Phase field modeling on initial microstructure effect on grain coarsening and concomitant property degradation in SOFC electrodes

Yinkai Lei [1,2], Tianle Cheng [1,3] and Youhai Wen [1]

[1]US Department of Energy, National Energy Technology Laboratory, Albany OR; [2]Oak Ridge Institute for Scientific Education, Oak Ridge, TN; [3]AECOM Corporation, Albany OR

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Introduction

Purpose of this research:

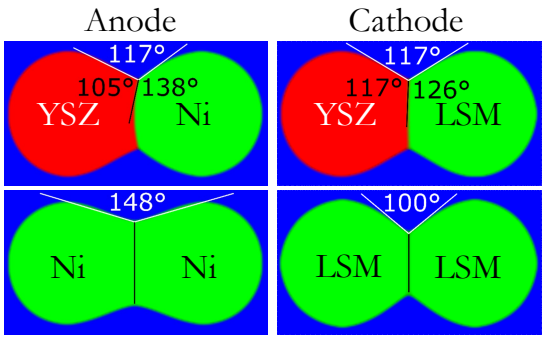
- Simulate microstructure evolution and concomitant property degradation in SOFC electrodes.
- Link attributes of initial microstructure to the rate of property degradation in SOFC electrodes.

Coarsening in SOFC electrodes:

- Driven by the interface curvature of particles/grains in different sizes.
- Leads to loss of TPB density, specific surface area and effective conductivity in both anode and cathode [1,2].

Phase field modeling

- Capable of simulating long term microstructure evolution.
- Properties of electrode can be extracted directly from simulated microstructures.
- The interfacial energy in our recently developed phase field model [1] can be easily tuned to match the interfacial energy of the real materials, i.e. Ni-YSZ for anode and LSM-YSZ for cathode.
- The mobility is tuned to match the self-diffusivity of Ni and LSM in bulk, while YSZ is kept static due to its slow self-diffusion.



Adapted from Ref. [1]

Attributes of initial microstructure

Composition

- Porosity: 30%.
- Ni/LSM: 25%~45%.
- YSZ: 45%~25%.

Average grain radius

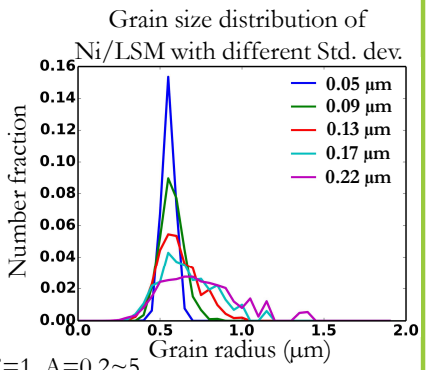
- YSZ: 0.55 μm
- Ni/LSM: 0.44~0.69 μm

Std. dev. of grain radius

- YSZ: 0.13 μm
- Ni/LSM: 0.05~0.22 μm

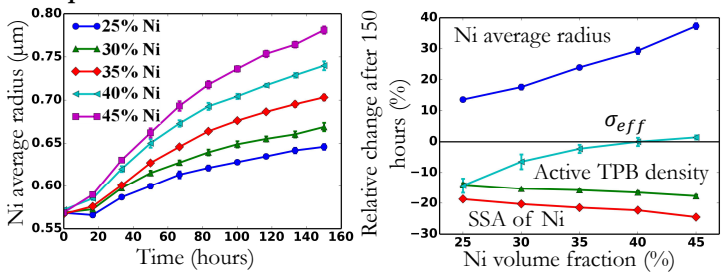
Grain shape

- Three principle axes: B=C=1, A=0.2~5
- Ellipsoid grains, A axis aligned in z-direction



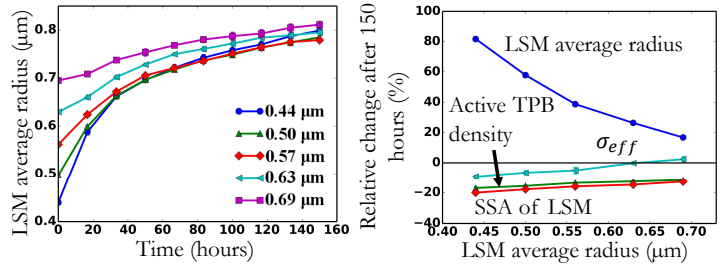
Results

Compositional effect



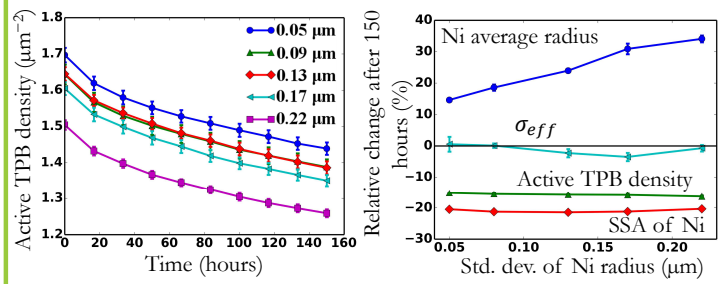
- The rate of grain coarsening and degradation of active TPB density and specific surface area (SSA) of Ni/LSM increase with increased Ni/LSM volume fraction.
- The degradation rate of effective conductivity decrease with increased Ni/LSM volume fraction.

Grain size effect



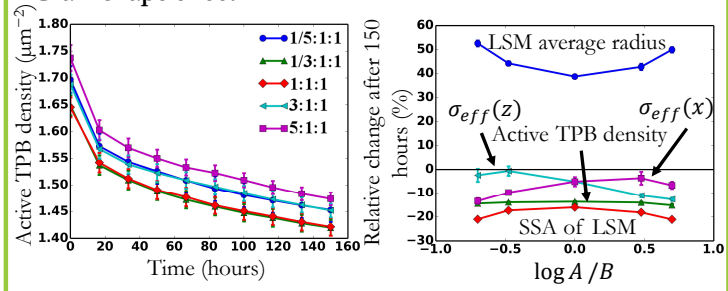
- Both the rate of coarsening and property degradation decrease with increased average grain size of Ni/LSM.

Std. dev. effect



- The rate of grain coarsening increase with increased standard deviation of Ni/LSM radius.
- The degradation rate of active TPB density, SSA and effective conductivity is insensitive to the standard deviation of Ni/LSM radius, but the value of properties depends on it.

Grain shape effect



- The rate of grain coarsening and degradation of SSA increase with increased aspect ratio.
- The degradation rate of active TPB density is insensitive to the grain shape.
- Anisotropic degradation rate of effective conductivity in the electrodes with non-equiaxed grains.

Conclusions

- The rate of coarsening and property degradation can be tuned by adjusting the composition, grain size and grain shape of the initial microstructures.
- Standard deviation of the initial grain size of Ni/LSM phase has limited effect on the rate of property degradation, but affects the value of properties.

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References

[1] Lei et al, J Power Sources, 345, 275-289 (2017)

[2] Zekri et al, Phys Chem Chem Phys, (2017), doi: 10.1039/C7CP02186K

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