Fundamental Studies of SOFC Materials

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UF-DOE HiTEC
Highlights of:

Determination of Electrochemical Performance and Thermo-Mechanical-Chemical Stability of SOFCs from Defect Modeling

*DOE SECA Contract No: DE-FC26-02NT41562*
*DOE Project Manager: Travis Schultz*

- Advance the fundamental understanding of the continuum-level electrochemistry of oxide mixed ionic-electronic conductors.
- Obtain fundamental constants required for implementing the continuum-level electrochemical model from experiment.
- Extend the models to multilayer structures and incorporate microstructural effects.
- Verify the models through experiment.
- Develop a transient version of the continuum-level electrochemical model.
- Obtain time constants for various transport processes from electrical impedance spectroscopy to examine the effects of transients on SOFC performance.
- Develop and deliver software modules for incorporation of the continuum-level electrochemical model into SOFC failure analysis software used by NETL, PNNL, ORNL and the SECA industrial teams.

Electrocatalytically Active High Surface Area Cathodes for Low Temperature SOFCs

*DOE EE/FE Contract No: DE-FC26-03NT41959*
*DOE Project Manager: Lane Wilson*

- Develop a fundamental understanding of heterogeneous electrocatalytic phenomena at the surface of ion conducting ceramics.
- Fabricate high surface area SOFC cathodes with controlled microstructure and porosity.
- Develop low ASR cathodes for low to intermediate temperature SOFCs.

UF - DOE High Temperature Electrochemistry Center

*DOE Advanced Research, HiTEC Contract No: DE-AC05-76RL01830*
*DOE Project Manager: Lane Wilson*

- Develop the fundamental understanding of ionic transport in, and electrocatalytic phenomena on the surface of, ion conducting materials, spanning the range from first-principles calculations and molecular dynamic simulations of ionic transport and gas-solid interactions to synthesis and characterization of novel ion conducting materials and electrocatalysts.
Defect Energetics and Mobility Based on:
- Crystal structure
- Cation radii
- Cation polarizability
- Cation oxidation state
- Etc.

Defect Concentration Dependence on:
- Defect formation energy
- Temperature
- $P_{O_2}$

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- Crystal structure
- Cation radii
- Cation polarizability
- Cation oxidation state
- Etc.

Defect Concentration Dependence on:
- Defect formation energy
- Temperature
- $P_{O_2}$

\[
C_V = \left[ \frac{3}{4} K_r \rho P_{O_2}^{-\frac{1}{4}} + \left( \frac{A}{2} \right)^\frac{3}{2} \right]^2
\]
EXTENSION OF MODEL TO THERMO-MECHANICAL PROPERTIES

Thermal expansion
\[ \frac{a - a_0}{a_0} = \alpha \Delta T \]

Chemical expansion
\[ \frac{a - a_0}{a_0} = \frac{\theta}{a_0} c_V \]

Thermo-chemical expansion
\[ \frac{a - a_0}{a_0} = \alpha \Delta T + \frac{\theta}{a_0} c_V \]

Lattice constant, \( a \), has linear relationship with \( c_V \)

Therefore, \( r \sim a \sim c_V \)

\[
c_V = \left[ \frac{3}{4} K_1 r P_0 \frac{1}{2} + \left( \frac{A}{2} \right)^{\frac{3}{2}} \right]^{\frac{2}{3}}
\]
Thermo-Chemical Expansion of GDC

Thermo-Chemical Expansion \( \Delta l / l_0 \times 10^{-6} \)

- Heat up in air
- Dry Argon
- 5% wet H\(_2\)/N\(_2\)
- 50% wet H\(_2\)/N\(_2\)
- Dry H\(_2\)
- Wet H\(_2\)
- Cool down in H\(_2\)
- Decreasing pO\(_2\)
EXTENSION OF MODEL TO THERMO-MECHANICAL PROPERTIES

\[ \frac{\Delta l}{l_0} = \alpha \Delta T + \theta \left( \frac{3}{4} K R P_{O_2} \frac{1}{4} + \left( \frac{1}{2} A \right)^{\frac{1}{2}} \right)^2 \]

EXTENSION OF MODEL TO THERMO-MECHANICAL PROPERTIES

Lattice constant, $a$, has linear relationship with $c_v$

Therefore, $r \sim a \sim c_V$

$E_{bond} = \frac{A}{r^m} - \frac{B}{r^n}$

A, B, n and m are constants

$Y_{bond} = \frac{1}{r_0} \left( \frac{d^2 E}{dr^2} \right)_{r=r_0}$

$\frac{Y}{Y^*} \approx \left( \frac{a}{a_0} \right)^{-(\delta+3)}$

$\frac{a}{a_0} = \theta c_V + 1$

$Y \approx Y^* \left( \theta c_V + 1 \right)^{-(\delta+3)}$

$\delta$ is equivalent to:

- $n$ (if $A$ is constant)
- $m$ (if $B$ is constant)

as oxygen vacancies are introduced

EXTENSION OF MODEL TO THERMO-MECHANICAL PROPERTIES
Experimental Validation

H₂, H₂/H₂O, N₂, Air

Gas flow controller

Sample

Tube Furnace

Oxygen Sensor

PO₂ = 0.22 atm
PO₂ = 9.5 x 10⁻⁵ atm
PO₂ = 1.8 x 10⁻¹⁷ atm
PO₂ = 4.5 x 10⁻²² atm
PO₂ = 5.1 x 10⁻²⁵ atm

Vacancies preserved by fast cooling

50°C/min

800°C, 5 hr

Fast cool

Time, hr

Temp. °C

P₀₂

A

B

C

D

E

F
Nanoindents

Size: ~0.6 µm

Depth: ~125 nm

• Effect of crystallographic orientation on elastic modulus and hardness evaluated statistically by applying many indents on grains of known orientation.

• In-plane anisotropy can be measured by changing the indent orientation.

SEM image of surface after thermal etch. Average grain size ~12 µm.
EXTENSION OF MODEL TO THERMO-MECHANICAL PROPERTIES
Experimental Validation - Nanoindents and Microstructure

Nanoindents

Size: ~0.6 µm
Depth: ~125 nm

- 100 indents were applied on the sample, which covered 100 µm X 100 µm (~25 different grains)

Modulus: 218.35±11.12 GPa
Hardness: 9.00±0.73 GPa

- The small variations imply that ceria is elastically isotropic.

SEM image of surface after thermal etch.
Average grain size ~12 µm.
Effect of Oxygen Vacancy Population on Elastic Modulus of Ceria

Y, GPa

log(Po2), atm

(measured in air)

experiment
Effect of Oxygen Vacancy Population on Elastic Modulus of Ceria

\[ Y(P_{O_2}) \approx Y^* (\theta c_V P_{O_2} + 1)^{(-\delta + 3)} \]

(measured in air)
Effect of Oxygen Vacancy Population on Elastic Modulus of Ceria

(measured in air)

\[ Y(P_{O_2}) \approx Y^* (\theta_{cV}(P_{O_2}) + 1)^{-(\delta+3)} \]

\[ Y, \text{ GPa} \]

\[ \log(Po2), \text{ atm} \]
Effect of Oxygen Vacancy Population on Elastic Modulus of Gadolinia-Doped Ceria (GDC)

Y, GPa

log(Po2), atm

(measured in air)

experiment
Effect of Oxygen Vacancy Population on Elastic Modulus of Gadolinia-Doped Ceria (GDC)

\[ Y(P_{O_2}) \approx Y^* (\theta c_Y (P_{O_2}) + 1)^{(-d+3)} \]

( measured in air )
Effect of Oxygen Vacancy Population on Elastic Modulus of Gadolinia-Doped Ceria (GDC)

\[ Y(P_{O_2}) \approx Y^*(\theta c_V(P_{O_2}) + 1)^{-(\delta+3)} \]

(measured in air)
Effect of Oxygen Vacancy Population on Elastic Modulus of Yttria-Stabilized Zirconia (YSZ) (measured in air)

Y, GPa

log(Po2), atm
Effect of Oxygen Vacancy Population on Elastic Modulus of Yttria-Stabilized Zirconia (YSZ)

Higher temperature and higher current will shift decrease in modulus to higher $P_{O_2}$
Effect of Oxygen Vacancy Population on Elastic Modulus of Ceria, GDC, YSZ

\[ Y(PO_2) \approx Y^* (\theta c_V (PO_2) + 1)^{-(\delta+3)} \]

Extend to Include Microstructural Effects:

\[ Y(p) = Y_{p=0} (1-p)^r \quad \text{where } p \text{ is porosity and } r \approx 2 \text{ for porous ceramics [1]} \]

\[ Y(PO_2, p) = Y^* (\theta c_V (PO_2) + 1)^{-(\delta+3)(1-p)^r} \]

EXTENSION OF MODEL TO THERMO-MECHANICAL PROPERTIES

\[ Y(P_{O_2}) \approx Y^* \left( \theta \left( \frac{3}{4} K_R^{1/2} P_{O_2}^{-1/4} + \left( \frac{1}{2} A \right)^{3/2} \right) + 1 \right)^{-(\delta+3)} \]

\[ \frac{\Delta l}{l_0} = \alpha \Delta T + \theta \left( \frac{3}{4} K_R^{1/2} P_{O_2}^{-1/4} + \left( \frac{1}{2} A \right)^{3/2} \right) \]

SAME!

\( K_R = \) Equilibrium constant for \( V_{O^{**}} \) formation

\( A = \) Dopant concentration

\( \theta = \) Empirical constant = \( 3.2 \times 10^{-3} \) nm\(^3\) [1,2]

**FUNDAMENTAL QUANTITATIVE DEFECT CONSTANTS**

\[ K_R \]

Thermodynamics of Oxides
•Computational and experimental thermodynamics of SOFC materials.

Equilibrium constant for \( V_{O^{\cdot \cdot}} \) formation

\[ O_{O^X} = V_{O^{\cdot \cdot}} + 2e' + 1/2O_2 \]

\[ K_R = \frac{[V_{O^{\cdot \cdot}}]^n P_{O_2}^{0.5}}{[O_{O^X}]} \]

Calculated Zr-O phase diagram

*UF-DOE HiTEC*
FUNDAMENTAL QUANTITATIVE DEFECT CONSTANTS

\[ \theta = ? \]

Computational Materials Thrust

• Large-scale molecular dynamics simulations to elucidate the effects ionic radius and polarizability of on ionic conductivity, the structure of vacancy clusters, and the mechanisms of oxygen transport.

• First principles, electronic structure simulations. Calculation of defect formation energy in oxides from first principles and thermodynamics. Study of oxygen reactions at surfaces and interfaces.

\[ E_{\text{bond}} = \frac{A}{r^m} - \frac{B}{r^n} \]

A, B, n and m are constants

UF-DOE HiTEC
FUNDAMENTAL QUANTITATIVE DEFECT CONSTANTS

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Defect formation energies as a function of $P_{O_2}$

Ab-initio calculation of ZrO$_2$ grain boundary and comparison with Z-contrast TEM image
FUNDAMENTAL PROPERTIES

**LaFeO₃**: Rhombohedrally distorted perovskite

**Calculated Lattice Constants**

- $a = 3.7822 \ \text{Å}$
- $c = 3.6493 \ \text{Å}$

**Cutoff Energy**: 500 eV  
**Exchange-Correlation approximation**: LDA  
**K-POINT spacing**: 2X2X2

**DEFECT EQUILIBRIA**

- **Brouwer Region I**
  - $c_e = 2c_{V_e}$

- **Brouwer Region IIa**
  - $c_{D} = 2c_{V_e}$

- **Brouwer Region IIb**
  - $c_{D} = c_h$

- **Brouwer Region III**
  - $3c_{V_e} + 3c_{V_B} = c_{h}$

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**Same approach being applied to perovskites**

- Defect equilibria already developed
- Structural optimization in progress

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CATHODE DEVELOPMENT

Optimize Microstructure for:

- **Activation Polarization**
  - Electrocatalytic Activity
    - Increase specific catalytic activity
    - Increase TPB
    - Dispersed catalyst

- **Ohmic Polarization**
  - Electronic vs. Ionic Transport
    - Electronic conduction path
    - Ionic conduction path

- **Concentration Polarization**
  - Gas transport
    - Graded porosity
    - Gas vs. solid state transport
CATHODE DEVELOPMENT - Electrocatalytic Activity

- **Temperature programmed reaction (TPR)**
  - Ramp temperature in reacting gas mixture to determine catalytic activity and selectivity
- **Temperature programmed desorption (TPD)**
  - Ramp temperature in He to determine adsorbed species
CATHODE DEVELOPMENT - Electrocatalytic Activity

Set up for $^{18}\text{O}_2$ probe molecule with $^{16}\text{O}$ oxide catalyst:

$^{18}\text{O}_2 = ^{18}\text{O}_2$ - phys-adsorbed

$^{18}\text{O}_2 = ^{18}\text{O}^{16}\text{O}$ - scrambled product

$^{18}\text{O}_2 = ^{16}\text{O}_2$ - lattice oxygen

Kinetics of scrambled product formation indicative of charge transfer reaction and surface exchange coefficient, $k_o$

NO used as probe molecule:

$\text{NO} = \frac{1}{2}\text{N}_2 + \frac{1}{2}\text{O}_2$

vs.

$\text{O}_2 = \text{O}_2$
Effect of B-site transition metal on catalytic activity:

- Cations with partially filled d-orbitals (Co, Ni) more active
- Ru most active
• Potential programmed reaction (PPR)
  – Ramp voltage in reacting gas mixture to determine catalytic activity and selectivity
• Potential programmed desorption (PPD)
  – Ramp voltage in He to determine adsorbed species

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CATHODE DEVELOPMENT - Electrocatalytic Activity

\[ \text{O}_\text{O}^x \leftrightarrow \text{V}_\text{O}^{18O} + 2e' + \frac{1}{2} \text{O}_2 \]

\[ K_R = \frac{k_o}{k_o} \]

Include:
- Electrode structure
- Current-voltage behavior: \( i_o \sim k_o, k = f(V) \)
CATHODE DEVELOPMENT - Electronic vs. Ionic Transport

Benchmark

C. Xia, Y. Zhang, M. Liu, Appl. Phys. Lett., Vol. 82, No. 6, 10 February 2003
CATHODE DEVELOPMENT - Electronic vs. Ionic Transport

C. Xia, Y. Zhang, M. Liu, Appl. Phys. Lett., Vol. 82, No. 6, 10 February 2003
Relative size of ionic/electronic conducting phase

- Same volume fractions
- ESB particle size reduction
CATHODE DEVELOPMENT - Electronic vs. Ionic Transport

Stability @ 650°C (100h) in air

Smaller ESB particle size increases stability

However, ASR still increases with time under current due to electromigration of Ag
New Cathode Materials - Pyrochlores

- High Electrical Conductivity $\sim 10^3$ Scm$^{-1}$
- Metallic (increases with decreasing temperature)

K. S. Lee, J. Solid state Chem. 131 (1997), 405
CATHODE DEVELOPMENT - Electronic vs. Ionic Transport

C. Xia, Y. Zhang, M. Liu, Appl. Phys. Lett., Vol. 82, No. 6, 10 February 2003
CATHODE DEVELOPMENT - Electronic vs. Ionic Transport

![Cathode Images and Diagram]

Interfacial resistance, $\Omega \cdot \text{cm}^2$

- **BRO$_7$s-ESBvm**
- **BRO$_7$vm-ESBvm**
- **BRO$_7$vm-ESBs**

Temperature range: 500°C to 700°C
EXTEND MODEL TO INCLUDE MICROSTRUCTURAL EFFECTS

CATHODE

\[ P_{O_2, \text{cathode-electrolyte interface}} = P_{\text{atmos}} - \left( P_{\text{atmos}} - P_{O_2 @ air} \right) \exp \left( \frac{kT}{4q} \frac{\tau_c}{D_c} \frac{L_c}{\varepsilon_c} J \right) \]

ANODE

\[ P_{H_2, \text{anode-electrolyte interface}} = P_{H_2 \text{@ fuel}} - \frac{kT}{2q} \frac{\tau_a}{D_a} \frac{L_a}{\varepsilon_a} J \]

\[ P_{H_2O, \text{anode-electrolyte interface}} = P_{H_2O \text{@ fuel}} + \frac{kT}{2q} \frac{\tau_a}{D_a} \frac{L_a}{\varepsilon_a} J \]

DEFECT CONCENTRATION

\[ K\big|_{J=0} \exp \left( \frac{q\eta}{kT} \right) = \frac{c_v c_e^2}{1 - c_v} P_{O_2}^{1/2} \]

ACTIVATION OVERPOTENTIAL

\[ J = J_0 \left[ \exp \left( \frac{q}{kT} \alpha \eta \right) - \exp \left( -\frac{q}{kT} (1 - \alpha) \eta \right) \right] \]

POTENTIAL

\[ \Phi_{\text{ext}} - \Phi_{th} = \frac{k_B T}{z_V q} \ln \frac{c_{V_L}}{c_{V_0}} = \frac{z_V u_e + u_V \left( 1 - \frac{\eta}{\Phi_{th} - \Phi_{ext}} \right)}{u_e - u_V \left( 1 - \frac{\eta}{\Phi_{th} - \Phi_{ext}} \right)} \]

\[ \Phi_{\text{ext}} - \Phi_{th} = \frac{k_B T}{z_V q} \ln \frac{c_{V_L}}{c_{V_0}} = \frac{u_e c_A / z_V}{u_e - u_V \left( 1 - \frac{\eta}{\Phi_{th} - \Phi_{ext}} \right)} \]

\[ \Phi_{\text{ext}} - \Phi_{th} = \frac{k_B T}{z_V q} \ln \frac{c_{V_L}}{c_{V_0}} = \frac{u_e c_A / z_V}{u_e - u_V \left( 1 - \frac{\eta}{\Phi_{th} - \Phi_{ext}} \right)} \]

S. Chan, K. Khor, Z. Xia, J. Power Sources, 93 (2001) 130
• Electrochemical model (with pore diffusion incorporated) matches “Virkar”* model, but with less fitting parameters, (3 vs. 10)

• Fitting parameters: $\tau_a/D_a$ (effective tortuosity anode), $\tau_c/D_c$ (effective tortuosity cathode) and $i_o$ (exchange current density).

EXTEND MODEL TO INCLUDE MICROSTRUCTURAL EFFECTS

I-V & power density curves can also be generated for mixed conducting materials:

- Electrolytes such as GDC (above)
  - Shows reduction in OCP and current density due to low $t_i$ at 800°C

- Cathodes such as LSF and LSCF (near future)
EXTEND MODEL TO INCLUDE MICROSTRUCTURAL EFFECTS

\[
\frac{\tau_a}{D_a} = \frac{\tau_c}{D_c} = 10^2 \text{ s/m}^2 \\
i_o = 0.1 \text{ A/cm}^2
\]

Model shows decrease in effective tortuosity (\(\tau/D\))
can dramatically increases power density
DECONVOLUTION OF CATHODE MECHANISM

Oxygen exchange at TPB (0.0001 s)

Ionic conductivity through electrolyte grain boundary

Ionic conductivity in the bulk electrolyte

Artifacts minimized by nulling

Dissociation and surface diffusion of O-species on LSM to TPB (0.18 s)

Oxygen diffusion through porous cathode (5.9 s)
# DECONVOLUTION OF CATHODE MECHANISM

<table>
<thead>
<tr>
<th>Step #</th>
<th>Process identity</th>
<th>“x” in ( R \propto pO_2^x )</th>
<th>( E_a ) (eV)</th>
<th>( \tau ) (s) at 800 °C</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Ionic diffusion through electrolyte bulk.</td>
<td>~0 Independent</td>
<td>1.10&lt;sup&gt;a&lt;/sup&gt; 1.05&lt;sup&gt;d&lt;/sup&gt;</td>
<td>-</td>
</tr>
<tr>
<td>2</td>
<td>Ionic diffusion across electrolyte grain boundary.</td>
<td>~0 Independent</td>
<td>1.04&lt;sup&gt;b&lt;/sup&gt; 1.16&lt;sup&gt;d&lt;/sup&gt;</td>
<td>-</td>
</tr>
<tr>
<td>3</td>
<td>Migration and incorporation of ( O^{2-} ) from TPB into YSZ.</td>
<td>~0 Independent&lt;sup&gt;a&lt;/sup&gt;</td>
<td>0.97&lt;sup&gt;a&lt;/sup&gt; 1.10&lt;sup&gt;a&lt;/sup&gt; 1.13&lt;sup&gt;b&lt;/sup&gt;</td>
<td>8.5 \times 10^{-5} 1.6 \times 10^{-5}&lt;sup&gt;a&lt;/sup&gt;</td>
</tr>
<tr>
<td>4</td>
<td>Dissociation and surface diffusion of O-species on LSM.</td>
<td>-0.15&lt;sup&gt;a,c&lt;/sup&gt; -0.268&lt;sup&gt;a,c&lt;/sup&gt;</td>
<td>1.2 1.61&lt;sup&gt;a&lt;/sup&gt; 1.69&lt;sup&gt;b&lt;/sup&gt;</td>
<td>0.18 0.016&lt;sup&gt;a&lt;/sup&gt;</td>
</tr>
<tr>
<td>5</td>
<td>Gas diffusion through porous electrode.</td>
<td>-1.1&lt;sup&gt;a&lt;/sup&gt; -1.02&lt;sup&gt;a,c&lt;/sup&gt;</td>
<td>~0 ~0&lt;sup&gt;a&lt;/sup&gt;</td>
<td>5.9 0.16&lt;sup&gt;a&lt;/sup&gt;</td>
</tr>
</tbody>
</table>

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DECONVOLUTION OF CATHODE MECHANISM

Microstructure/Impedance - LSCF Sintering Temperature Effect

- Highest temperature coarsens microstructure - multiple changes to impedance

Powder supplied by NexTech
Focused Ion Beam
• Enables 3-D analysis of electrode microstructure
  - Particle-size, pore-size, & distribution
  - Triple-phase boundary density
  - Tortuosity

QUANTIFYING MICROSTRUCTURE
QUANTIFYING MICROSTRUCTURE

AREA FRACTION

- Measure grain to interface line distance
- **LSM-YSZ Grain Interface**
- **Pore-YSZ Interface**

- Sample shown is screen-printed LSM sintered at 1350° C

![Image](image_url)

**Total Grain Interface: 8.1 um**
**Total Pore Interface: 4.9 um**

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AREA FRACTION

By combining consecutive line analysis, area density analysis is achieved.

Percent of grain density per total area is current approach.

Example: 67% grain-to-interface density

\[
\begin{array}{c}
\text{Lg/Total: 64\%} \\
\text{Lg/Total: 71\%} \\
\text{Lg/Total: x\%} \\
\text{Lg/Total: x\%} \\
\end{array}
\]
QUANTIFYING MICROSTRUCTURE

VOLUME FRACTION

- Measure grain and pore area
- By analyzing over multiple evenly spaced slices, volume fraction can be determined.

- Ex.: 89% Area Grain
- Sample shown is screen-printed LSM sintered at 1350°C

Total Grain Interface: 8.1 um
Total Pore Interface: 4.9 um
QUANTIFYING MICROSTRUCTURE

VOLUME FRACTION

By combining consecutive area analysis, a volume density analysis can be achieved.
QUANTIFYING MICROSTRUCTURE

TRIPLE PHASE LINE DENSITY

- Calculate triple phase boundary density
- Triple-phase points

Sample shown is screen-printed LSM sintered at 1350°C

LSM

YSZ

13 μm

Triple Phase Points: 9

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By connecting all of the triple phase points, the interface lines can be determined in the sample.
QUANTIFYING MICROSTRUCTURE

Butler-Volmer Equation:

\[ J = J_0 \left[ \exp(q_0 \eta_{act}/kT) - \exp(-q(1-\alpha)\eta_{act}/kT) \right] \]

\[ J_0 = j_0 \times A_{TPB} = L_{TPB} \times w_{TPB} \]

LSM/YSZ  
\[ w_{TPB} \approx \text{Debye length} \]

LSM/GDC, LSCF/YSZ, LSCF/GDC  
\[ w_{TPB} > \text{Debye length} \]

\[ w_{TPB} = f(\text{geometry, contact area, material property}) \]
QUANTIFYING MICROSTRUCTURE

Tortuosity

\[ \tau = \frac{z_{\text{path}}}{z_{\text{thickness}}} \]

 LSM (Nextech) on YSZ

Consecutive 50nm slices
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