Background and Motivation
The performance of solid oxide fuel cells (SOFCs) can be improved by introducing nanoparticles onto the electrode backbone to influence both the microstructural properties and electrochemical activity of the electrode. However, the amount of improvement is in some way limited by the properties of the backbone.

Purpose of the Study
This study focuses on the optimization of the microstructure of a Lanthanum Strontium Manganese (LSM)/Yttria-Stabilized Zirconia (YSZ) backbone for nanoparticle infiltration via an in-house-developed multiphysics simulation.

Electrochemical model
• Butler-Volmer model (anode)
\( i_{\text{an}} = \frac{\beta_{\text{an}} F \nu_{\text{an}}}{R T} \exp \left( \frac{-\theta_1 F \nu_{\text{an}}}{R T} \right) \)
• Multistep oxygen reduction reaction (ORR) model (cathode)
\( \text{surface adsorption and dissociation (sob)}: \quad \frac{1}{2}O_2 + e^- + \text{ORR} \)
\( \text{surface charge transfer (act)}: \quad \frac{1}{2}O_2 + e^- + \text{ORR} \)
\( \text{incorporation (inc)}: \quad \frac{1}{2}O_2 + e^- + \text{ORR} \)
\( \text{bulk charge transfer (bt):} \quad \beta_{\text{bt}} \frac{1}{2}O_2 + e^- + \text{ORR} \)

Performance improves via nanoparticle infiltration
• After infiltration, the charge transfer resistance, especially the surface adsorption and dissociation step, is significantly reduced, while the concentration resistance is slightly increased.
• Ohmic resistance dominates the resistance of infiltrated backbone.

Multiphysics Modeling

Baseline LSM/YSZ backbones

LSM/YSZ infiltrated with nano-LSC

Summary
• Multiphysics simulations with multistep ORR mechanism were developed and calibrated to investigate the performance of LSM/YSZ composite backbones before and after nanoparticle infiltration.
• For baseline backbones and infiltrated backbones, the backbone LY_64-P_22 (\( V_{\text{LSM/YSZ}} = 50\% \) with finest grain size) shows the best performance, while the backbone LY_64-P_00 (\( V_{\text{LSM/YSZ}} = 60\% \) with coarsest grain size) shows the largest resistance.
• The infiltration mainly promotes the charge transfer, especially the surface adsorption and dissociation step, of cathode. After infiltration, the ohmic resistance becomes more dominant over polarization resistance.

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