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

<table>
<thead>
<tr>
<th>Pathways</th>
<th>Reaction steps</th>
<th>Process description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Surface</td>
<td>$1(2O_{a} + s^{\text{ads}}O_{ad})$</td>
<td>Dissociate oxygen adsorption (S: surface adsorption site)</td>
</tr>
<tr>
<td>S2</td>
<td>$O_{i} + e^{\text{ads}} + O_{ad}$</td>
<td>Oxygen-intermediate formation (1st step charge-transfer)</td>
</tr>
<tr>
<td>S3</td>
<td>$O_{ad} + s^{\text{ads}}O_{ad}$</td>
<td>Surface diffusion towards TPB</td>
</tr>
<tr>
<td>S4</td>
<td>$O_{ad} + e^{\text{ads}} + O_{ad}$</td>
<td>TPB incorporation of oxygen intermediates (2nd step charge-transfer)</td>
</tr>
<tr>
<td>Bulk</td>
<td>$B_{i} + V_{\text{Omic}} + e^{\text{ads}} + O_{ad}$</td>
<td>Reaction of vacancy from MIEC bulk with surface oxygen intermediates</td>
</tr>
<tr>
<td>B4</td>
<td>$O_{ad} + s^{\text{ads}}O_{ad} + V_{\text{Omic}} + s^{\text{ads}}O_{ad}$</td>
<td>2PB exchange between YSZ and MIEC (surface adsorption site)</td>
</tr>
</tbody>
</table>

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.

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

Acknowledgements

- This work was performed in support of the US Department of Energy National Energy Technology Laboratory’s ongoing Solid Oxide Fuel Cell research activity under the Research Support Services contract 89243318CFE000003.