Nanoscale Architectural Engineering for High-Performance Solid Oxide Fuel Cells

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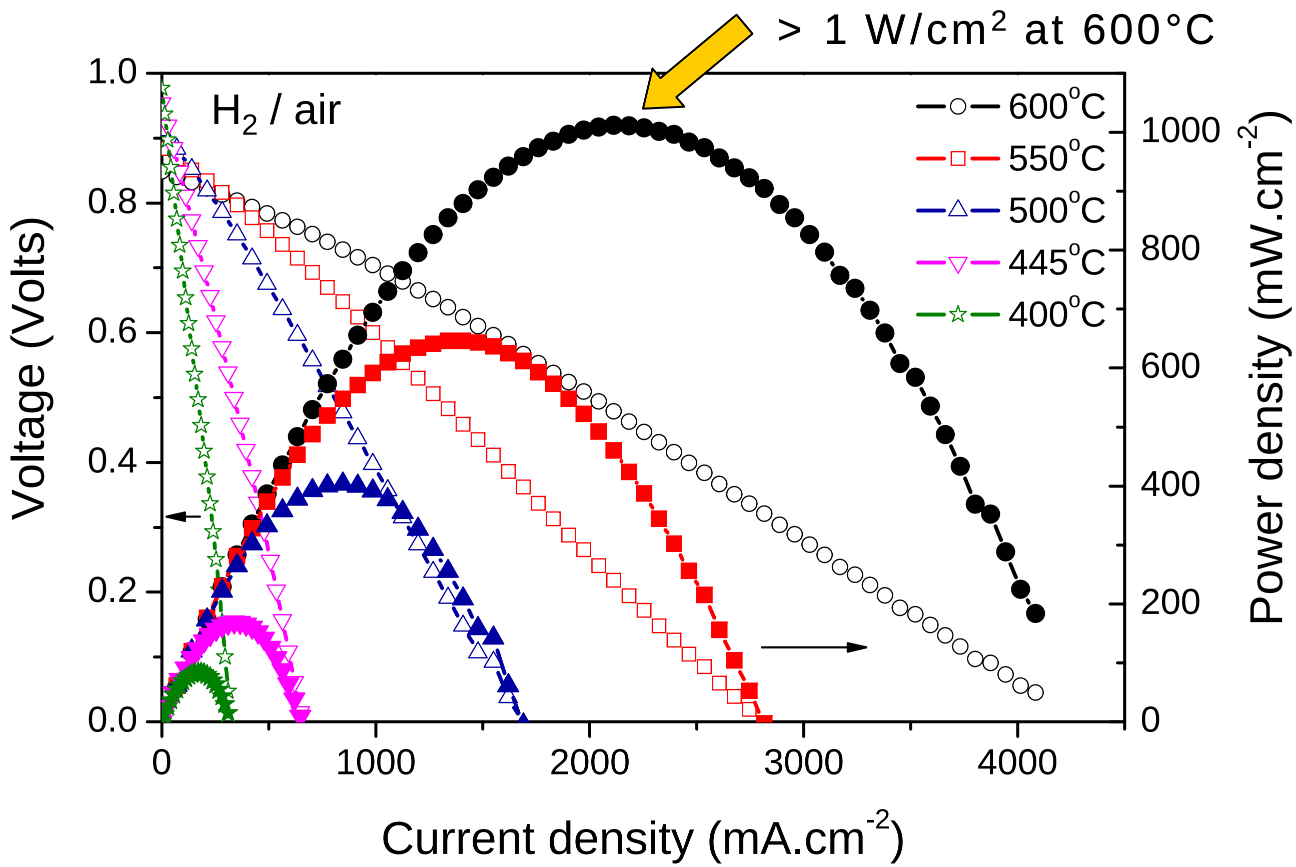
Vision and Objectives

- 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

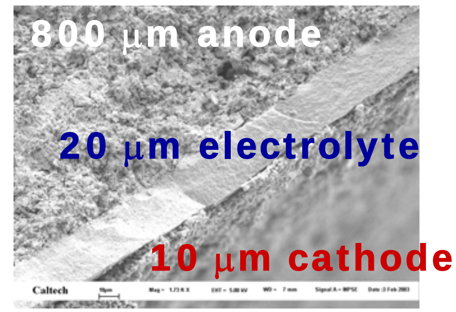
Conventional powder processing

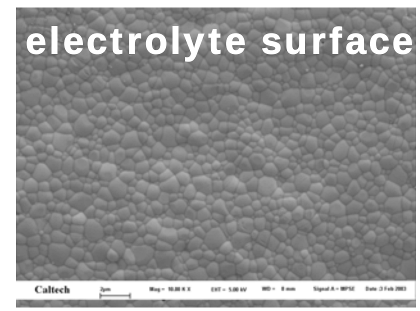


High power density reproduced in other labs

SDC = samaria doped ceria BSCF = $Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{3-\delta}$

Ni-SDC | SDC | BSCF

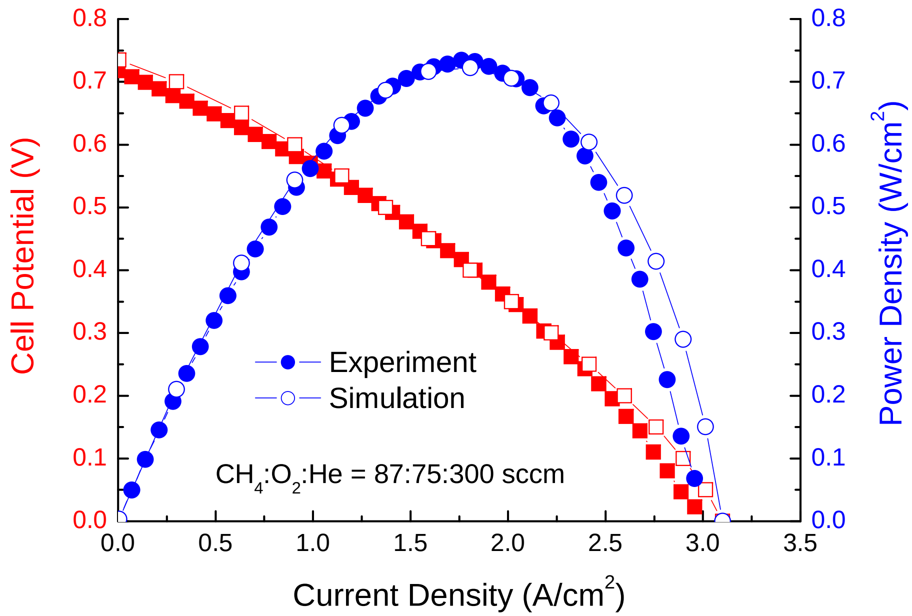




Z. Shao and S. M. Haile, *Nature* **431**, 170-173 (2004).

Computational Modeling

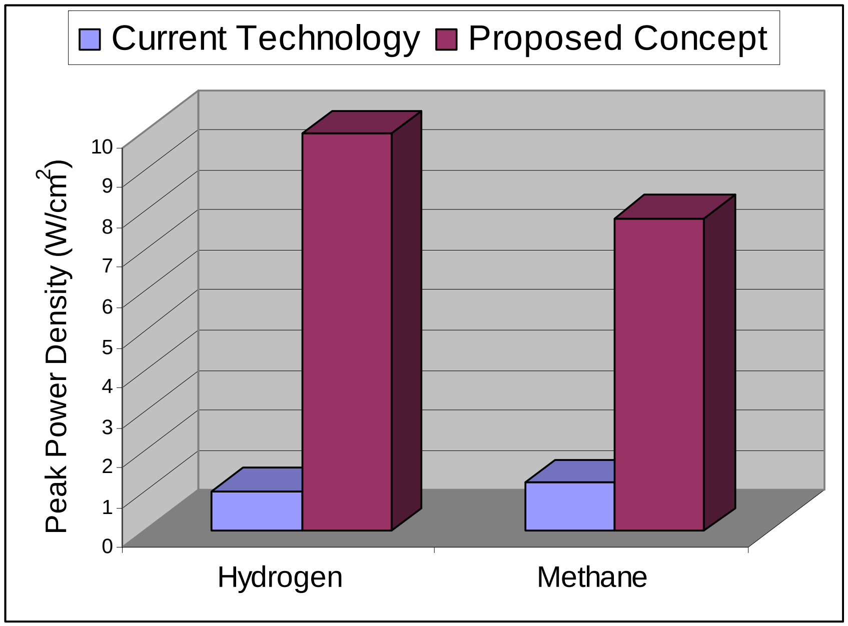
Model validation



- Parameters obtained independently
- Model predicts experimental results

Model predictions

- architectural design
- 10x increase in power



Based on fundamentals

Y. Hao, Z. Shao, J. Mederos, W. Lai, D. G. Goodwin and S. M. Haile, *Solid State Ionics* **177**, 2013-2021 (2006).

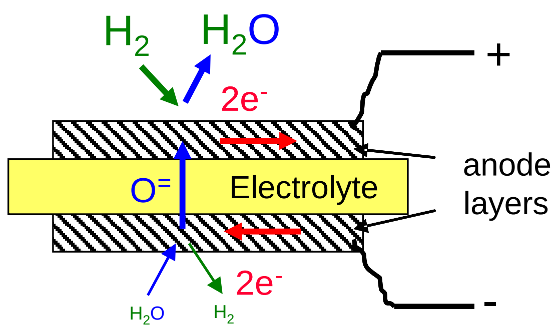
Hypotheses

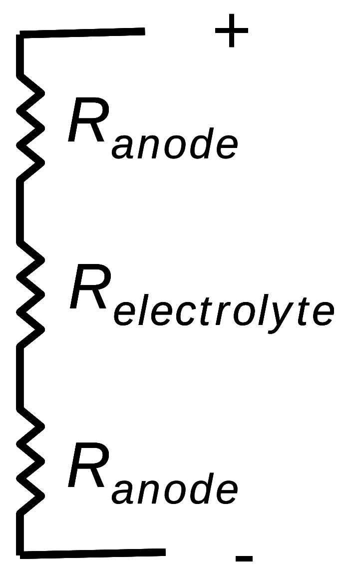
- Fuel electro-oxidation occurs on ceria surface, not limited to triple points
- Of the electrodes, anode is rate limiting
  - Cathode is fastest component
- Cathode is surface area limited
  - Bulk diffusion is rapid
- Electrolyte is grain boundary limited
- Prove hypotheses:
  - Lasting science & technological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

Hydrogen electro-oxidation

- Impedance measurement

$$H_2 + O^{=} \rightarrow H_2O + 2e^-$$

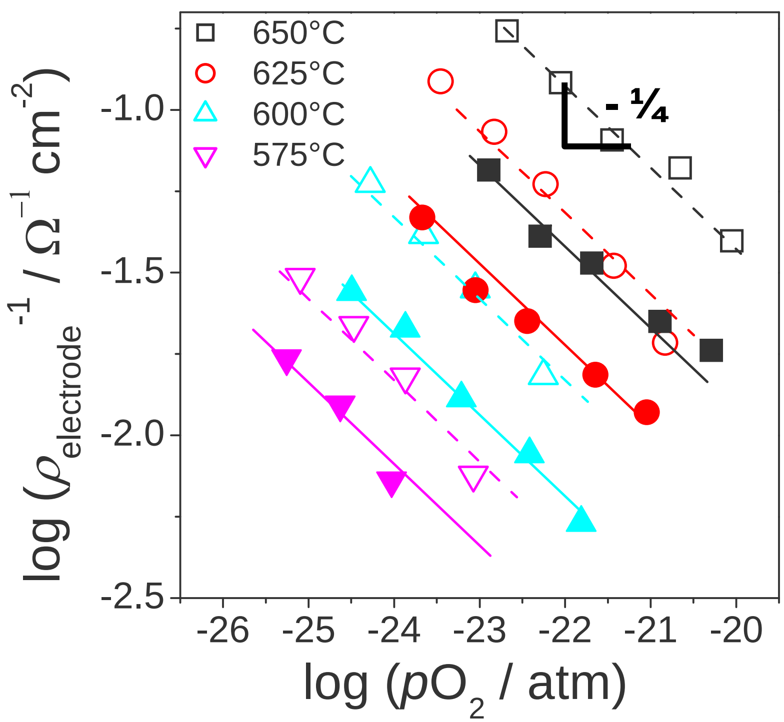




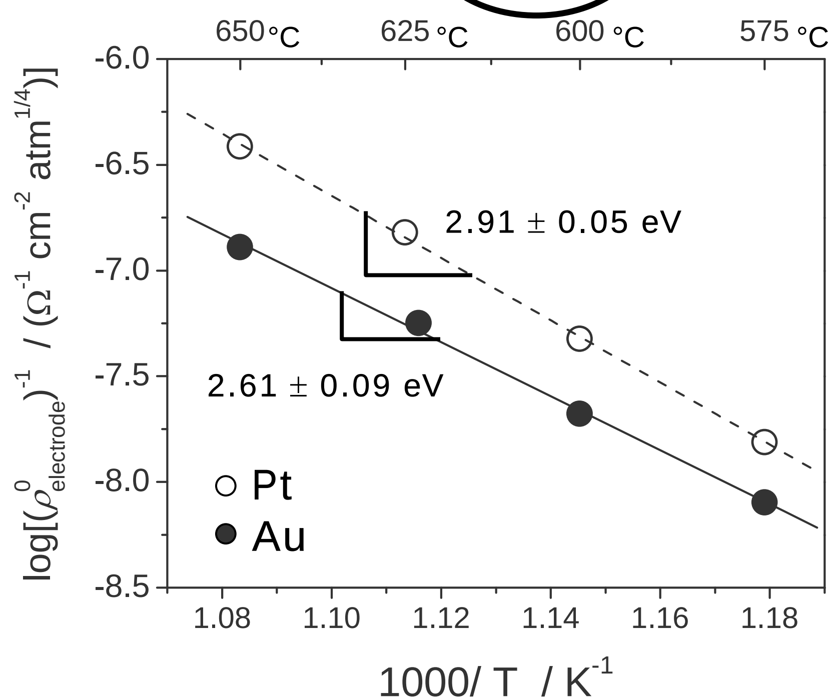
- Measurement also yields
  - ionic conductivity, electronic conductivity, electronic charge carrier concentration

Hydrogen electro-oxidation

open: Pt closed: Au



fit to $1/\rho_{electrode} = 1/\rho^{0}_{electrode} \bullet p_{O_2}^{-1/4}$



very different metals, similar behavior

matches electronic conductivity

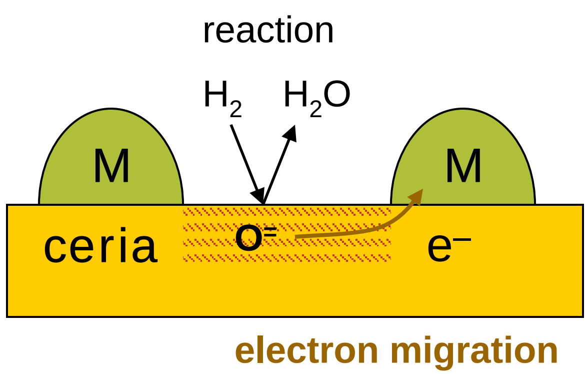
	$\sigma^{0}_{electronic}$
Pt|SDC15|Pt	2.41 $\pm$0.01 eV
Au|SDC15|Au	2.76 $\pm$ 0.05 eV

W. C. Chueh, W. Lai and S. M. Haile, *Solid State Ionics* (2008).

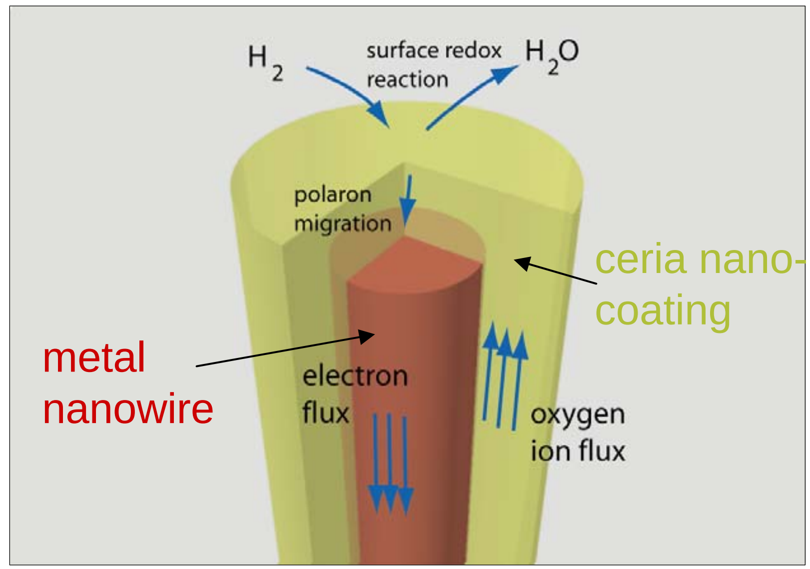
Hydrogen electro-oxidation

$H_2 + O^= \leftrightarrow H_2O + 2e^-$

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



Target architecture



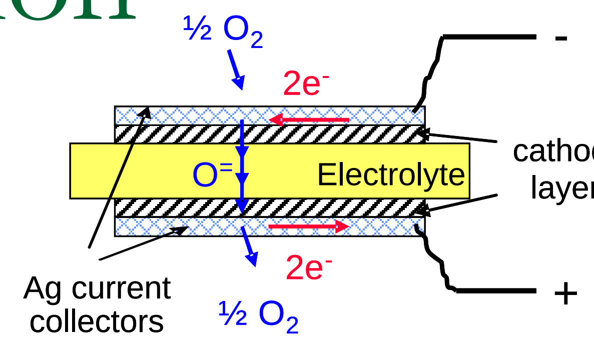
- "Triple points" not required
- Flexibility in choice of metal
- Oxide coating stabilizes structure
- Ceria is non-coking

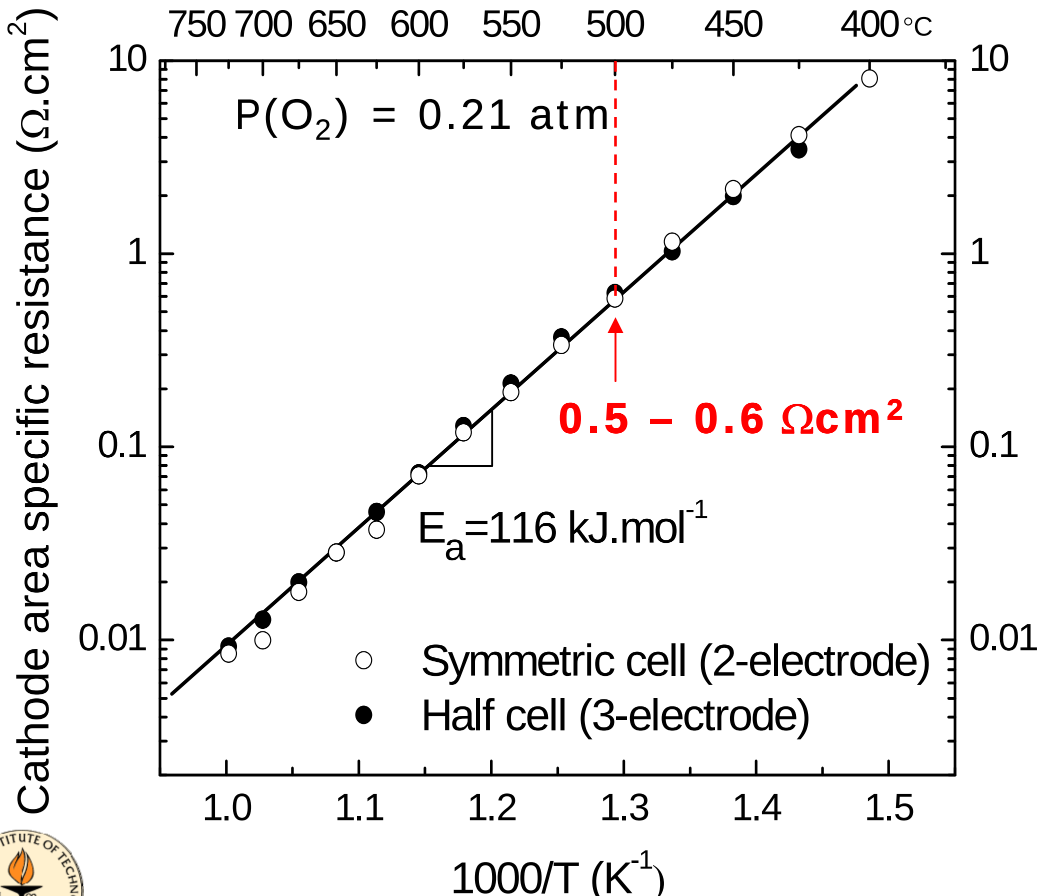
W. Lai and S. M. Haile, *J. Amer. Cer. Soc.* **88**, 2979–2997 (2005).

Oxygen electro-reduction

- Impedance measurement

$\frac{1}{2} O_2 + 2e^- \rightarrow O^=$



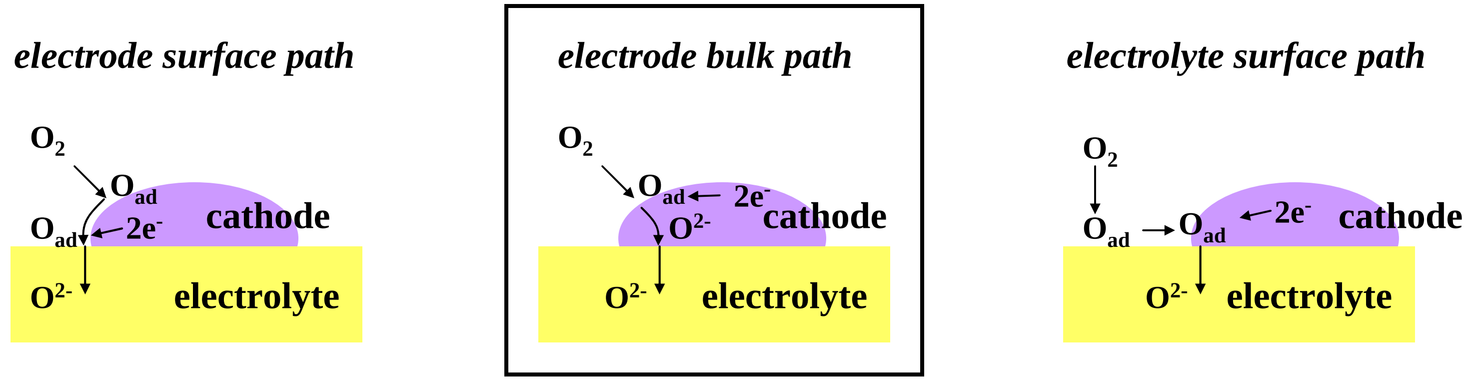


- Activation energy matches that for oxygen surface exchange (113 kJ.mol^{-1})
- Exchange rate measured indep'ly by O_2 permeation
- Bulk diffusion is fast (46 kJ.mol^{-1})
- Other 'advanced' cathodes
  - (PrSm)CoO_3: 5.5 Ωcm^2
  - (LaSr)(CoFe)O_3: 48 Ωcm^2

Z. Shao and S. M. Haile, *Nature* **431**, 170-173 (2004).

Oxygen electro-reduction

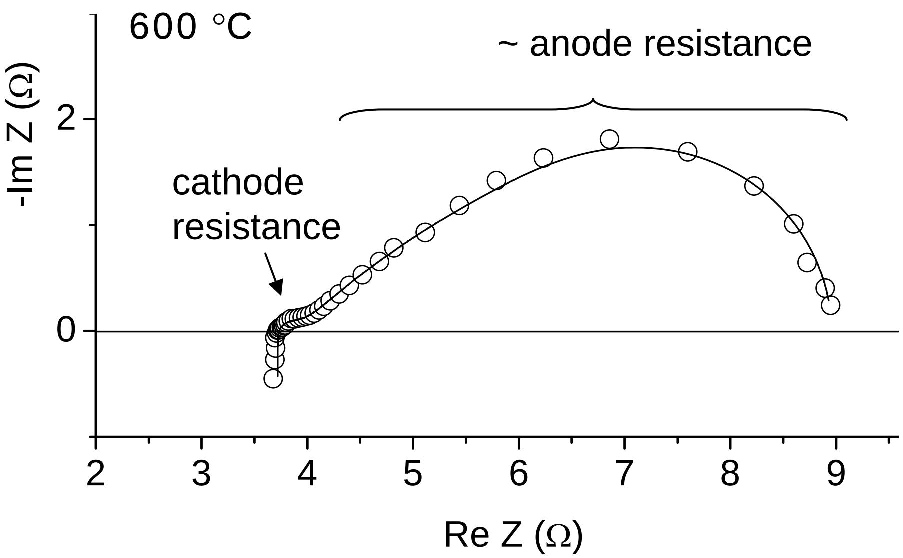
- Reaction pathways



- $(Ba_{0.5}Sr_{0.5})(Co_{0.8}Fe_{0.2})O_{3-\delta}$
  - Exceptionally high oxygen vacancy diffusivity
  - Exceptionally high vacancy concentration (δ ~ 0.4)
  - No indication of vacancy ordering/clustering
  - Surface related step is rate-limiting ← *maximize surface area*

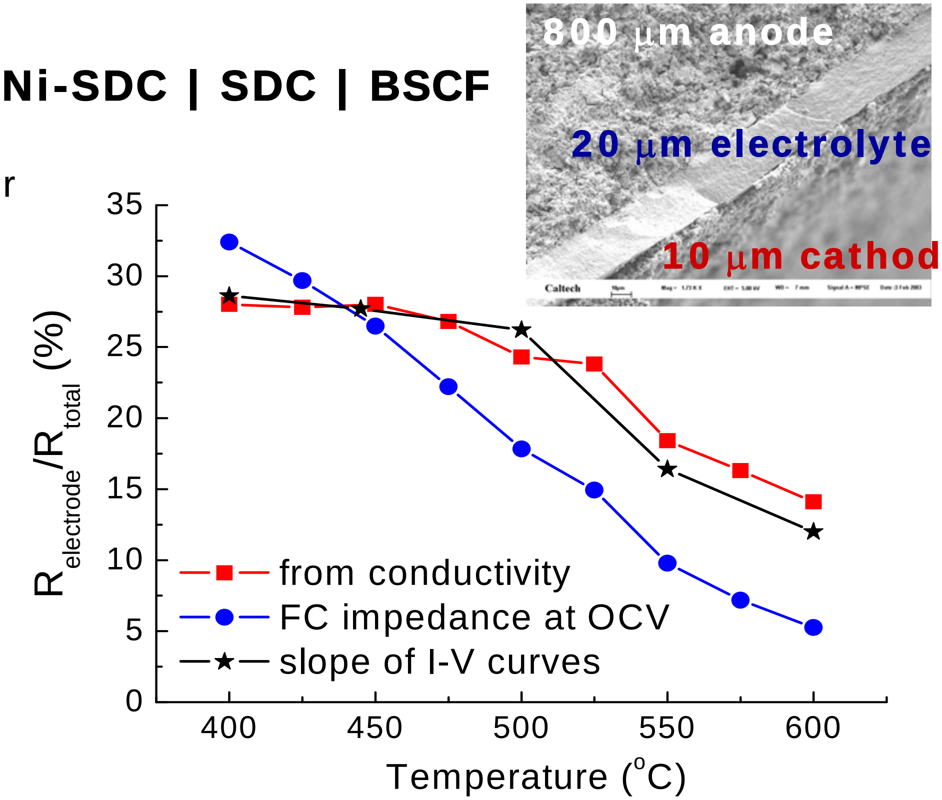
Performance limiters

Pt | SDC15 | BSCF



H_2/air

Ni-SDC | SDC | BSCF



- 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?