Nanoscale Architectural Engineering for High-Performance Solid Oxide Fuel Cells

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Vision and Objectives

- Fuels cells are the most efficient, clean way to convert from chemical to electrical energy
- Solid oxide fuel cells offer fuel flexibility
- Potential near-term CO$_2$ emissions reduction (due to high efficiency)
  - No need to wait for hydrogen
- Barrier is cost
  - What matters is not absolute cost
  - It is cost/power (at ‘reduced’ temperatures)
- Dramatic improvements in performance
  - Imply lower cost/power and acceptance
State-of-the-art SOFCs

Conventional powder processing

> 1 W/cm² at 600°C

H₂ / air

Voltage (Volts)

Current density (mA.cm⁻²)

Power density (mW.cm⁻²)

0.0 0.2 0.4 0.6 0.8 1.0

0 1000 2000 3000 4000

0 200 400 600 800 1000

Ni-SDC | SDC | BSCF

800 μm anode

20 μm electrolyte

10 μm cathode

electrolyte surface


High power density reproduced in other labs

SDC = samaria doped ceria

BSCF = Ba₀.₅Sr₀.₅Co₀.₈Fe₀.₂O₃₋δ
Computational Modeling

Model validation

- Parameters obtained independently
- Model predicts experimental results

Model predictions
- architectural design
- 10x increase in power

Hypotheses

- Fuel electro-oxidation occurs on ceria surface, not limited to triple points
- Of the electrodes, anode is rate limiting
  - Cathode is fastest component
- Cathode is surface area limited
  - Bulk diffusion is rapid
- Electrolyte is grain boundary limited
- Prove hypotheses:
  - Lasting science & technological advances
Hydrogen electro-oxidation

- Impedance measurement

\[ \text{H}_2 + \text{O}^- \rightarrow \text{H}_2\text{O} + 2\text{e}^- \]

- Measurement also yields
  - ionic conductivity, electronic conductivity, electronic charge carrier concentration
**Hydrogen electro-oxidation**

very different metals, similar behavior  
matches electronic conductivity

$$\frac{1}{\rho_{\text{electrode}}} = \frac{1}{\rho^0_{\text{electrode}}} p_{O_2}^{-1/4}$$

$\sigma^0_{\text{electronic}}$

<table>
<thead>
<tr>
<th>Electrode</th>
<th>$\sigma^0_{\text{electronic}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pt</td>
<td>SDC15</td>
</tr>
<tr>
<td>Au</td>
<td>SDC15</td>
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</tbody>
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Hydrogen electro-oxidation

\[ \text{H}_2 + \text{O}^= \leftrightarrow \text{H}_2\text{O} + 2\text{e}^- \]

- Independent of metal
- Activation energy matches \( \sigma_{\text{electronic}} \)
- Reaction on ceria
- Rate-limiting step:

Target architecture

- “Triple points” not required
- Flexibility in choice of metal
- Oxide coating stabilizes structure
- Ceria is non-coking

Oxygen electro-reduction

- Impedance measurement

\[
\frac{1}{2} \text{O}_2 + 2e^- \rightarrow \text{O}^=\]

- Activation energy matches that for oxygen surface exchange (113 kJ.mol\(^{-1}\))

- Exchange rate measured indep’ly by \text{O}_2 permeation

- Bulk diffusion is fast (46 kJ.mol\(^{-1}\))

- Other ‘advanced’ cathodes
  - (PrSm)CoO\(_3\): 5.5 Ωcm\(^2\)
  - (LaSr)(CoFe)O\(_3\): 48 Ωcm\(^2\)

\[E_a=116 \text{kJ.mol}^{-1}\]

\[P(\text{O}_2) = 0.21 \text{atm}\]

\[0.5 - 0.6 \ \Omega\text{cm}^2\]

Oxygen electro-reduction

- **Reaction pathways**

  - **Electrode surface path**
    - $\text{O}_2$ ad → 2e$^-$ cathode
    - O$_2^-$ electrolyte

  - **Electrode bulk path**
    - $\text{O}_2$ ad → 2e$^-$ cathode
    - O$_2^-$ electrolyte

  - **Electrolyte surface path**
    - $\text{O}_2$ ad → 2e$^-$ cathode
    - O$_2^-$ electrolyte

- **(Ba$_{0.5}$Sr$_{0.5}$)(Co$_{0.8}$Fe$_{0.2}$)O$_{3-\delta}$**
  - Exceptionally high oxygen vacancy diffusivity
  - Exceptionally high vacancy concentration ($\delta \sim 0.4$)
  - No indication of vacancy ordering/clustering
  - Surface related step is rate-limiting

  $\leftarrow$ maximize surface area
Performance limiters

- Depending on the cell (electrode fabrication)
  - Anode can dominate: slow electro-oxidation reactions
  - Electrolyte can dominate: resistive grain boundaries
  - Cathode is always negligible
Target fuel cell architecture

- **Anode**
  - High surface-area, porous metal *coated with doped ceria*
  - Overall thickness?

- **Electrolyte**
  - 10 μm; clean or parallel grain boundaries

- **Cathode**
  - High surface-area, porous BSCF
  - Overall thickness?