Modeling Interdiffusion Across Solid YSZ-LSM Interface

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Introduction and Objectives

Knowledge of the interface chemistry is centrally important for designing SOFCs with improved durability since:

- Electrode transport and exchange processes are strongly affected by the local surface and interface chemistry
- Small changes in the TPB chemistry can drastically modify the SOFC oxygen exchange rates

Modeling this phenomena can give an insight into the improvement of SOFCs

Defect Chemistry/Reaction Pathway

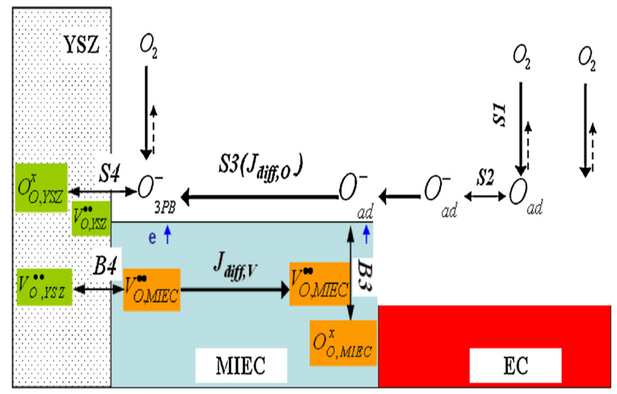
Pathways	Reaction steps		Process description
Surface	S1	$1/2O_2 + S \underset{k_{S1}^-}{\overset{k_{S1}}{\longleftrightarrow}} O_{ad}$	Dissociate oxygen adsorption (S: surface adsorption site)
	S2	$O_{ad} + e^- \underset{k_{S2}^-}{\overset{k_{S2}}{\longleftrightarrow}} O_{ad}^-$	Oxygen intermediate formation (1st step charge-transfer)
	S3	$O_{ad}^- \underset{k_{S3}^-}{\overset{k_{S3}}{\longleftrightarrow}} O_{TPB}^-$	Surface diffusion towards 3PB
	S4	$O_{TPB}^- + e + V_{O,YSZ}^{\bullet\bullet} \underset{k_{S4}^-}{\overset{k_{S4}}{\longleftrightarrow}} O_O^x$	3PB incorporation of oxygen intermediates (2nd step charge-transfer)
Bulk	B3	$O_{ad}^- + V_{O,MIEC}^{\bullet\bullet} + e^- \underset{k_{B3}^-}{\overset{k_{B3}}{\longleftrightarrow}} O_{O,MIEC}^x$	Reaction of vacancy from MIEC bulk with surface oxygen intermediates
	B4	$O_{O,MIEC}^x + V_{O,YSZ}^{\bullet\bullet} \underset{k_{B4}^-}{\overset{k_{B4}}{\longleftrightarrow}} O_{O,YSZ}^x + V_{O,MIEC}^{\bullet\bullet} + S$	2PB exchange between YSZ and MIEC(S: surface adsorption site)

Kinetic Model

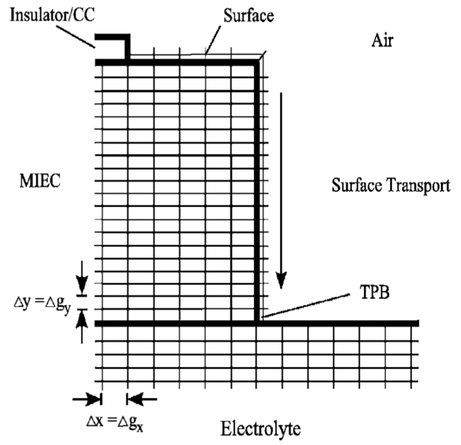
The interface model is solved using a phase field approach. The Poisson-Cahn equation evaluates the interfacial diffusion, while the Allen-Cahn equation tracks the presence of intermediate phases.

Fundamental Equations	
Poisson-Cahn	$\frac{\partial c_i}{\partial t} = \nabla \cdot [M_c(\nabla \mu)]$
Allen-Cahn	$\frac{\partial p_k}{\partial t} = M_k \left(\frac{\partial f}{\partial p_k} \right)$
Free Energy	$F(c,p) = \int \left[f_0(c,p) + \frac{1}{2}\sum_{i=1}^{2}\sum_{j=1}^{M_i}(\nabla p_j) + \frac{1}{2}\sum_{i=1}^{2}\sum_{j=1}^{2}\left(\nabla c_i \cdot \nabla c_j\right)^2 \right] dv$
Electrostatic Potential	$\frac{d^2\varphi}{dx^2} = -\frac{F}{\varepsilon_r \varepsilon_0}(2N_v - N_a)$

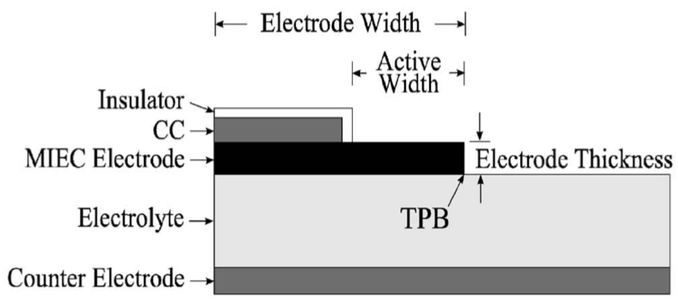
Results and Figures



(a) Schematic of oxygen reduction on MIEC Cathode



(b) Finite volume discretization



(c) 2D model domain

Figure a. shows the reaction pathway of the proposed mechanism. The schematic shows the triple phase boundary and bulk incorporation. This mechanism will be discretized, similarly to Figure b, but with an adaptive refined mesh towards the interface. Figure c, is a 2D cross-sectional of the model

Conclusions and Future Work

The model will need to be able to handle the boundary of the MIEC and Electrolyte. This problem is being addressed by incorporating the mesh adaptability of MOOSE. The process will be outlined as followed:

- Refine the mesh of the MIEC
- Write and modify kernels in MOOSE to model the SOFC
- Fine tune the mobility parameters within the model using the sequential Monte Carlo routine
- Incorporate final model into overall NETL model

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