On the Mechanisms of Cathode Degradation in SOFCs: A Phase-Field Model

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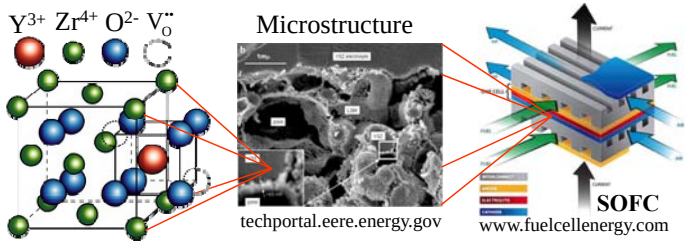
Office of Research and Development

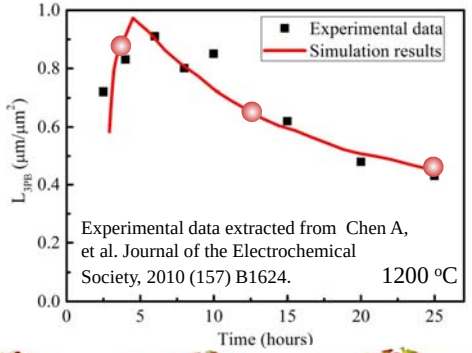
Objectives

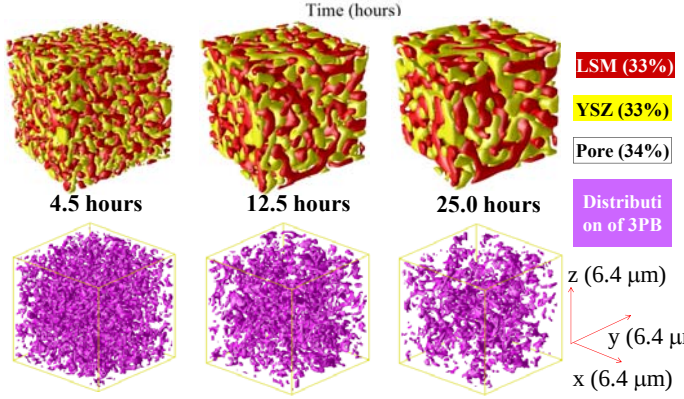
Understanding the mechanisms of cathode degradation from the level of microstructure



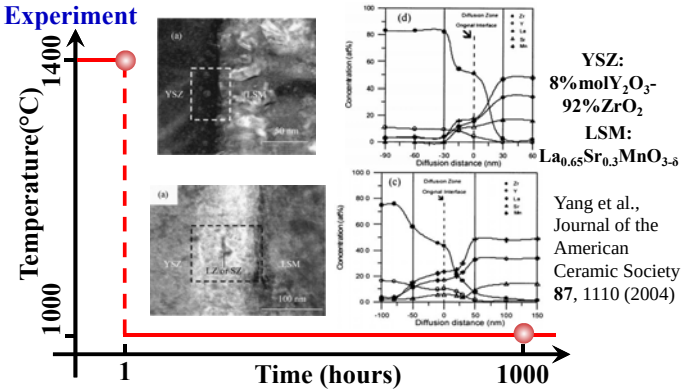
- **Modeling time-dependent changes in the morphology of electrode**
  - **Coarsening (particle growth), 3PB length, …**
- **Modeling time-dependent changes in the distributions of ions**
  - **Cation interdiffusion, oxygen vacancy / electron diffusion…**

Morphological evolution

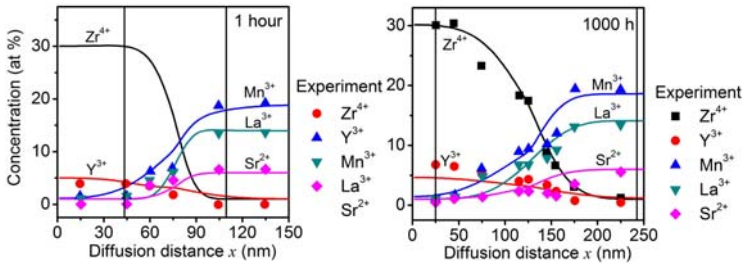




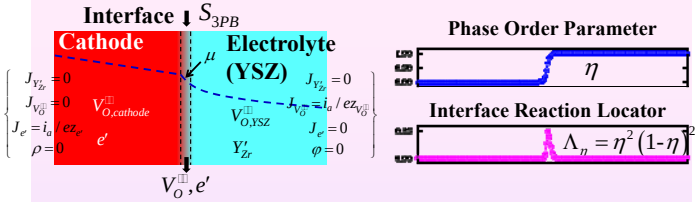
Cation interdiffusion



Phase-field simulations



Oxygen vacancy / electron diffusion



Schematic of one-dimensional electrochemical phase-field model across the cathode/electrolyte interface. The phase order parameter and interface reaction locator are shown on the right.

❑ **Thermodynamics of diffusion**

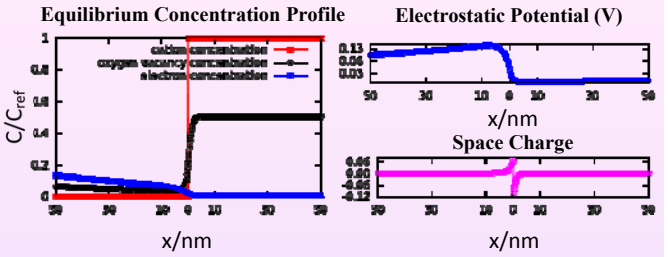
- **Electrochemical potential**

$$\bar{\mu}_i = \mu_i^o + k_B T \ln X_i + z_i e\varphi, \qquad i \in \left\{V_O^{\square}, e', Y'_{Zr}\right\}$$

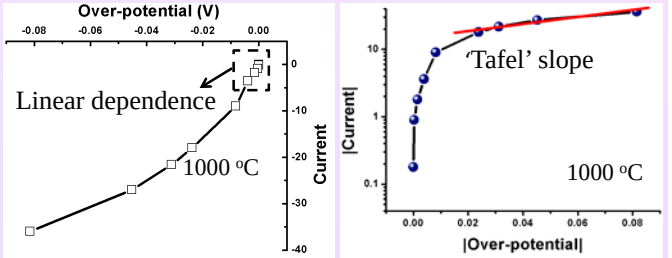
- **Diffusion and Poisson's equation**

$$\begin{cases} \dfrac{\partial c_i(x,t)}{\partial t} = -\nabla \cdot J_i = \nabla \cdot D_i \nabla c_i(x,t) + \nabla \cdot \dfrac{D_i z_i e c_i}{k_B T} \nabla\varphi - \left|J_i^{ext}\right| K \Lambda_\eta, \quad K = 1 \Big/ \int_0^{+\infty} \Lambda_\eta dx, \\ \varepsilon_0 \varepsilon \nabla^2 \varphi = -e \sum_i z_i c_i(x) = -2e c_{V_O^{\square}}(x) + e c_{e'}(x) + e c_{Y'_{Zr}}(x) \end{cases}$$

❑ **Results**



Equilibrium profiles of concentration, electrostatic potential and space charges under flux $J_{e'}^* = 50$, $J_{V_O^{\square}}^* = -25$.



Magnitude of the current as a function of the over-potential

Summary

Phase-field models are developed to simulate/predict:

- three-dimensional cathode microstructure (including 3PB) evolution during coarsening
- cation interdiffusion profiles across an electrode-electrolyte interface
- oxygen vacancy / electron diffusion across an electrode-electrolyte interface under electric current loading

These models can be adapted to describe the microstructure coarsening and ionic diffusion in SOFC anodes.

Acknowledgement

As part of the National Energy Technology Laboratory's research portfolio, this work was conducted under the RES contract DE-FE0004000.