Optimum Microstructure and Phase Composition of Solid Oxide Fuel Cell Electrodes with Infiltrated Nanocatalysts

Shiwoo Lee[1,2], Tao Yang[1,2], Bo Guan[1,3], Harry W. Abernathy[1,2], Thomas L. Kalapos[1,2], Gregory A. Hackett[1]

[1]U.S. DOE, National Energy Technology Laboratory, Morgantown WV; [2]Leidos Research Support Team, Morgantown WV; [3]West Virginia University, Morgantown WV

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Introduction

Background & Motivation

- Infiltration with nanocatalysts has been widely adopted as a post-processing of electrode fabrication due to its simplicity and efficiency in improving electrochemical activity of composite electrode backbones.
- However, the conventional electrode scaffold or backbone was not designed for the additional process. A conventional electrode backbone is required to be modified for the additional infiltration process for optimization in performance.

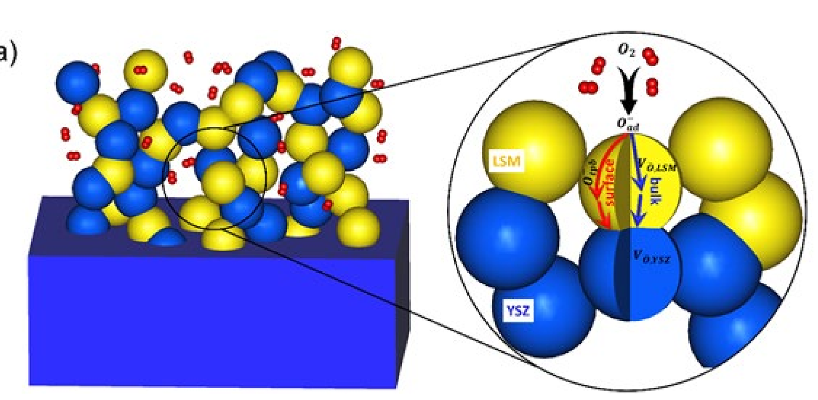
Purpose of the study

- To understand whether the conventional SOFC cathode microstructure, typically optimized without considering the performance change associated with infiltration, needs to be adjusted to benefit fully from the infiltrated nanocatalysts.

Methodology

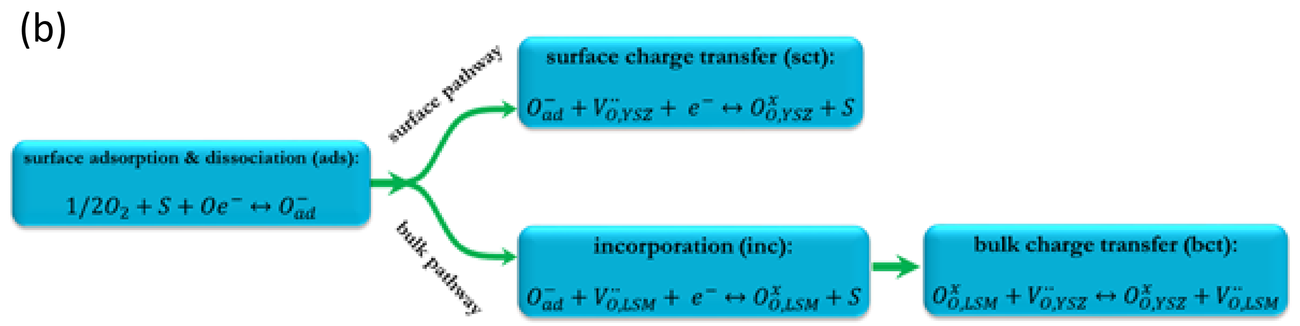
Calibrated Multistep ORR modeling

(a)



- Sketch of parallel surface and bulk pathways for oxygen reduction between LSM and YSZ:
- (a) 3D sketch,
- (b) pathways with detailed reaction steps.

(b)



- The developed multiphysics model considers all the basic physical/electrochemical processes occurring within the SOFCs.
- Mathematically, these highly coupled processes are formulated by sets of partial differential equations with specific expressions for different corresponding physics.

Charge conservation (electron-conducting phase)

$$a_{int} C_{DL} \frac{\partial}{\partial t}(\varphi_e - \varphi_i) + \nabla \cdot (-\sigma_e \nabla \varphi_e) = i_F$$

Species transport

$$\varepsilon \frac{\partial \phi}{\partial t} = \nabla \cdot \left(D_\phi^{eff} \nabla \phi\right) - S_\phi$$

- In our study, the complicated nonlinear coupled system of partial differential equations is solved, numerically, by in-house developed FORTRAN codes..

References

- T. Yang et al., *Journal of The Electrochemical Society*, 166(8), pp F448-F457, 2019.
- T. Yang et al., *International Journal of Hydrogen Energy,* 43(32), pp 15445-15456, 2018.
- T. Yang et al, *Physical Chemistry Chemical Physics*, 19(45), pp 30464 – 30472, 2017.
- T. Yang et al., *International Journal of Electrochemical Science*, 12, pp 6801-6828, 2017.

Results

Baseline LSM-YSZ backbones (Volume fractions & Grain size)

Parameters:

1) Volume fraction

$V_{LSM}:V_{YSZ} = 40\%:60\%, 50\%:50\%$, or $60\%:40\%$

2) Grain size

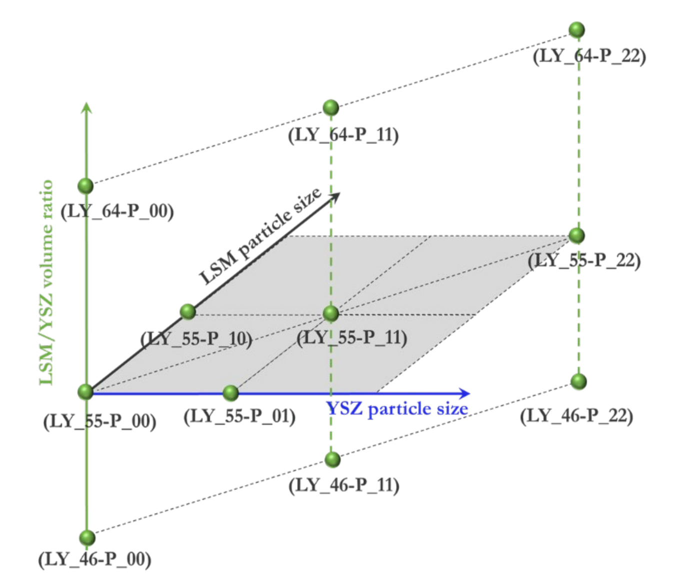
$\beta = 0$: baseline (P-0)
$\beta = 1$: finer grain (P-1)
$\beta = 2$: finest grain (P-2)

$$r_{LSM} = 0.67^{\beta_{LSM}} \cdot r_{LSM,ref}$$
$$r_{YSZ} = 0.5^{\beta_{YSZ}} \cdot r_{YSZ,ref}$$

$r_{LSM,ref} = 0.57 \times 10^{-6} m$
$r_{YSZ,ref} = 0.35 \times 10^{-6} m$

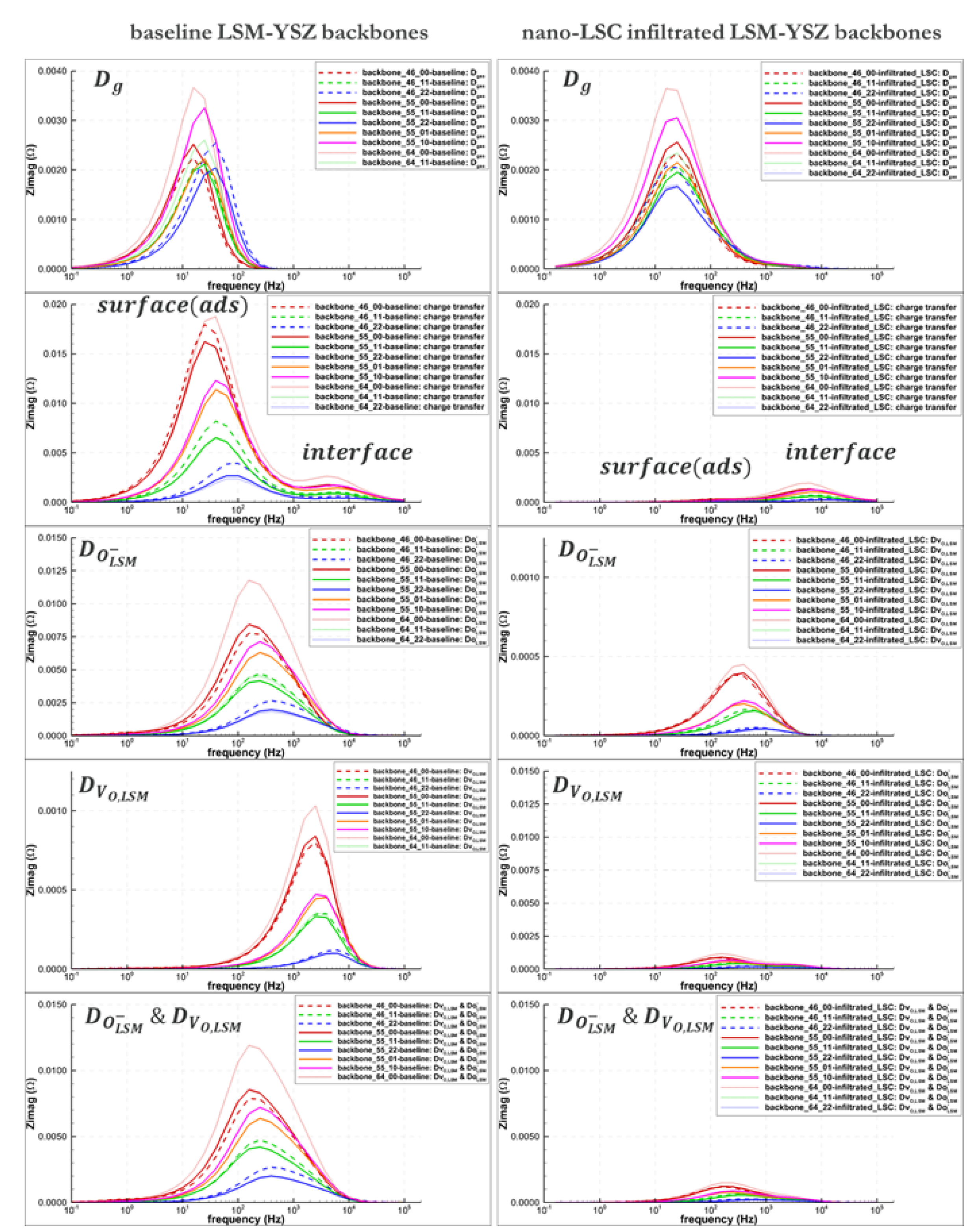
Sample notation

ex) LY_46-P_21
volume fraction: $V_{LSM}:V_{YSZ} = 40\%:60\%$
grain size: $\beta_{LSM} = 2$, $\beta_{YSZ} = 1$

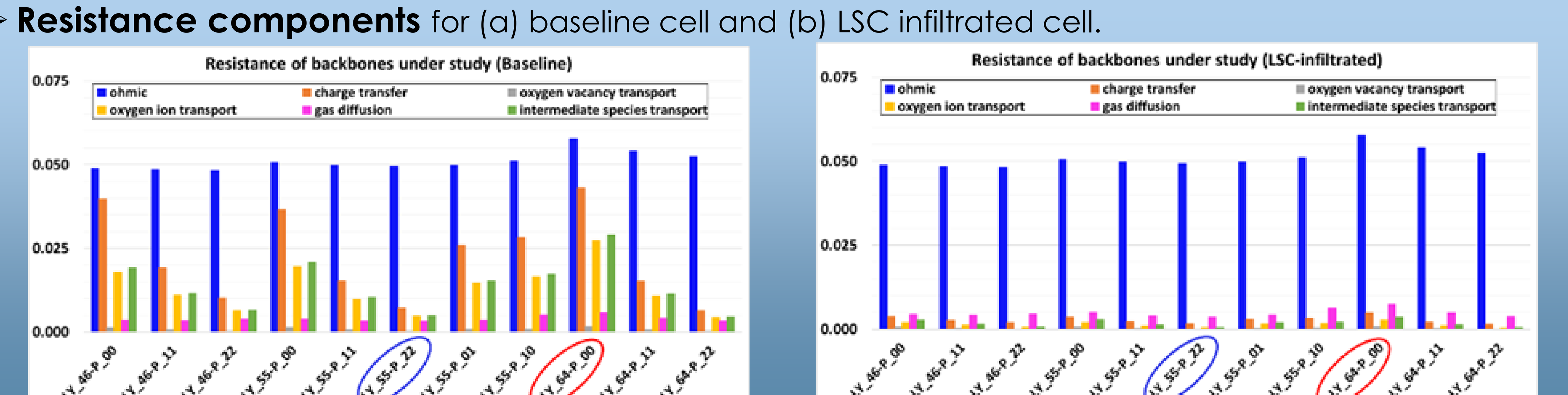


Total 11 backbones with different LSM/YSZ volume fractions and grain sizes. The name of backbones, LY_*ab*-P_*cd*, indicates the volume ratio (*ab*) and the size scale (*cd*) of LSM/YSZ.

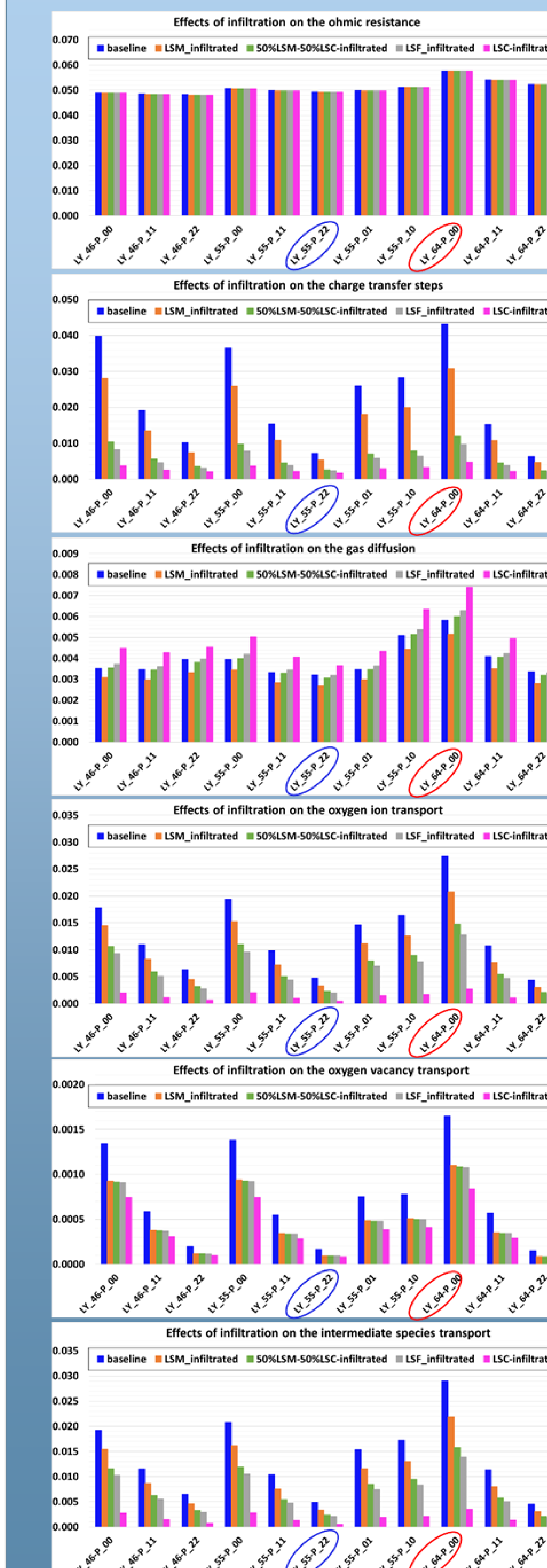
Resistance components associated with reaction steps and species transport for baseline LSM/YSZ composite cathode and nano-LSC infiltrated backbones



Resistance components for (a) baseline cell and (b) LSC infiltrated cell.



Effects of different infiltration materials on each reaction/transportation processes in oxygen reduction reactions:



Summary

- The infiltrated nanoparticles with higher ORR activity (e.g., LSF, LSC, 50%LSM-50%LSC) significantly affected the surface adsorption/dissociation step and the transport of oxygen ion and oxygen vacancy. The gas diffusion and interface charge transfer step were only slightly affected.
- The change of rate-limiting steps in ORR mechanism was observed for materials with LSC infiltrated cathode.
- The ohmic resistance was the largest resistance component for the infiltrated backbones. The technology for ohmic resistance reduction is necessary for further improvements of infiltrated cathodes.
- The thorough analysis of performance change with different infiltrates helped filter out the optimum backbone for infiltration technology

U.S. DEPARTMENT OF ENERGY

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