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

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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.

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

The authors would like to thank Drs. Kirk Gerdes, Gregory Hackett, Harry Abemuth, Long-Qing Chien, Paul Salvador, William Epling and Tom Kalapos for valuable technical discussions. This project was supported in part by an appointment to the Internship/Research Participation Program at the National Energy Technology Laboratory, US Department of Energy, administered by the Oak Ridge Institute for Science and Education.

Acknowledgement:
The authors would like to thank Drs. Kirk Gerdes, Gregory Hackett, Harry Abemuth, Long-Qing Chien, Paul Salvador, William Epling and Tom Kalapos for valuable technical discussions. This project was supported in part by an appointment to the Internship/Research Participation Program at the National Energy Technology Laboratory, US Department of Energy, administered by the Oak Ridge Institute for Science and Education.

References

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.