**Phase-Field Modeling of Three-Phase SOFC Cathode Microstructures**

**National Energy Technology Laboratory-The Pennsylvania State University**

Linyun Liang1,2, Qun Li1,2, Kirk Gerdes1, and Long-Qing Chen1,2

1US DOE-National Energy Technology Laboratory

2The Pennsylvania State University

e-mail: [lul22@psu.edu](mailto:lul22@psu.edu) Phone: (814) 865-0389

The cathode microstructure is known to have a large impact on the performance of solid oxide fuel cells (SOFCs). Due to the high operating temperature, the life time and degradation of cathodes are major concerns for commercial applications. It is generally accepted that the performance of a cathode is largely governed by triple phase boundary (TPB) densities where the main reduction reaction occurs. In this work, a phase-field model for describing three-phase cathode microstructures (i.e., electrode-phase, electrolyte-phase and pore-phase) and their evolutions in SOFCs is proposed based on the diffuse-interface theory. Conserved composition and non-conserved grain orientation order parameters are simultaneously chosen to describe the coupled phase coarsening and grain growth in cathodes. The dihedral angles at the triple phase junction are determined by the experimental measurements of surface and interfacial energies. The simulated results well produce the three-phase cathode microstructures and their coarsening processes. The TPB length density measured as a function of evolution time indicates that the major degradation happens in the early stage. The extracted tortuosities from simulated cathode microstructures in terms of coarsening time and molar fractions of solid phases are also discussed. This work can contribute to the microstructural optimization of SOFC performance and to the understanding of long-term baseline degradation.