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Numerical simulation and experimental characterization of the performance evolution of a liquid antimony anode fuel cell

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HIGHLIGHTS

- Long term discharging test of a liquid antimony anode fuel cell.
- Mechanistic modeling of liquid antimony anode fuel cell.
- Observation and analytical explanation of the fuel cell performance evolution.

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ABSTRACT

A solid oxide fuel cell (SOFC) with a liquid antimony anode is fabricated based on a smooth single crystal YSZ electrolyte substrate and a porous Pt cathode. The performance of the liquid antimony anode was tested under "battery mode", with the anode chamber shielded in argon throughout the test and the cathode exposed to air. Polarization curves were taken and a long term constant potential discharging test was carried out afterwards. Taking electrochemical reaction, mass transport and microstructure of the liquid Sb anode into consideration, a one dimensional mathematical model was built and then validated by the polarization curve and the constant potential discharging performance curve obtained during the test. This model analyzes the metallic Sb distribution in the anode during cell operation, explains the cell performance evolution base on the microstructural development of the liquid Sb anode and simulates how the anode microstructure affects the cell performance.

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1. Introduction

Liquid antimony (Sb) anode solid oxide fuel cell is a promising power generation technology that could convert the carbon fuel directly into electricity [1–3]; the fuel cell exhibits stable performance [4] and satisfying tolerance of impurities during operation. Both Sb and Sb_2O_3 are in their liquid phase under cell operation circumstances, a special characteristic that provides extra convenience for mass and charge transfer in the anode region, and the mixed conducting structure formed by electrochemical oxidation of metallic Sb could promote the cell performance [2]. The liquid Sb anode showed excellent performance during operation both in battery mode [5] (Sb direct electrochemical oxidation with oxygen ions) and in fuel cell mode [6].

It's widely believed that metallic antimony is electrochemically oxidized into antimony trioxide (Sb_2O_3) when fuel cell is operating [6,7]. Therefore, to investigate the liquid Sb anode working process, one should closely evaluate the electrochemical oxidation of metallic Sb:

$$2Sb + 3O^{2-} \rightarrow Sb_2O_3 + 6e^- \quad (1)$$

For detailed research on this reaction, the liquid Sb anode should be operated under an inert atmosphere without any fuel supplement; this operation mode can also be noted as the "battery mode" of liquid Sb anode.

The interface between liquid antimony anode and the electrolyte also plays an important role in fuel cell performance. Because the electrochemical oxidation of liquid metallic Sb in the anode is a liquid–solid biphasic reaction, its reaction kinetics could be greatly influenced by the interface topological structure [7]. To simplify this effect, we choose a smooth interface for experimental tests.

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Nomenclature

Abbreviation

EIS	electrochemical impedance spectrum
OCV	open circuit voltage
SOFC	solid oxide fuel cell
TPB	triple phase boundary
YSZ	yttrium stabilized zirconium

English letter

A	pre-exponential factor of the Arrhenius form (in terms of m, mol and s)
c	concentration of species (mol m^{-3})
c_{Sb}^{ini}	the initial concentration of metallic Sb (mol m^{-3})
c_{Sb}	the metallic Sb concentrations in the liquid anode (mol m^{-3})
$c_{Sb_2O_3}^{ini}$	the initial concentration of antimony oxide (Sb_2O_3) (mol m^{-3})
$c_{Sb_2O_3}$	the Sb_2O_3 concentrations in the liquid anode (mol m^{-3})
D^{eff}	effective diffusion coefficient (m^2 s^{-1})
D_{Kn}^{eff}	effective Knudsen diffusion coefficient (m^2 s^{-1})
D_{mole}^{eff}	effective molecular diffusion coefficient (m^2 s^{-1})
$D_{Sb-Sb_2O_3}$	binary diffusion coefficient of Sb in Sb_2O_3(m^2 s^{-1})
E	activation energy (kJ mol^{-1})
F	Faraday constant (96,384C mol^{-1})
i_0	exchange current density (A m^{-2})
k	reaction rate constant (in terms of m, mol and s)
M	molecular weight (kg mol^{-1})
n_t	total number of electronic and ionic conducting particles
$n_{t,an}$	total number of electronic and ionic conducting clusters in anode
n_{ep}	fraction number of electronic conductor particles
n_{ip}	fraction number of ionic conductor particles
n_{Sb}	fraction number of Sb clusters
$n_{Sb_2O_3}$	fraction number of Sb_2O_3 clusters
p	pressure (Pa)
P_{ep}	whole range connection probability of electronic conductor particles
P_{ip}	whole range connection probability of ionic conductor particles
P_{Sb}	whole range connection probability of Sb clusters
$P_{Sb_2O_3}$	whole range connection probability of Sb_2O_3 clusters
$\bar{r}$	average pore radius of cathode (m)
r_{ep}	mean radius of the electronic conductor particle in cathode (m)
R	gas constant (8.314 mol^{-1} K^{-1}) or source term of mass balance equation (mol m^{-3} s^{-1})
$R_{Sb,\ elec}$	rate of Sb oxidation by electrochemical reaction (mol m^{-3} s^{-1})
$\dot{s}_{Sb,elec}$	electrochemical consumption rate Sb (mol m^{-2} s^{-1})
$S_{TPB,an}$	electrochemical active area in anode per unit volume (m^2 m^{-3})
$S_{TPB,ca}$	TPB active area in cathode per unit volume (m^2 m^{-3})
T	temperature (K)
$Q_{elec,an}$	electronic current source in anode (A m^{-3})
$Q_{elec,ca}$	electronic current source in cathode (A m^{-3})
$Q_{ion,an}$	ionic current source in anode (A m^{-3})
$Q_{ion,ca}$	ionic current source in cathode (A m^{-3})
V	diffusion volume
$V_{elec,an}$	electronic potential in anode (V)
$V_{elec,ca}$	electronic potential in cathode (V)
$V_{ion,an}$	ionic potential in anode (V)
$V_{ion,ca}$	ionic potential in cathode (V)
$V_{ion,el}$	ionic potential in electrolyte (V)
$V_{ref,an}$	reference potential in anode equal to OCV (V)
$V_{ref,ca}$	reference potential in cathode set to zero (V)
W	molecular weight of gas species (kg mol^{-1})
x	molar fraction
X	specific dimension of metallic antimony/antimony oxide cluster
Z	mean coordination number of electronic and ionic conductor particles
Z_{an}	mean coordination number of Sb and Sb_2O_3 clusters in the anode
Z_{ep}	coordination number of electron conductor particles
Z_{ip}	coordination number of ionic conductor particles
Z_{Sb}	coordination number of Sb clusters
$Z_{Sb_2O_3}$	coordination number of Sb_2O_3 clusters
$Z_{Sb\text{-}Sb}$	coordination number between two metallic Sb clusters
$Z_{Sb-Sb_2O_3}$	coordination number between Sb and Sb_2O_3 clusters
$Z_{Sb_2O_3-Sb_2O_3}$	coordination number between two metallic Sb_2O_3 clusters

Greek letters

α_{an}	anode charge transfer coefficient
α_{ca}	cathode charge transfer coefficient
β	cathode electrochemical kinetics parameter
ε	porosity of cathode
η_{an}	anode overpotential (V)
η_{ca}	cathode overpotential (V)
θ	contact angle between the electronic and ionic conductors (rad)
$\sigma_{elec,ca}^{eff}$	corresponding electronic conductor phase effective conductivity in cathode (S m^{-1})
$\sigma_{ion,ca}^{eff}$	corresponding ionic conductor phase effective conductivity in cathode (S m^{-1})
$\sigma_{elec,an}^{eff}$	corresponding electronic conductor phase effective conductivity in anode (S m^{-1})
$\sigma_{ion,an}^{eff}$	corresponding ionic conductor phase effective conductivity in anode (S m^{-1})
$\sigma_{ion,el}^{eff}$	corresponding ionic conductor phase effective conductivity in electrolyte (S m^{-1})
τ	tortuosity of cathode
$\partial\Omega$	computational domain

Subscripts

an	anode
ac	anode chamber
ca	cathode
cc	cathode chamber
el	electrolyte
elec	electronic
ep	electronic conductor particle
g	gas phase species
ion	ionic
ip	ionic conductor particle
Kn	Knudsen
mole	molecular
ref	reference
t	total

Superscripts

0	parameter at equilibrium conditions
bulk	bulk phase
eff	effective
TPB	triple phase boundary

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