

Engineering of microstructure and design of a planar composite SOFC cathode: a numerical analysis

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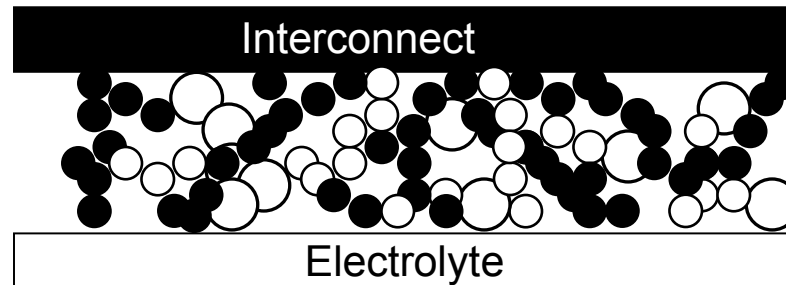
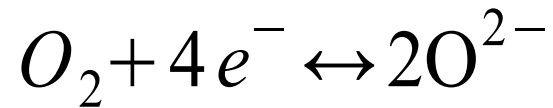
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Objective

- To study the transport of oxygen gas, electrons and ions and how they are influenced by cathode microstructure and design
- Focus on engineering of high performance composite cathode

SOFC Cathode

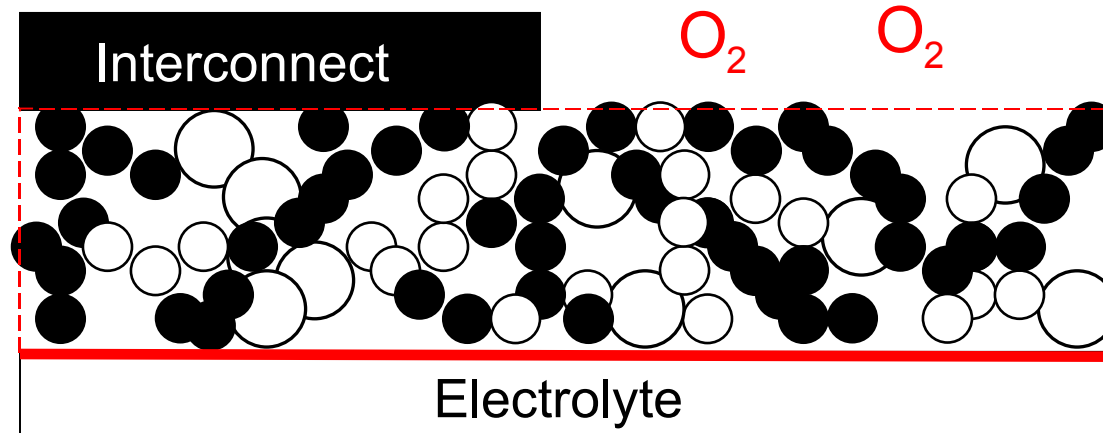
- LSM is the cathode material
- YSZ is the electrolyte material



● LSM particle ○ YSZ particle

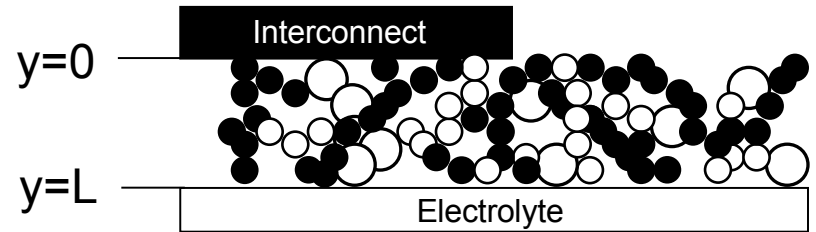
Model Development

Model Geometry



Model Equations

$$\nabla \cdot (\Gamma_i^{ref} \nabla \varphi_i) = S_i$$



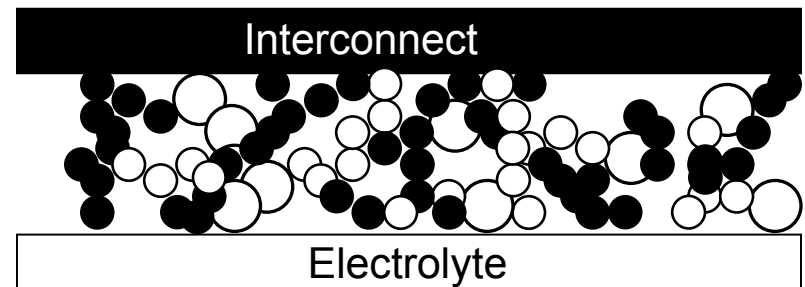
	Γ	φ	S_i
Electronic charge	σ_{el}^{eff}	φ_{el}	$\lambda_{TPBL} (i_{anodic} - i_{cathodic})$
Ionic charge	σ_{io}^{eff}	φ_{io}	$-\lambda_{TPBL} (i_{anodic} - i_{cathodic})$
O ₂ species	$D_{O_2-N_2}^{eff}$	[O ₂]	$-\frac{\lambda_{TPBL}}{4F} (i_{anodic} - i_{cathodic})$

Effective Transport Coefficients

Highly influenced by microstructural properties

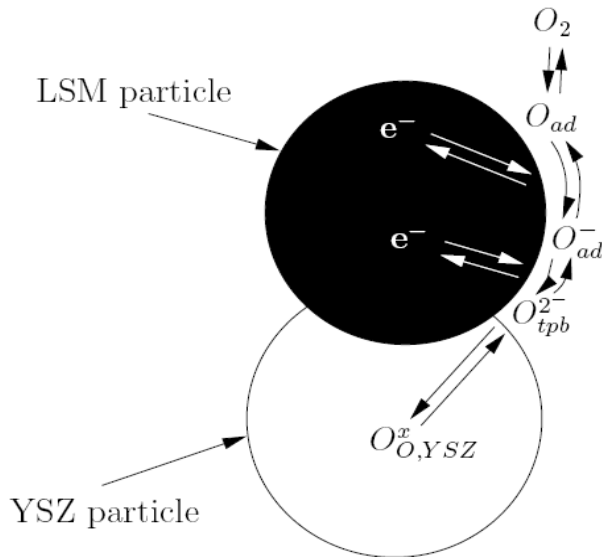
$$\sigma_i^{eff} = f\left(\varepsilon, \theta_i, P(\theta_i)\right)$$

$$D_{O_2-N_2}^{eff} = f\left(\varepsilon, \tau\right)$$



Cathode Kinetics

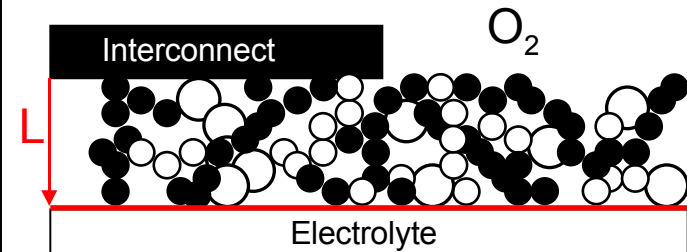
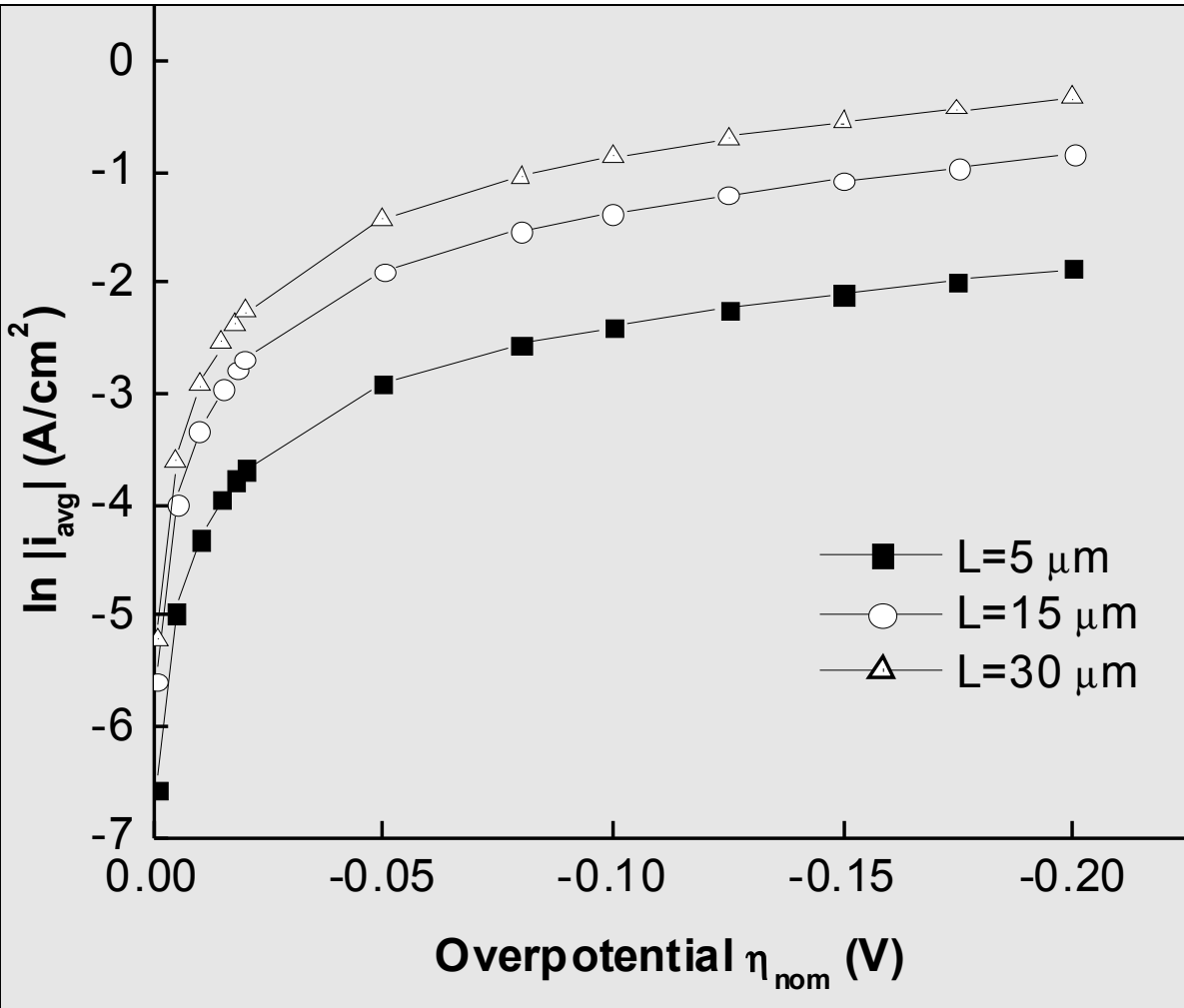
$$i = i_0^{ref} \left(\frac{pO_2}{pO_2^{ref}} \right)^\gamma \left[\exp\left(\alpha_a \frac{F}{RT} \eta \right) - \exp\left(-\alpha_c \frac{F}{RT} \eta \right) \right]$$



Equation	γ	α_a	α_c
$O_{2(g)} \rightleftharpoons 2O_{ad}$	1		
$O_{ad} + e^- \rightleftharpoons O_{ad}^-$	3/8	3/2	1/2
$O_{ad}^- \rightleftharpoons O_{TPB}^-$	1/4	1	1
$O_{TPB}^- + e^- + V_{\ddot{O}}^x \rightleftharpoons O_{O}^x$	1/8		

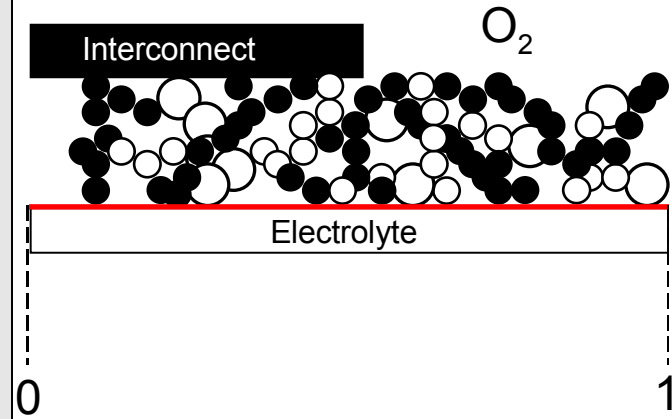
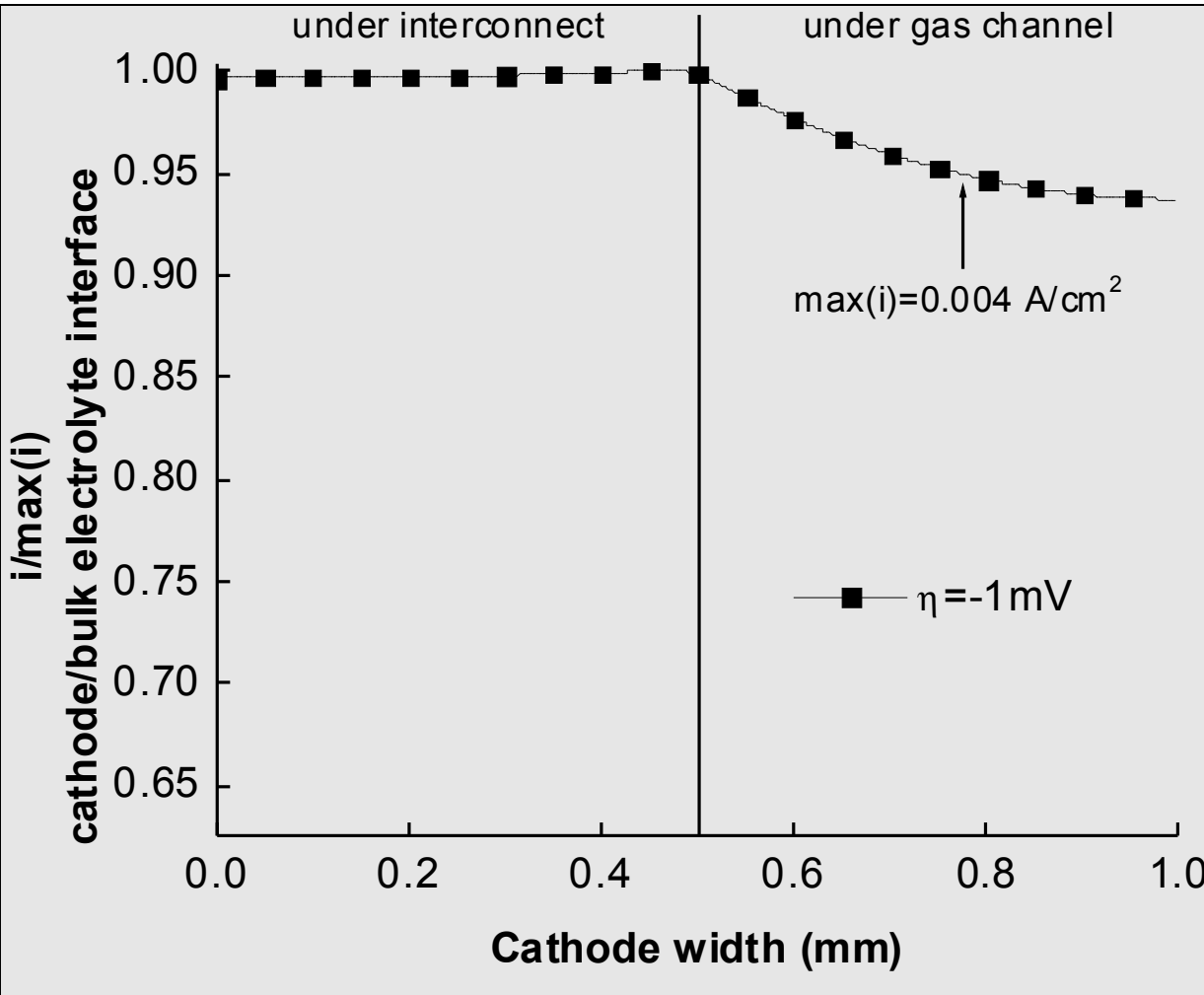
Results

Cathode Polarization Curve

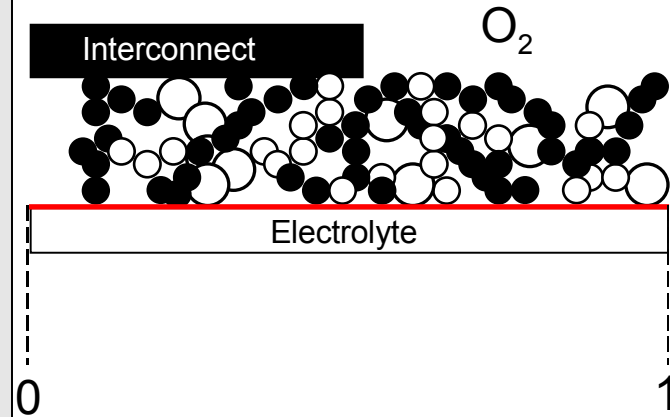
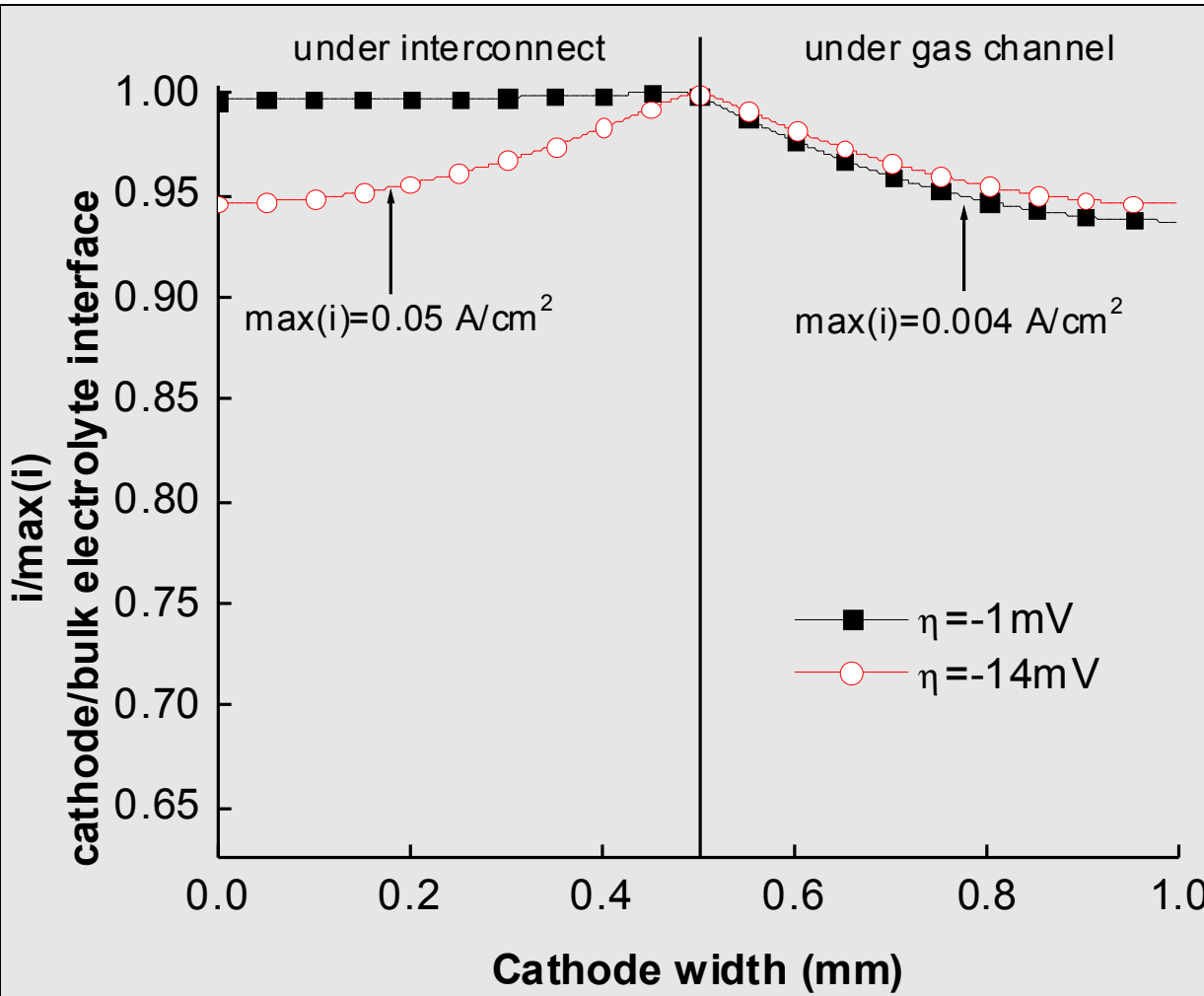


Only a small part of the story

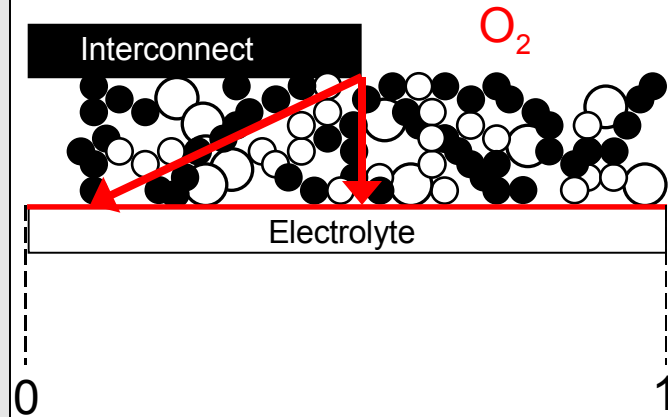
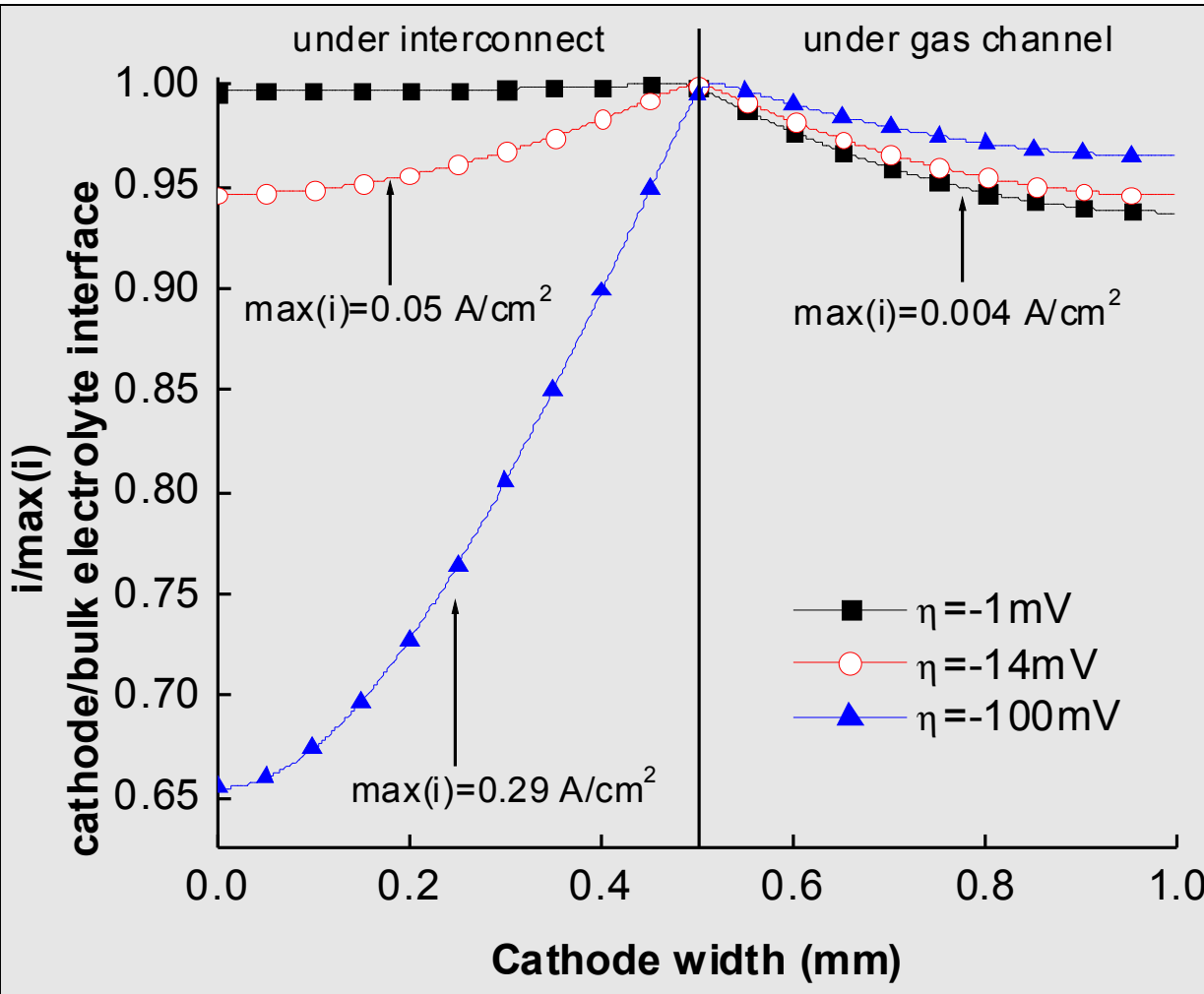
Current density distribution



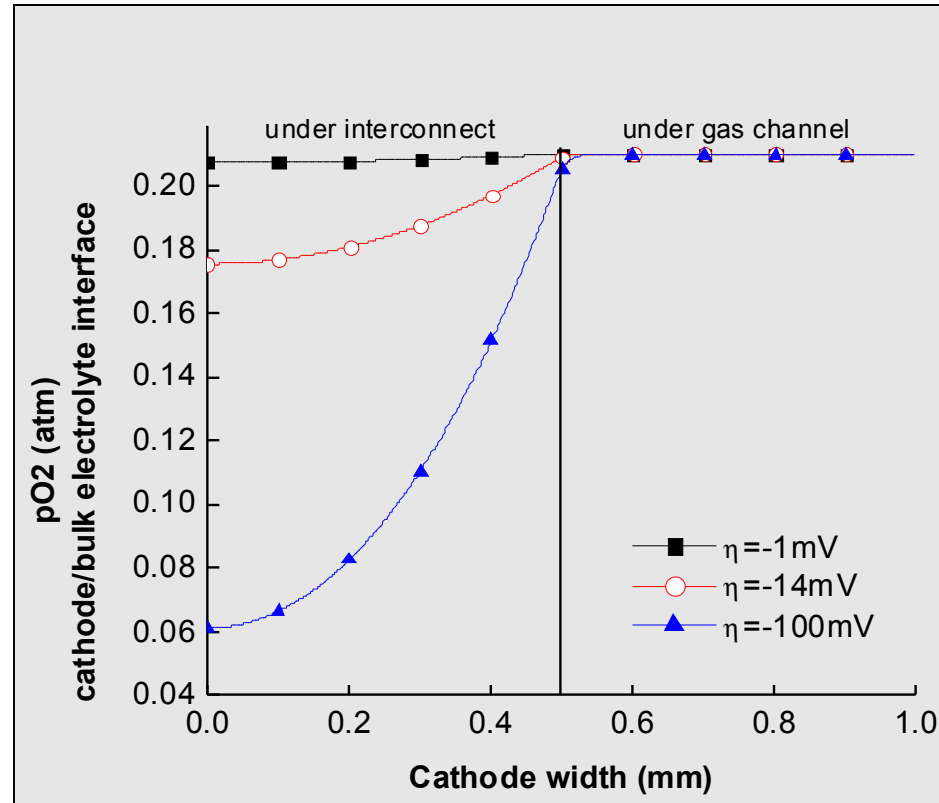
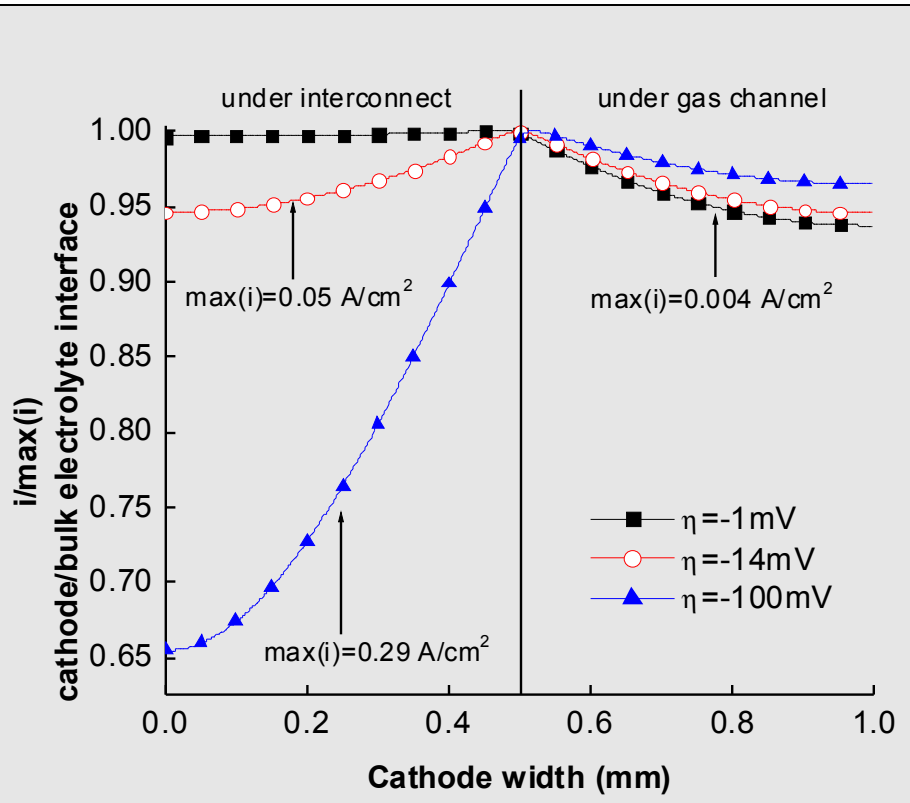
Current density distribution



Current density distribution

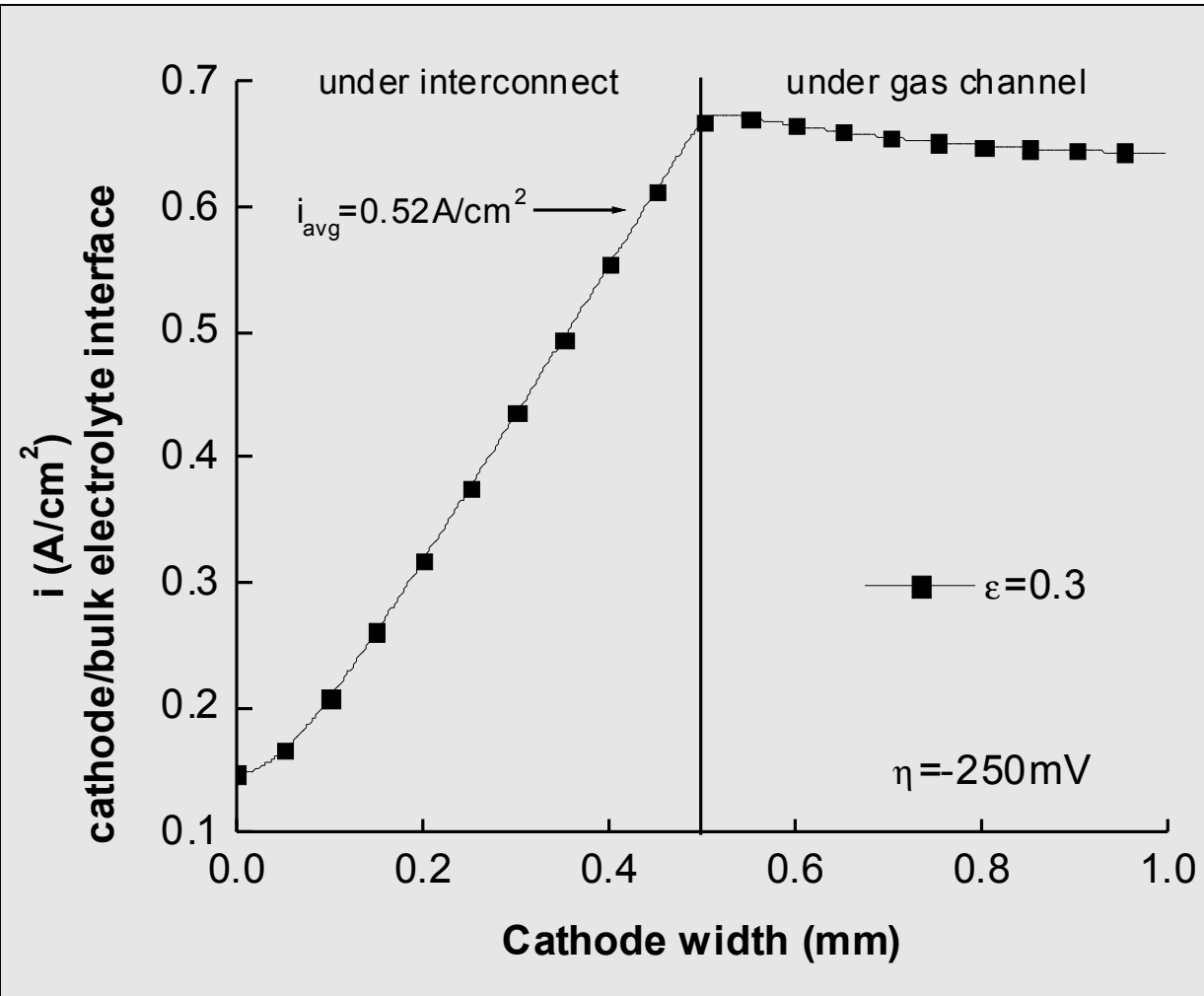


Current & P_{O2} Distribution

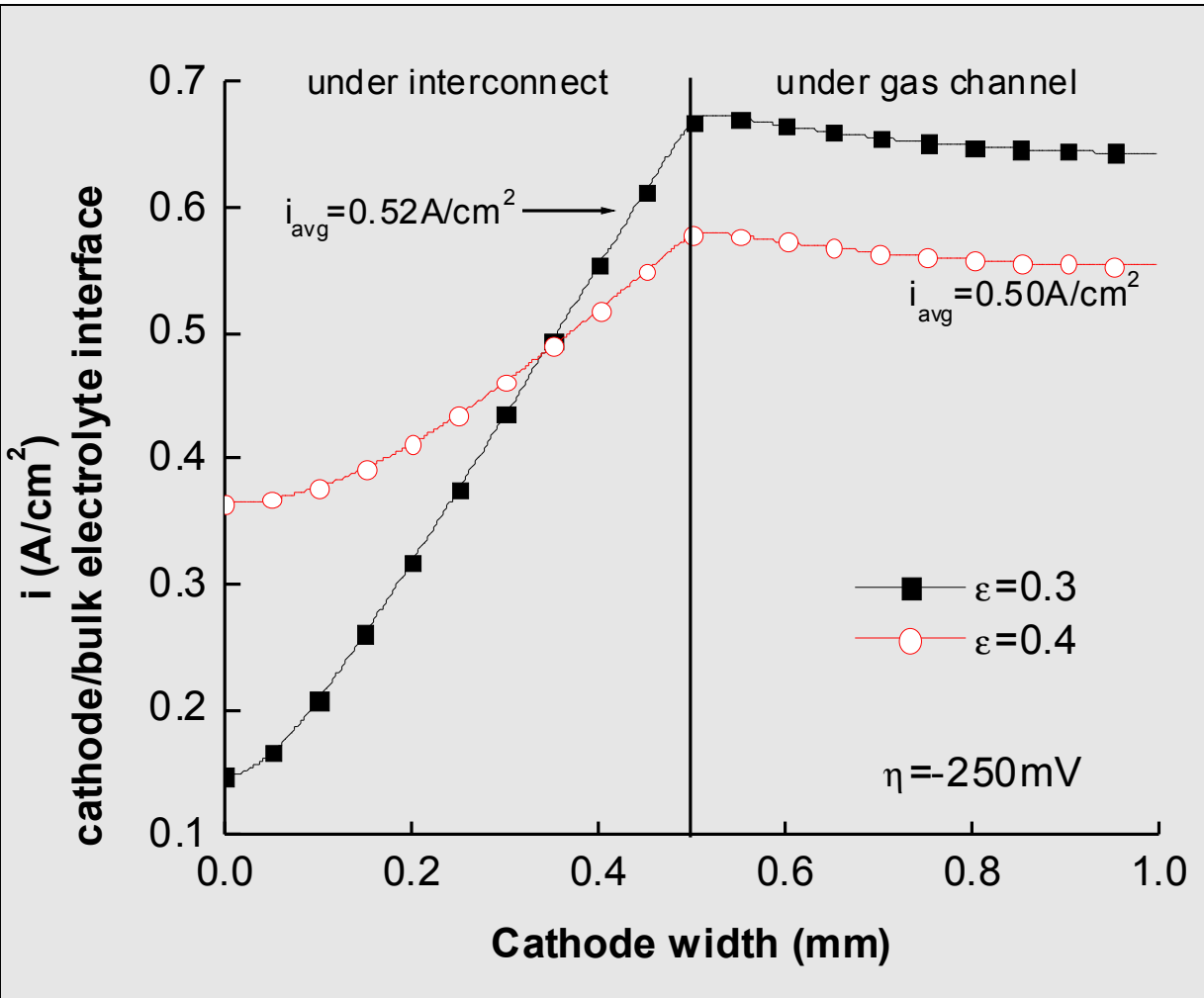


Effect of Porosity

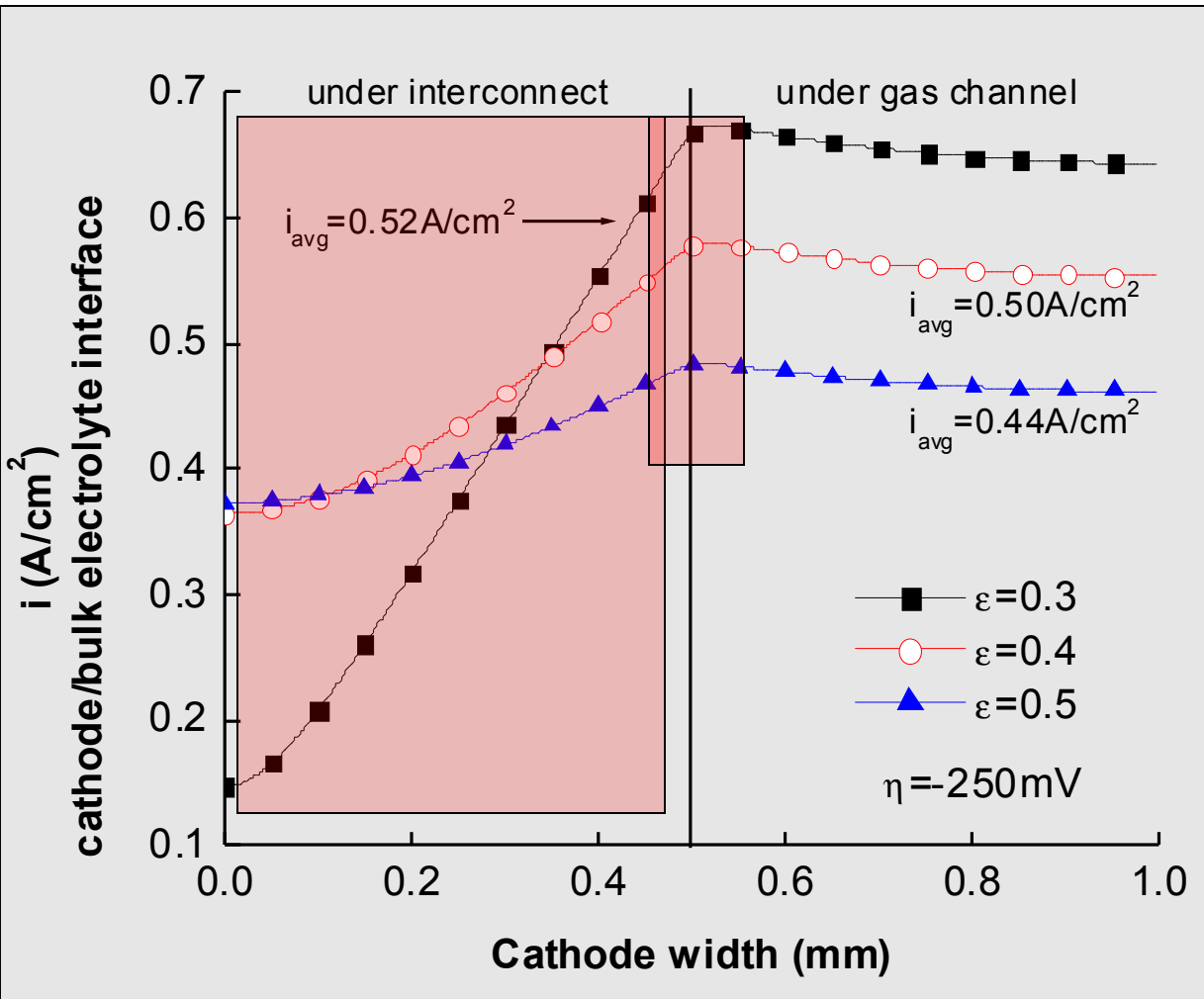
Effect of Porosity



Effect of Porosity



Effect of Porosity



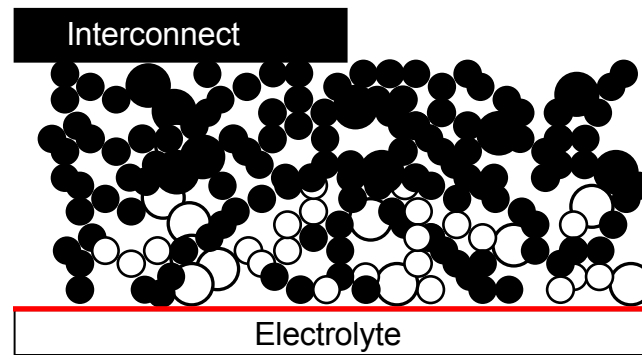
1. Low porosity increases resistance to oxygen diffusion
3. Low porosity increases TPBL

Engineering Cathode Geometry

- Must increase oxygen concentration underneath current collector but at the same time we should maintain a low porosity

Engineering Cathode Geometry

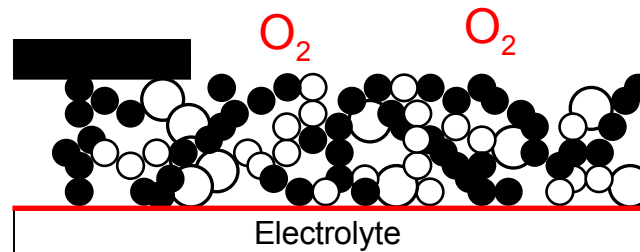
- Two possibilities:
 1. Add a gas diffusion layer (GDL)



6. Reduce interconnect coverage

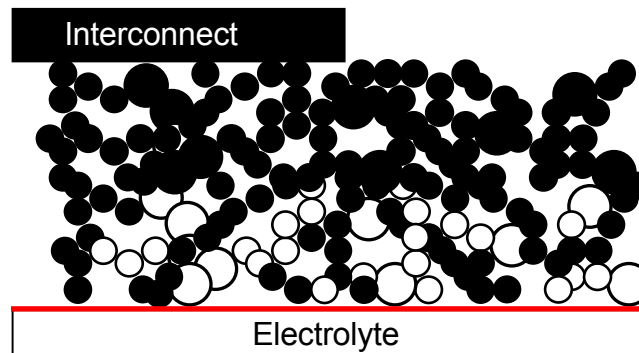
Engineering Cathode Geometry

- Two possibilities:
 1. Add a gas diffusion layer
 2. Reduce interconnect coverage

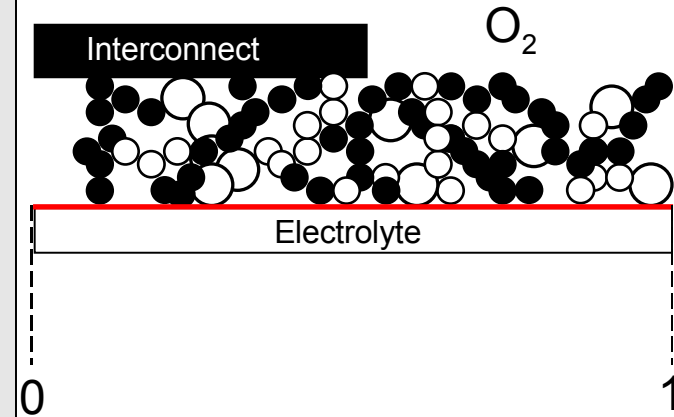
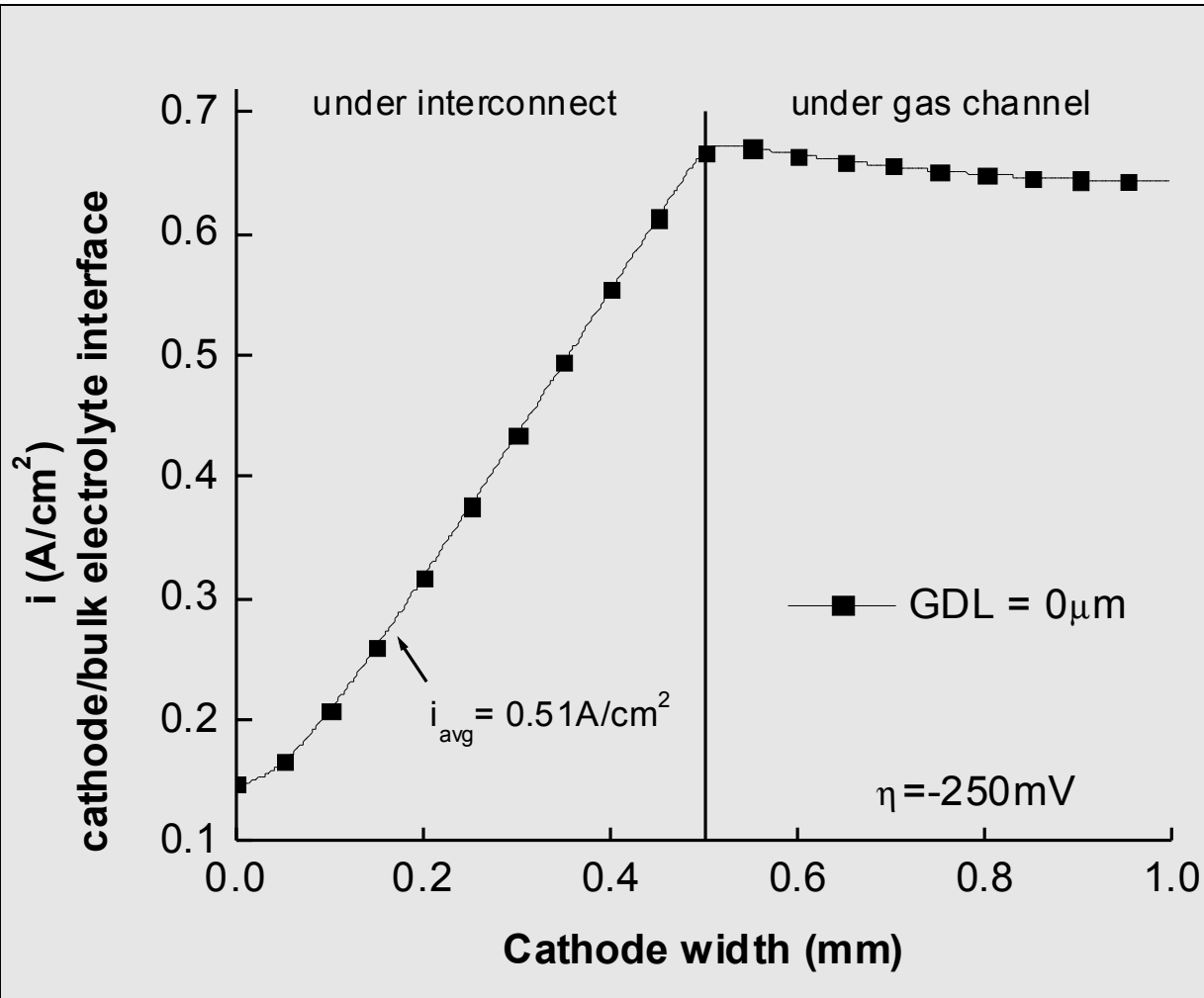


Influence of GDL

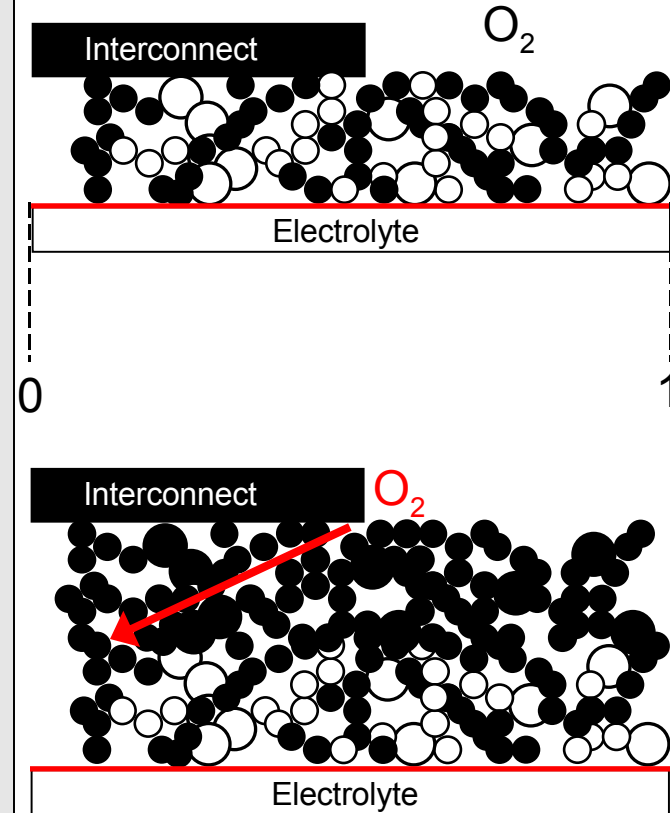
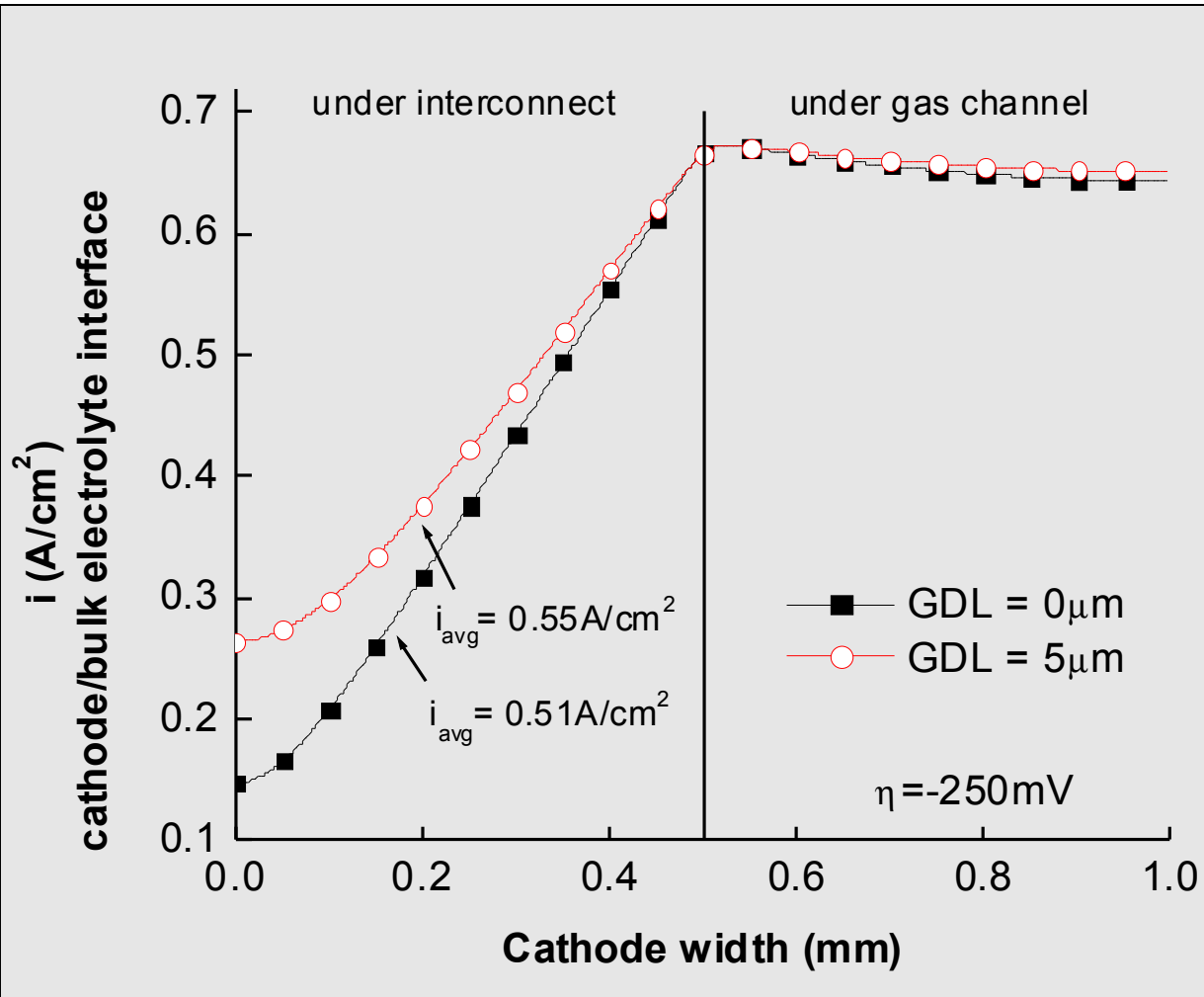
1. Add a gas diffusion layer (GDL)



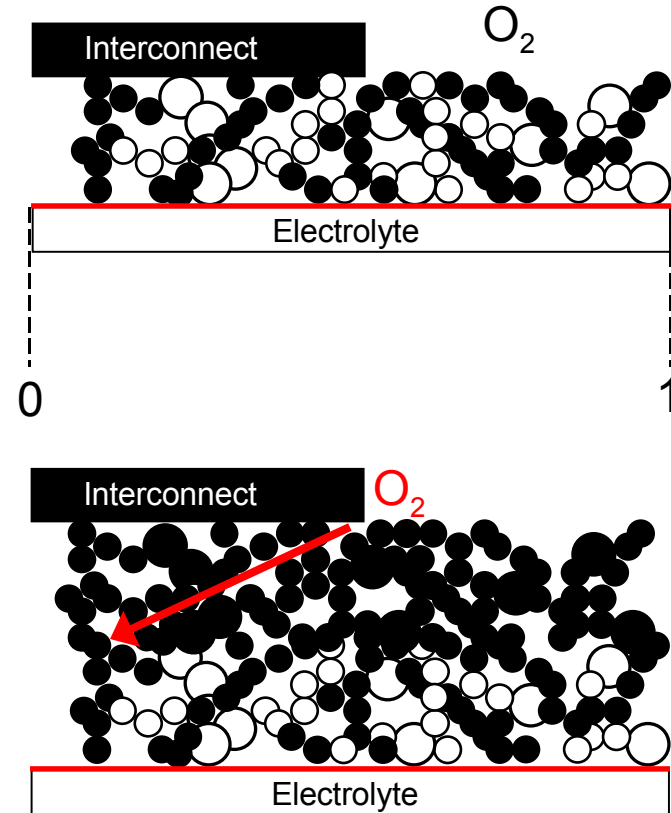
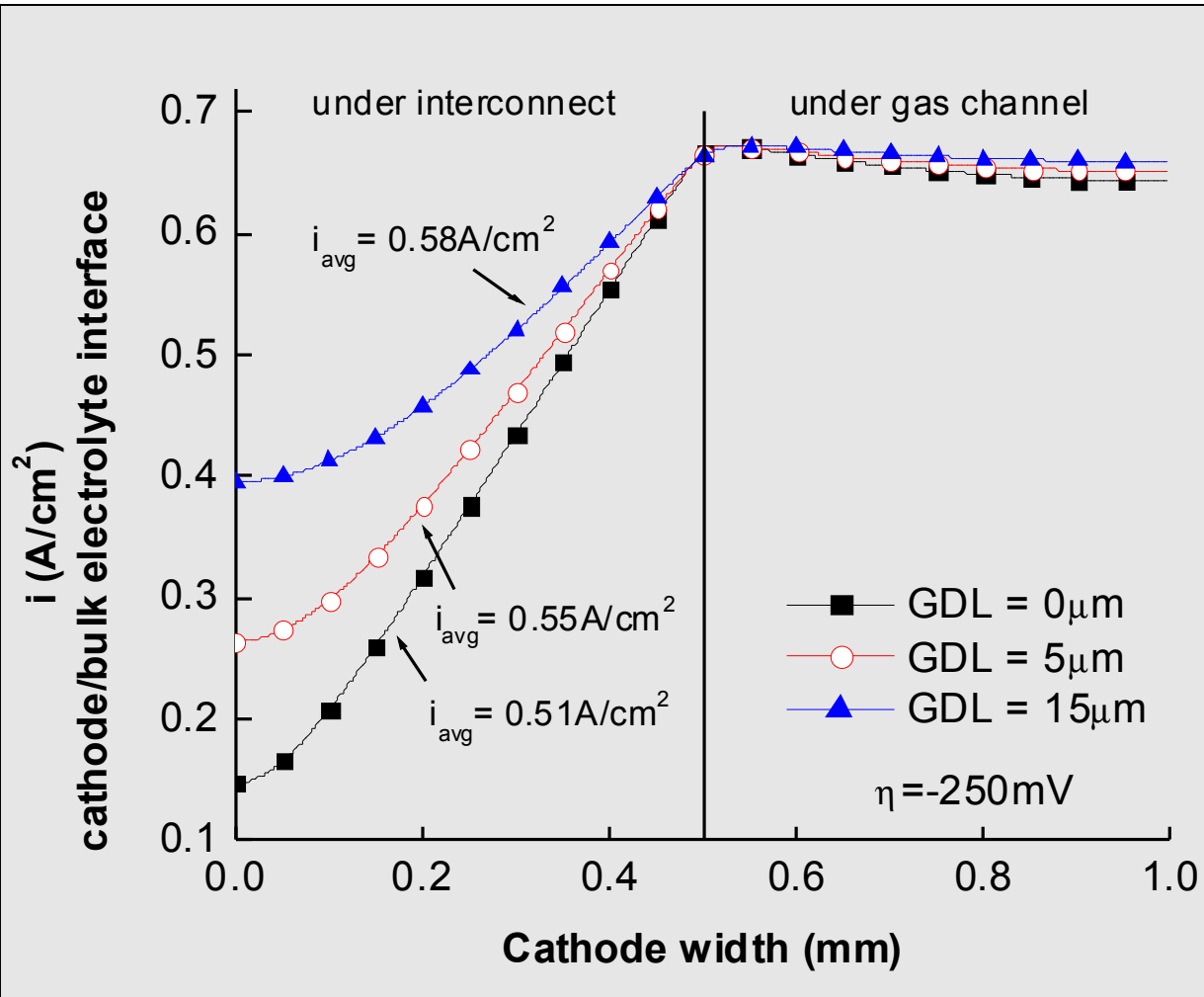
Effect of GDL



Effect of GDL

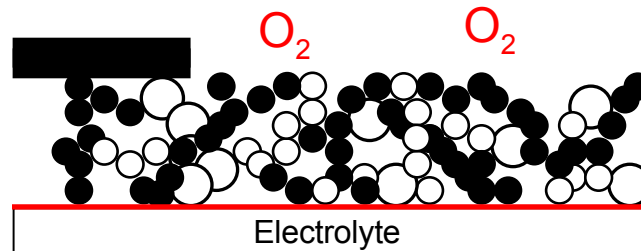


Effect of GDL

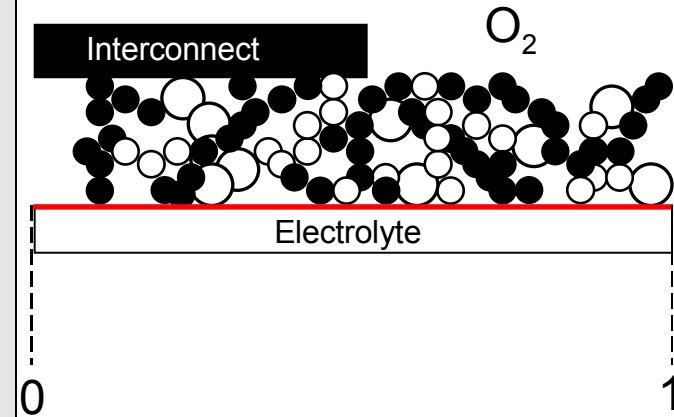
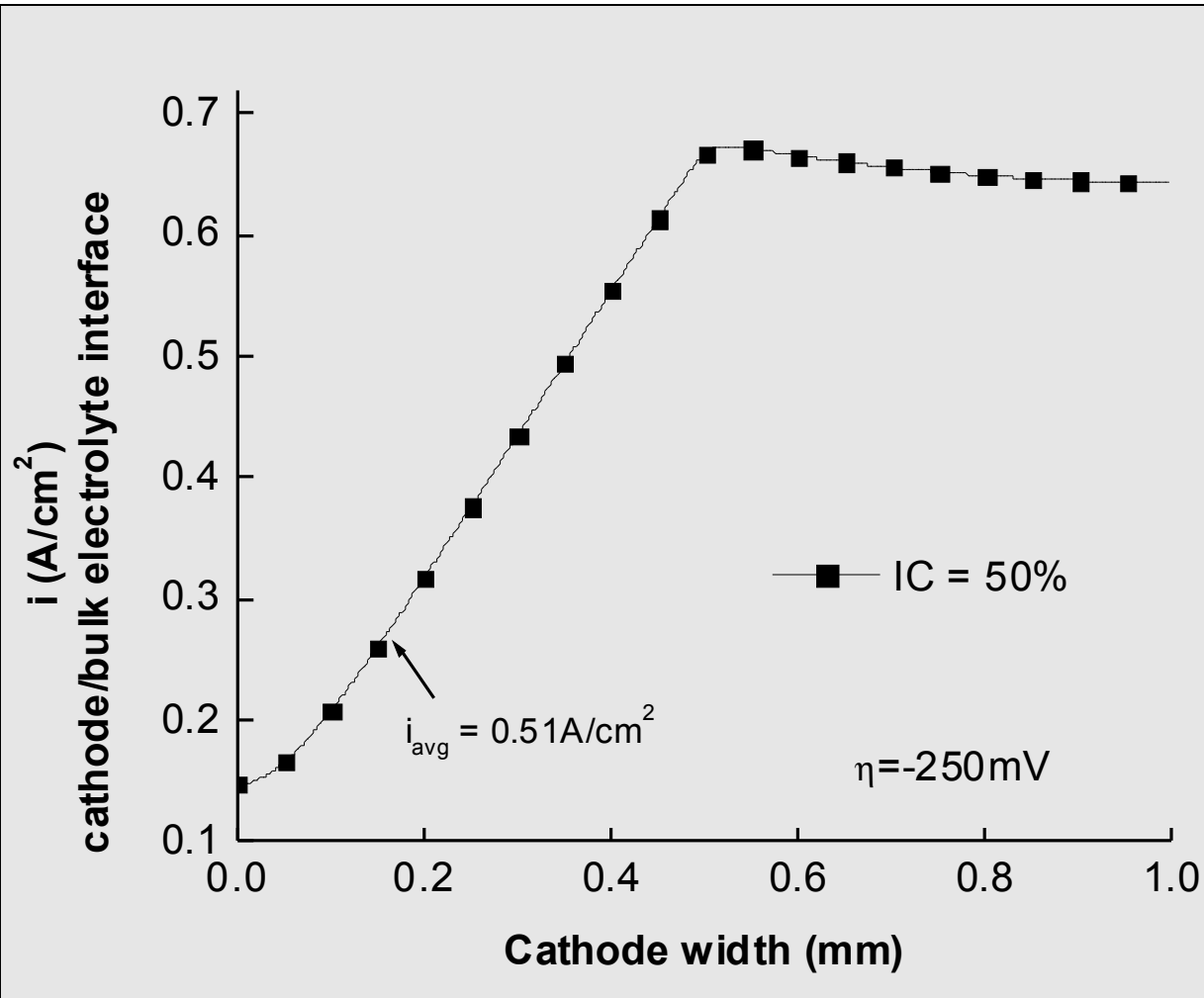


Influence of Interconnect Coverage

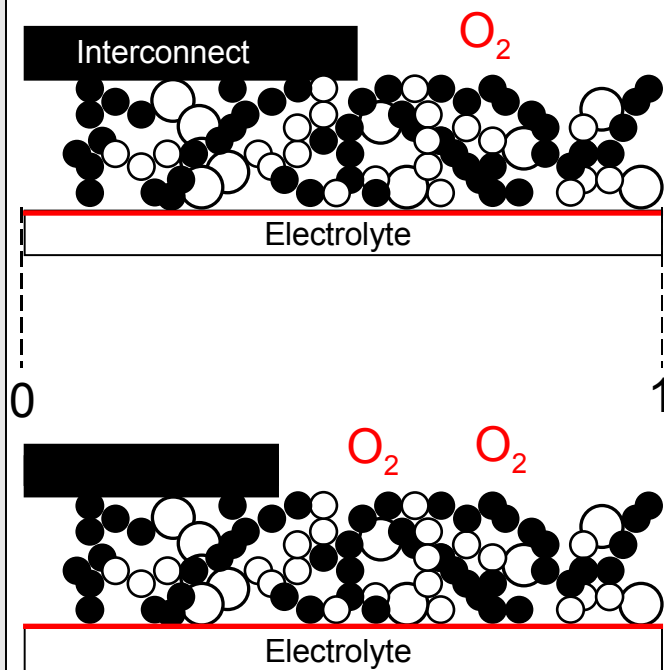
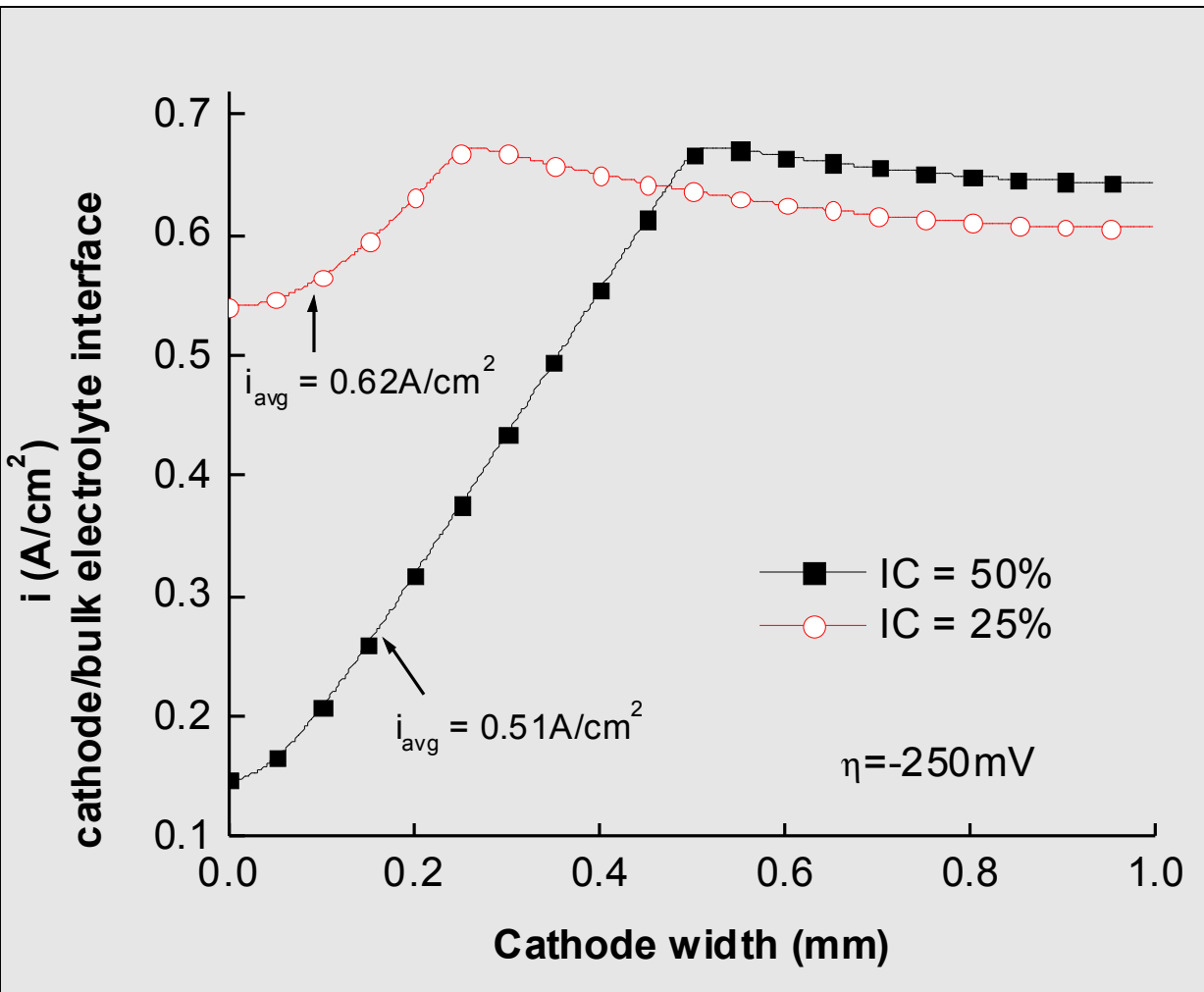
1. Add a gas diffusion layer
2. Reduce interconnect coverage



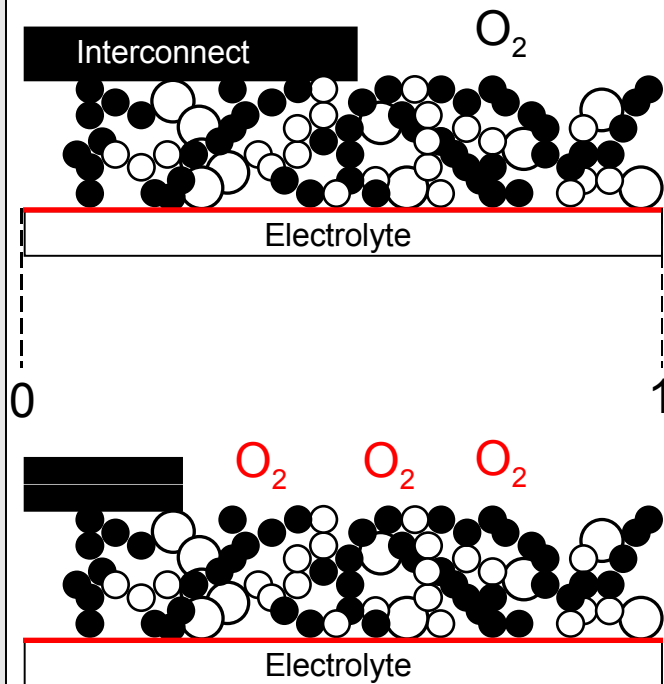
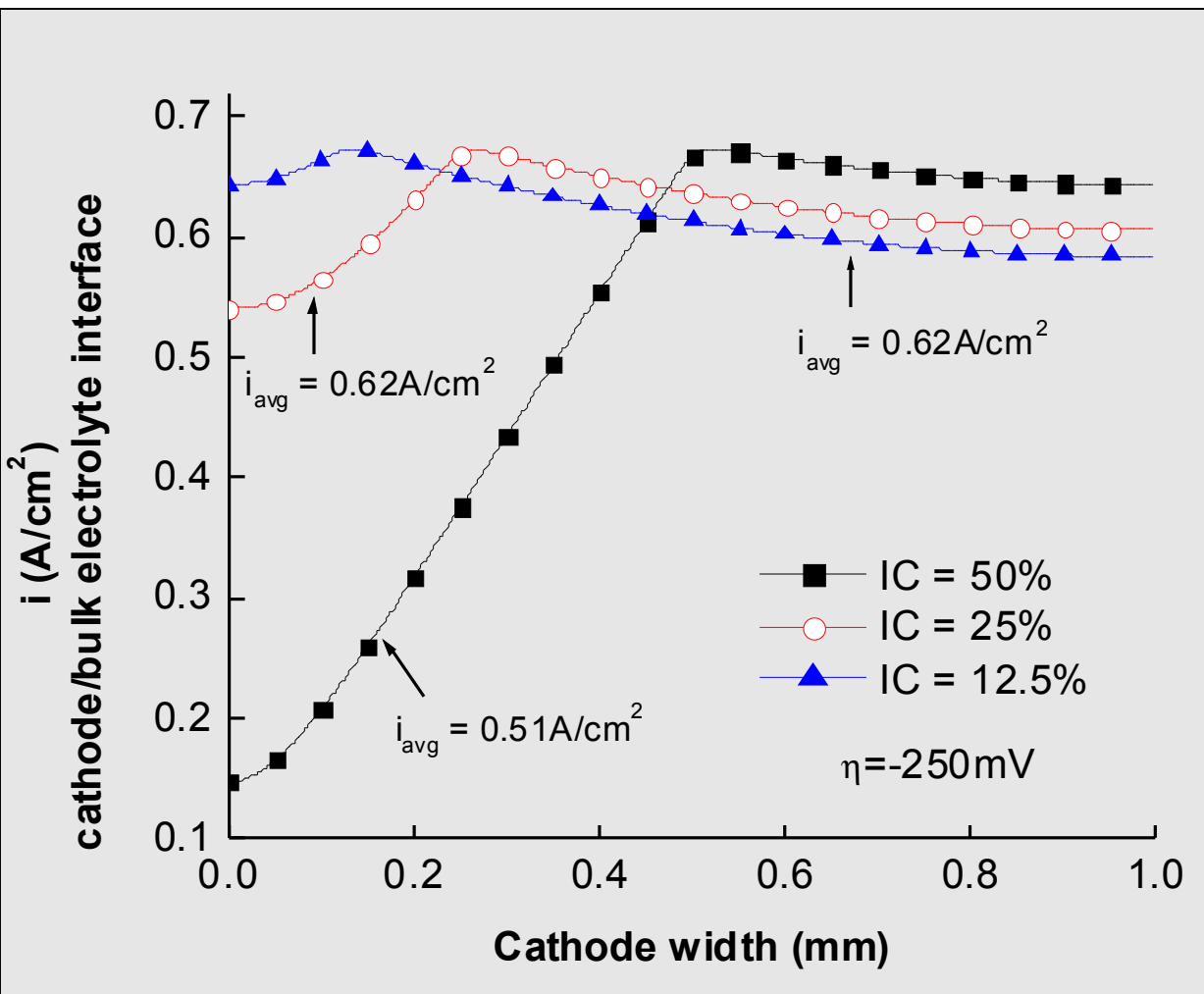
Effect of Interconnect Coverage



Effect of Interconnect Coverage



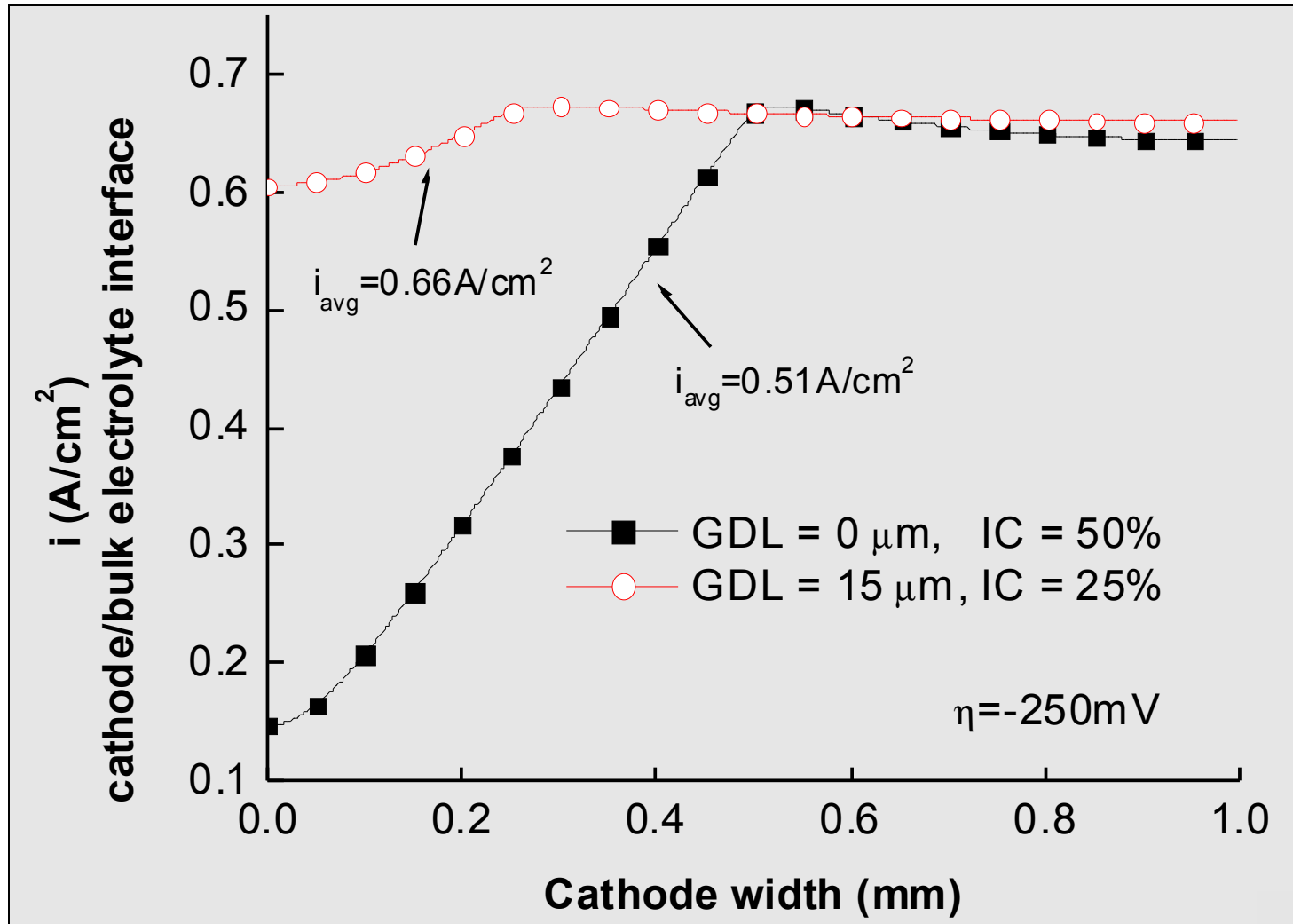
Effect of Interconnect Coverage



Combined Effects

2. Add a gas diffusion layer
4. Reduce interconnect coverage

Engineered Cathode Design



Conclusions

- Typical performance data such as a polarization curve only provides averages
- Both microstructural and geometric factors affect current density distribution
 - Activity of cathode depends on transport of participating reactants and not merely TPB
- High performance cathode can be designed by careful engineering of microstructure and geometry

Acknowledgments

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