduction or oxidation-induced strain $\boldsymbol{\varepsilon}^r$ is evaluated by the multiplication of the change in the vacancy δ by the reduction expansion coefficient β , and the thermal strain $\boldsymbol{\varepsilon}^\theta$ is calculated by multiplying the change in temperature θ and the thermal expansion coefficient α . The standard Dirichlet boundary condition is used in the deformation problem.

3. Analysis procedure

In the electrochemo-mechanical multiphysics analysis procedure, we first generate a model and mesh for the cell. Next, operation conditions such as the temporal temperature, the partial pressure of hydrogen, current, and voltage are input. Then, we perform electrochemical analysis and visualize the result. For use in the deformation analysis, the obtained results for temporal chemical strain and thermal strain in the electrochemical analysis are saved. Finally, the boundary condition of the cell is input, a mechanical simulation is performed, and the results are visualized.

4. Numerical results and discussion

4.1. Simulation for a button cell composed of LSCF/8YSZ/Ni-YSZ

On the basis of the developed method, we conduct electrochemo-mechanical analysis under the stress-free assumption during sintering. The analysis model is shown in Fig. 1. Our anode-supported button cell model consists of a nickel/yttria-stabilized zirconia (Ni-YSZ) for anode, an 8 mol% yttria stabilized zirconia (8YSZ) for electrolyte, and a $\text{La}_{0.6}\text{Sr}_{0.4}\text{Co}_{0.2}\text{Fe}_{0.8}\text{O}_{3-\delta}$ (LSCF) for cathode. The thicknesses of the layers of the cell composed of LSCF/8YSZ/Ni-YSZ are 0.02 mm for LSCF, 0.01 mm for 8YSZ and 0.4 mm for Ni-YSZ. The electrochemical and mechanical boundary conditions are shown in Fig. 2. Open circuit voltage condition is imposed on the surface of the electrolyte (Fig. 2(a)). A rigid body is used to express the holding and support jig (Fig. 2(b)). As the control condition shown in Fig. 3, the simulation starts at 900 °C under the assumption of sintering of the button cell, then decreases to 700 °C, and again increased to 900 °C considered to be the operation temperature. Here, the simulation is not conducted at lower temperature than 700 °C, because the change in oxygen vacancy concentration is kinetically negligible due to the high cooling rate

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