SOFC Materials Development and Degradation Modeling

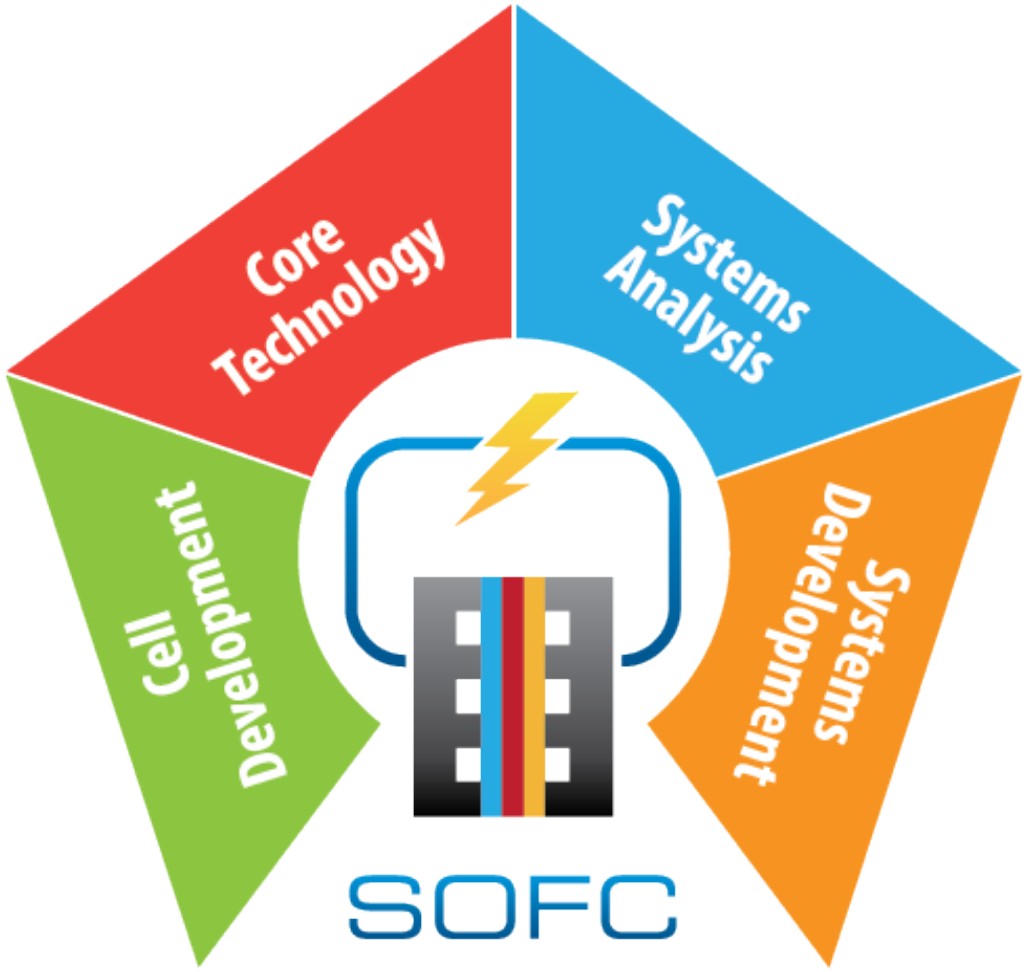
U.S. DOE Hydrogen and Fuel Cells Program Annual Merit Review and Peer Evaluation Meeting

Gregory A. Hackett, Ph.D. NETL Research and Innovation Center

June 13, 2018

Outline

- **NETL Research Team (EY18)**
- **NETL Research Portfolio Update**
  - Cell and Stack Degradation Evaluation and Modeling Progress
  - Electrode Engineering Research and Development Progress



NETL SOFC Research Team (EY18)

NETL (Federal Staff)
- Gregory Hackett, Team Lead (NETL)
- Travis Shultz (NETL)
- Rich Pineault (NETL)
- Yves Mantz (NETL)
- Paul Ohodnicki (NETL)
- Yuhua Duan (NETL)
- Slava Romanov (NETL)
- Youhai Wen (NETL)
- Dustin McIntyre (NETL)
- Jonathan Lekse (NETL)
- Christopher Matranga (NETL)

Carnegie Mellon University
- Paul Salvador (MSE)
- Shawn Litster (MechE)
- Tony Rollett (MSE)
- Tim Hsu (MSE, grad. student)
- Rubayyat Mahbub (MSE, grad. Student)
- Grigorios Panagakos (MSE)

NETL (Post-Doctoral Researchers)
- Yueh-Lin Lee (ORISE)
- Billy Epting (ORISE)
- Giuseppe Brunello (ORISE)
- Hunter Mason (ORISE)
- Tao Yang (ORISE)
- Yinkai Lei (ORISE)
- Beom Tak Na (ORISE-PM)
- Na Li (ORISE - Joining Soon)

NETL (Site Support Contracts)
- Tom Kalapos (AECOM)
- Harry Abernathy (AECOM)
- Shiwoo Lee (AECOM)
- Arun Iyengar (KeyLogic)
- Lynn Fan (AECOM)
- Rick Addis (USSE2)
- Tianle Cheng (AECOM)
- Yang Yu (AECOM)
- Youngseok Jee (AECOM)
- Jian (Jay) Liu (AECOM - July)

West Virginia University
- Harry Finklea (Chemistry)
- Ismail Celik (MAE)
- David Mebane (MAE)
- Elizabeth Ridgeway (MAE, Undergraduate)
- Ed Sabolsky (MAE)
- Xueyan Song (MAE)
- Xingbo Liu (MAE)
- Yun Chen (WV Research Corporation)
- Ozcan Ozmen (MAE, Ph.D. Student)

Clemson University
- Kyle Brinkman (MSE)

Penn State University
- Long-Qing Chen (MSE)

University of Wisconsin-Madison
- Dane Morgan (MSE)
- Ryan Jacobs (MSE)

Wake Forest University
- Michael Gross (Chemistry)
- Sixbert Muhoza (Chemistry, Ph.D Student)

Currently 50 SOFC Team Members

Cell and Stack Degradation

Predictive Modeling Toolset

Enabling SOFC Technology through R&D at NETL

Predictive Modeling – Reduction of Cost for SOFC Systems

TOOL RELEASE
Release of SOFC Predictive Modeling Toolset into public domain

DEMONSTRATION
Fully integrate all degradation models into SOFC operation model

MATURATION
Demonstration of degradation models integration into SOFC operation model

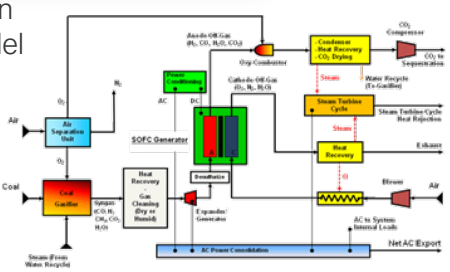
DEVELOPMENT
Critical SOFC degradation modes identified, expansion of SOFC operation model

DISCOVERY
Proof of Concept

Concept to Market Readiness

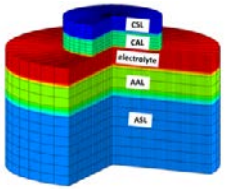
2020 — *Demonstrate how microstructure and operating conditions affect plant-level cost-of-electricity*

Integrated Gasification Fuel Cell System Model

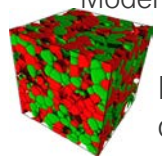


2018-19 — *Scale-bridge from microscale to cell to stack/system level (collaborate with PNNL)*

SOFC Operation "Multi-physics" Model



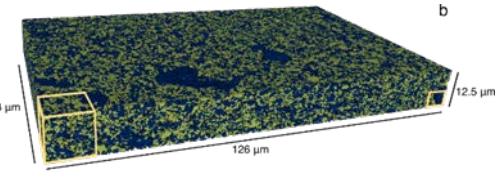
2015-18 — *Use of plasma-FIB to create world's largest reconstruction of commercial developer cells*



Particle coarsening degradation model

2013-15 — *Use of focused-ion beam (FIB) to reconstruct electrodes, evaluate operationally-relevant properties*

Cathode microstructure reconstruction



2012 — *Concept of Predictive "Hurricane" Model for SOFC*

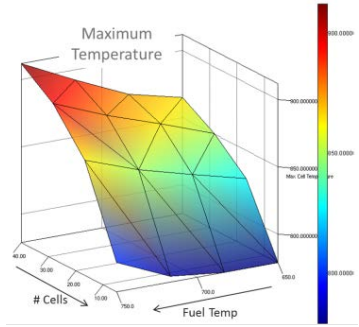
Hurricane prediction concept

Background

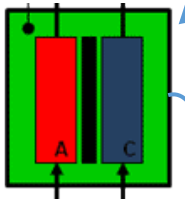
NETL/PNNL Collaboration to Complete Scaling Process

Need design and engineering at several scales to facilitate wide-scale SOFC commercialization

Link NETL and PNNL models at different scales to inform system level and life cycle analyses



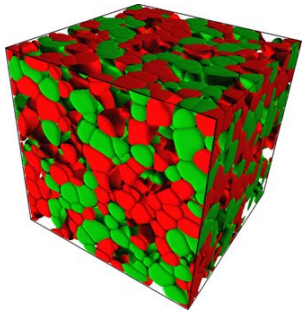
Response Surface Analysis

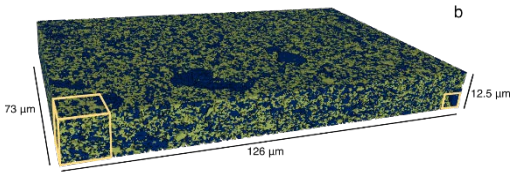


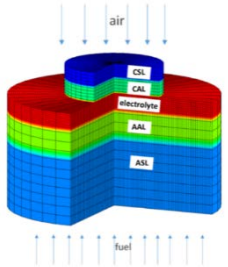
Reduced Order Model (ROM)

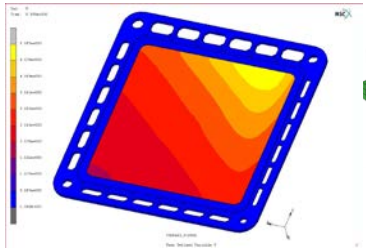
Stack Details

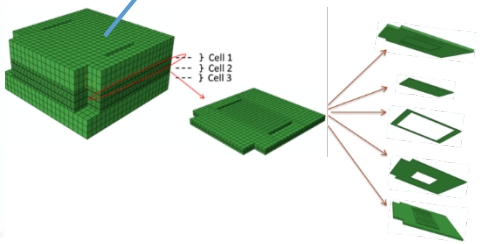
Increasing Scale

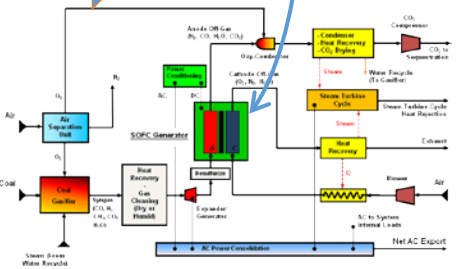








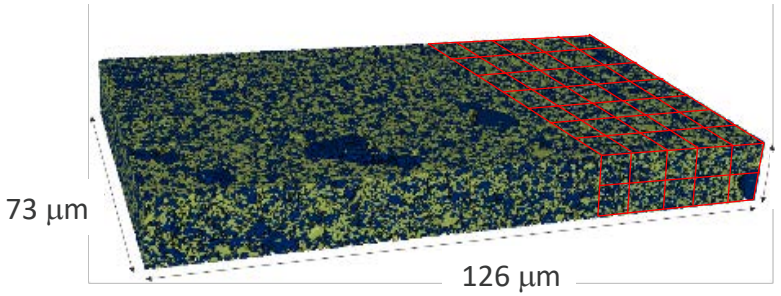




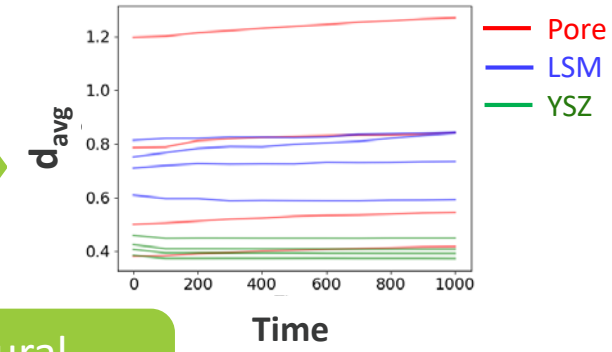
Electrode Microstructure | Single Cell | Multi-Cell Stack | IGFC System Model

NETL | ***PNNL*** | ***NETL***

Integrated Cell Degradation Model

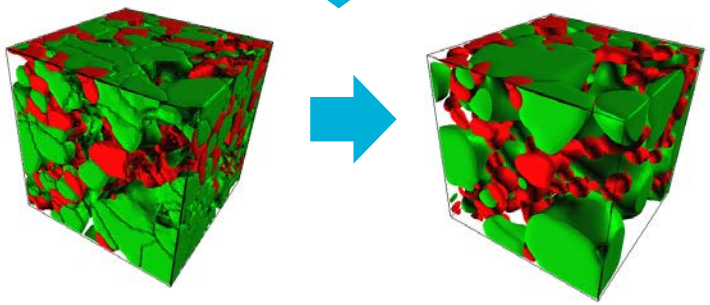


3D Reconstruction of SOFC Electrodes

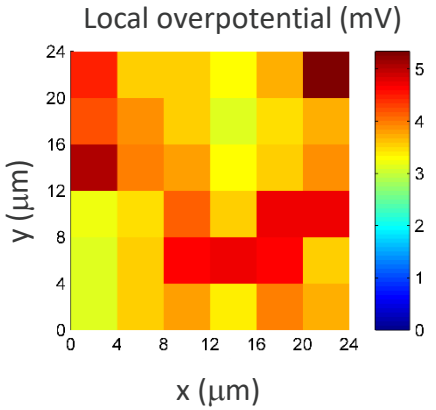


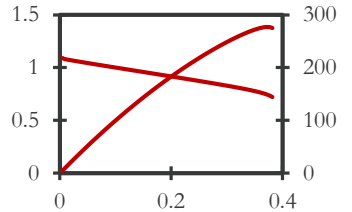
Microstructural Analysis

Degradation Models

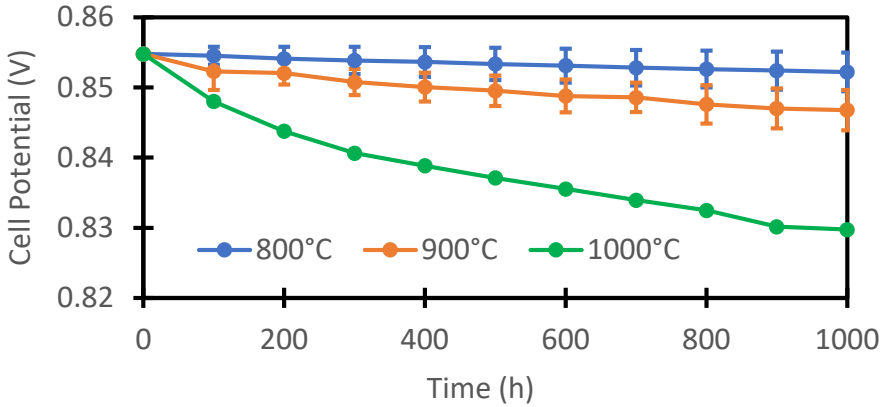


Multiphysics Performance Model





Degradation of Cell Performance

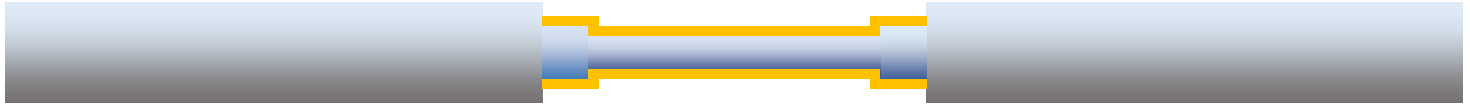


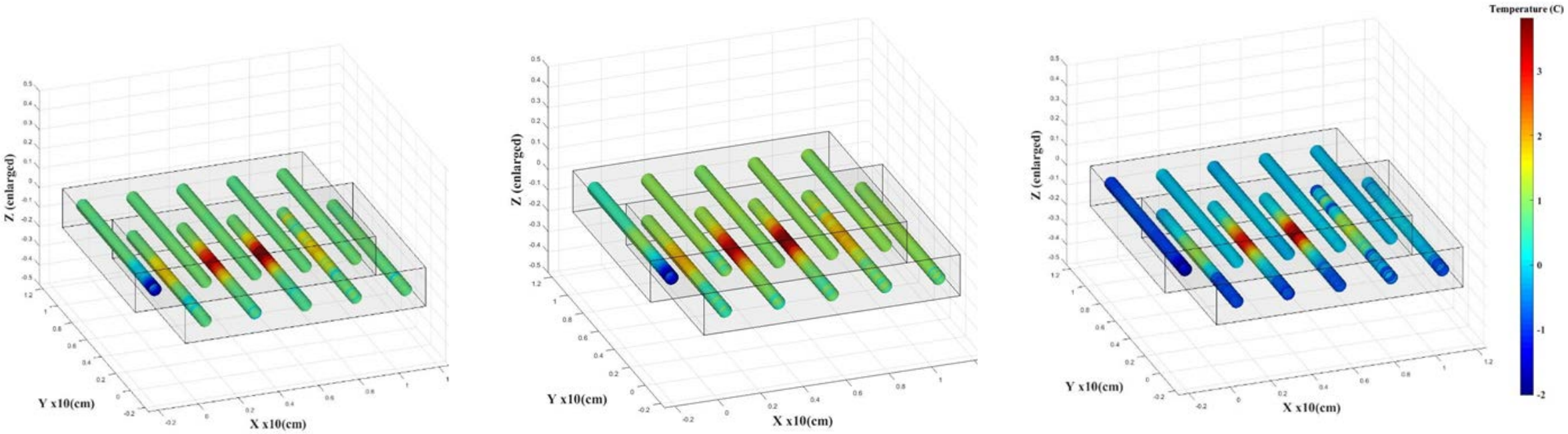
Cell and Stack Degradation

Technologies and Toolsets Under Development

High Temperature Optical Fiber Sensor

Distributed In-situ Temperature and Gas Composition Sensing



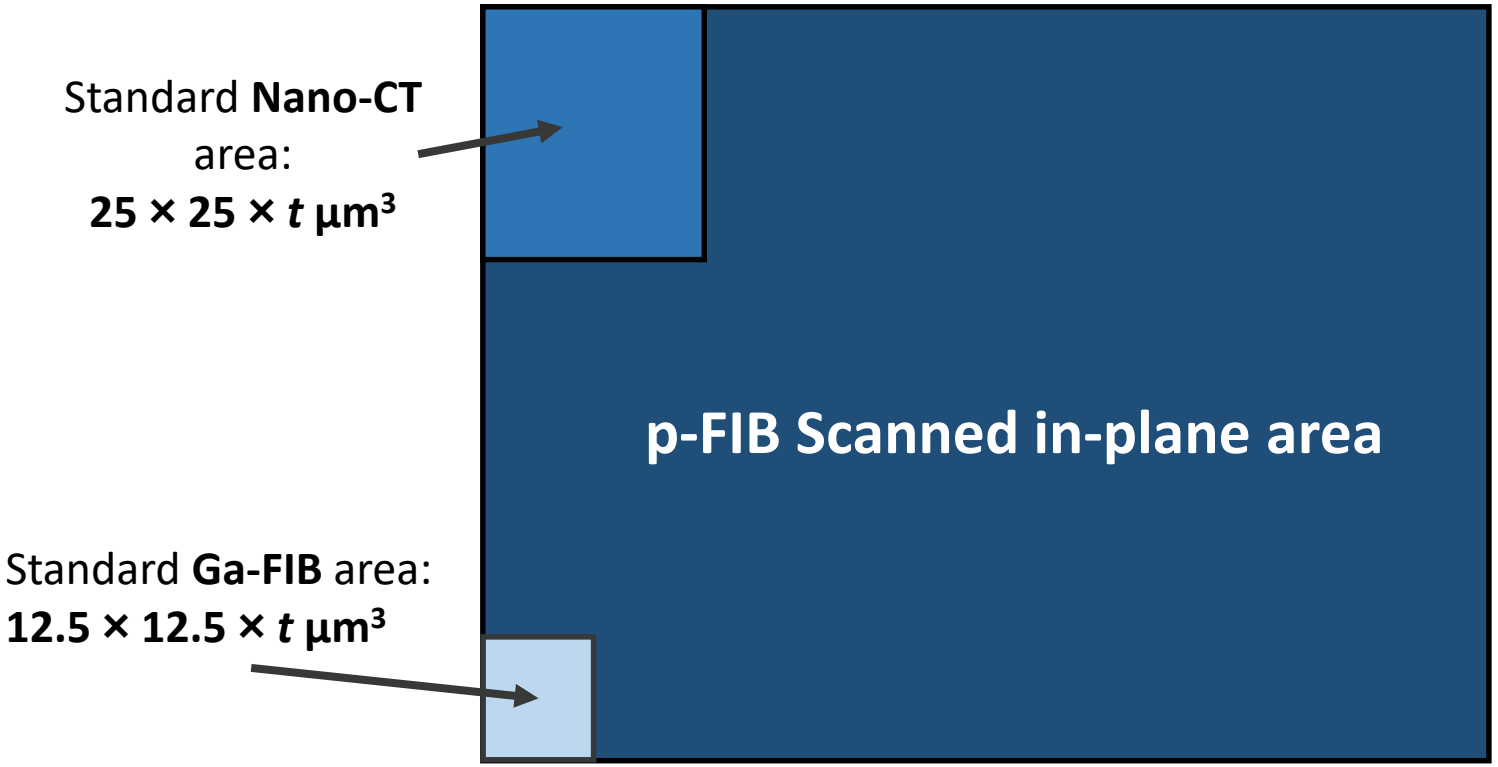


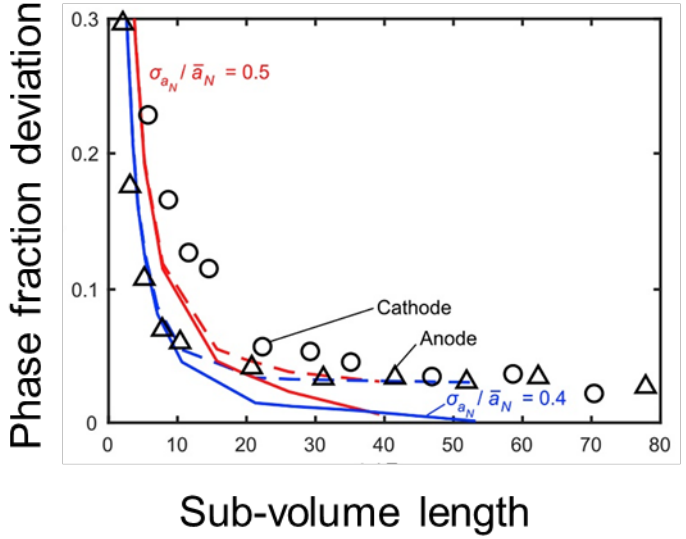
Thermal transients at 30, 60, and 90 s measured from 5×5 cm^2 ASC at 750° C with H_2 fuel after load (2 A) was drawn

3-D Reconstruction of Electrodes

Service CURRENTLY Available to Industrial Partners

- Complete/in progress reconstruction data for cells fabricated by four commercial developers





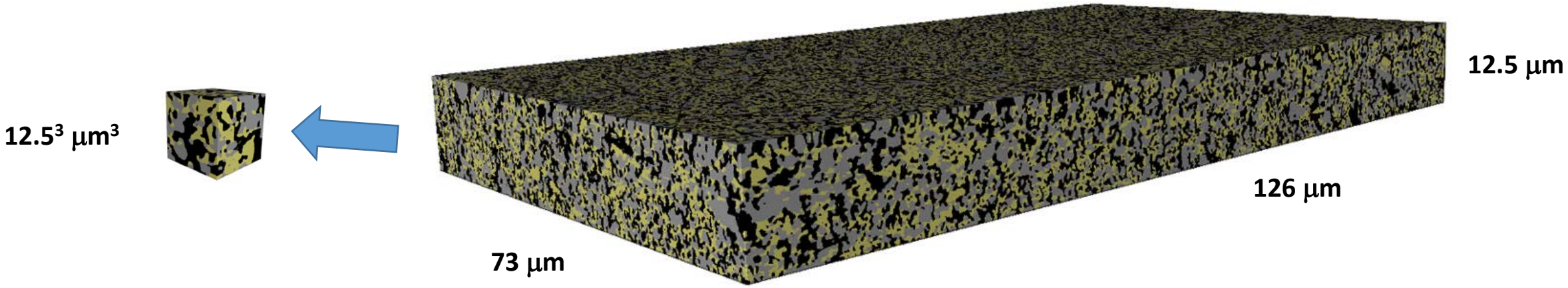
Heterogeneity in real electrodes

p-FIB can capture ≈ 50-200 × Ga-FIB area and ≈ 10-50 × Nano-CT area

3-D Reconstruction Analysis

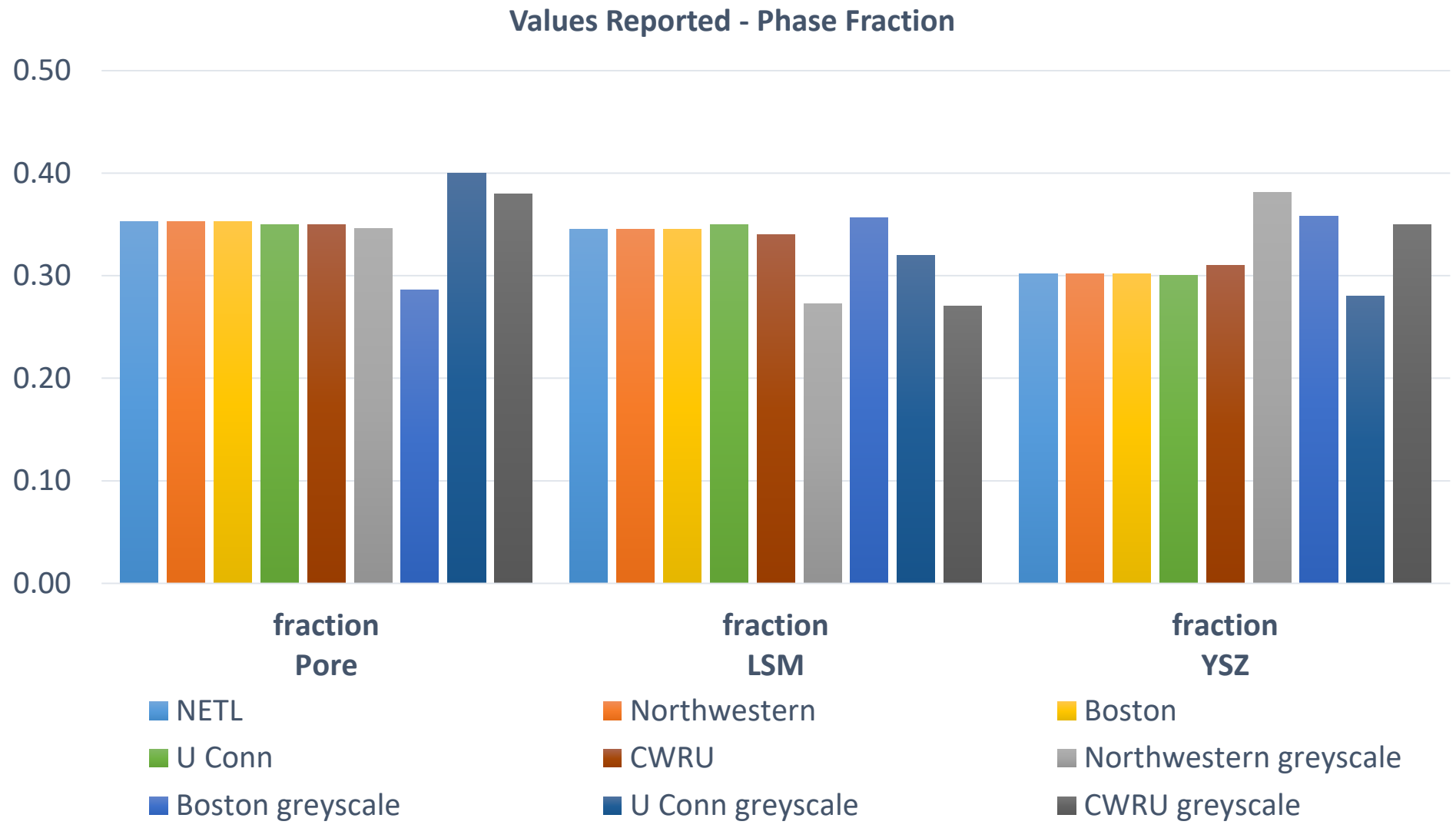
Comparing Analyses from Multiple Academic Groups

- **Five major research groups were given the same reconstruction dataset to compare segmentation procedure and microstructural analysis algorithms**
  - Northwestern, Boston University, UConn, Case Western Reserve
  - Carnegie Mellon works directly with NETL
- **Microstructure data was run through NETL multiphysics model to gauge impact in variance**



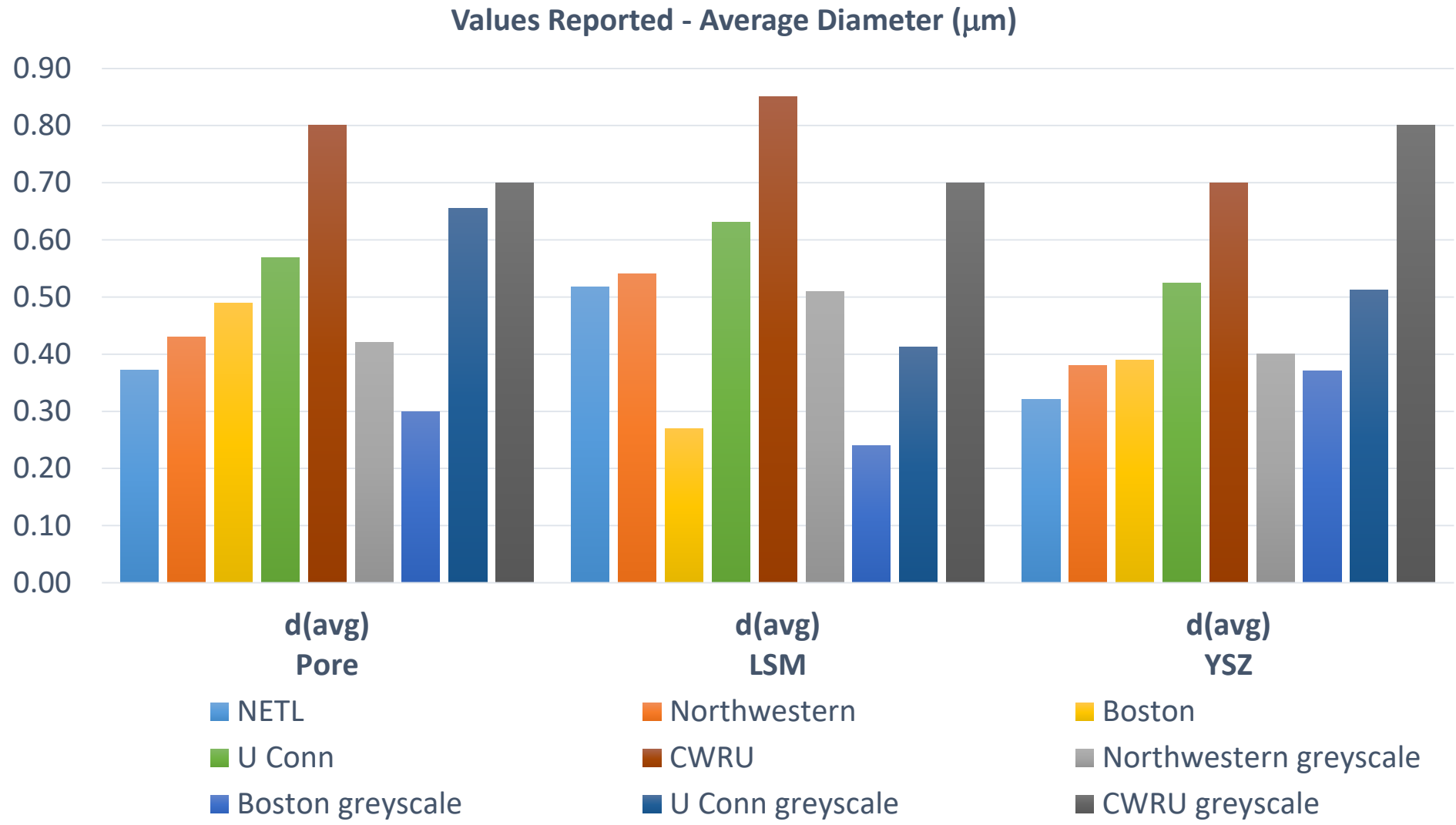
Parameter Distributions

Phase Fraction



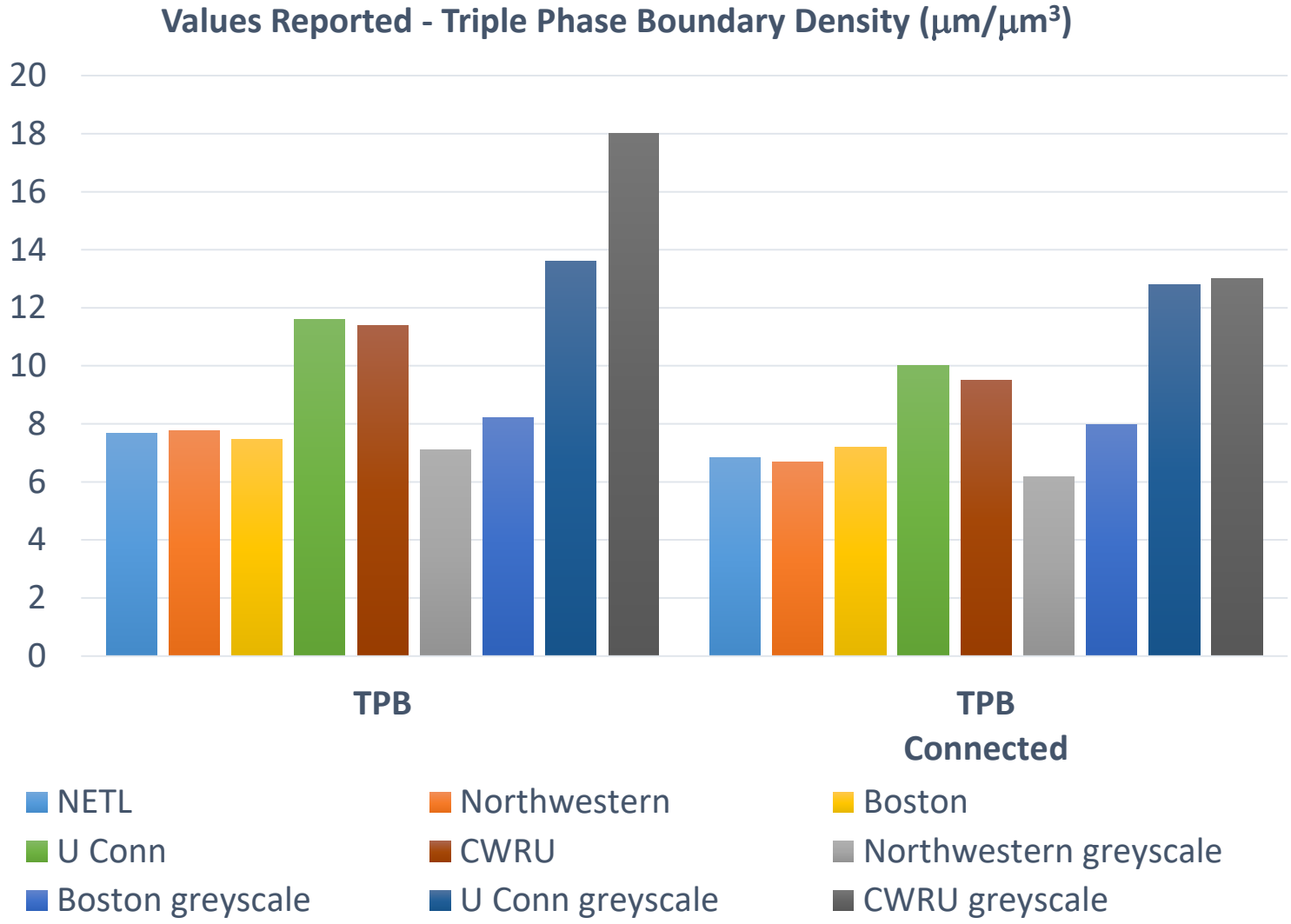
Parameter Distributions

Phase Particle Size



Parameter Distributions

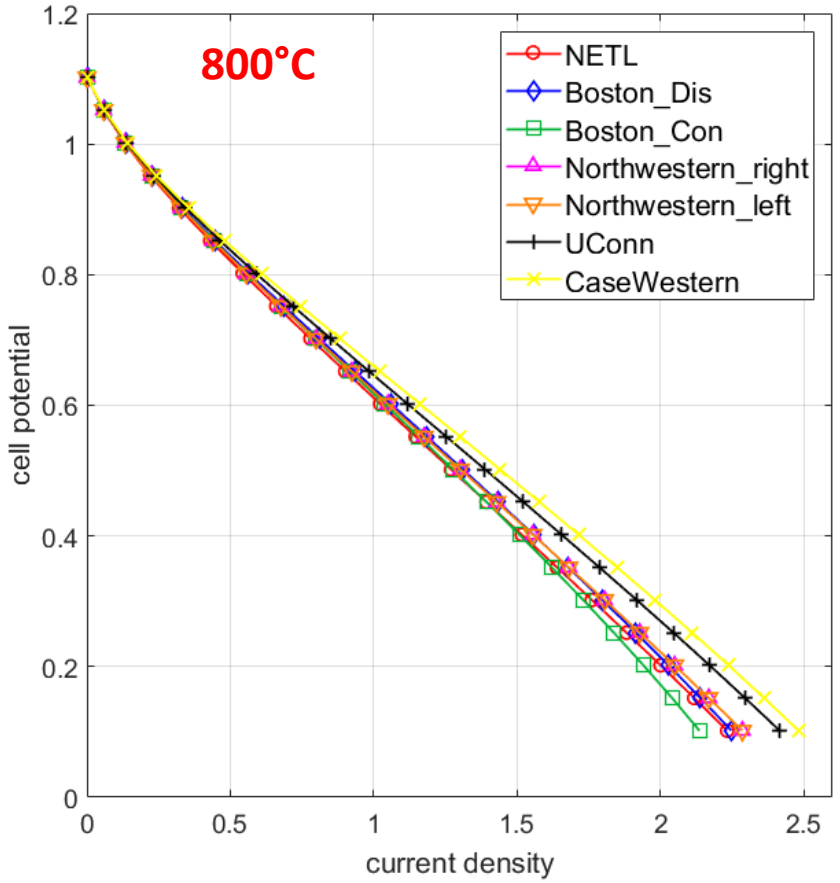
Triple Phase Boundary Density



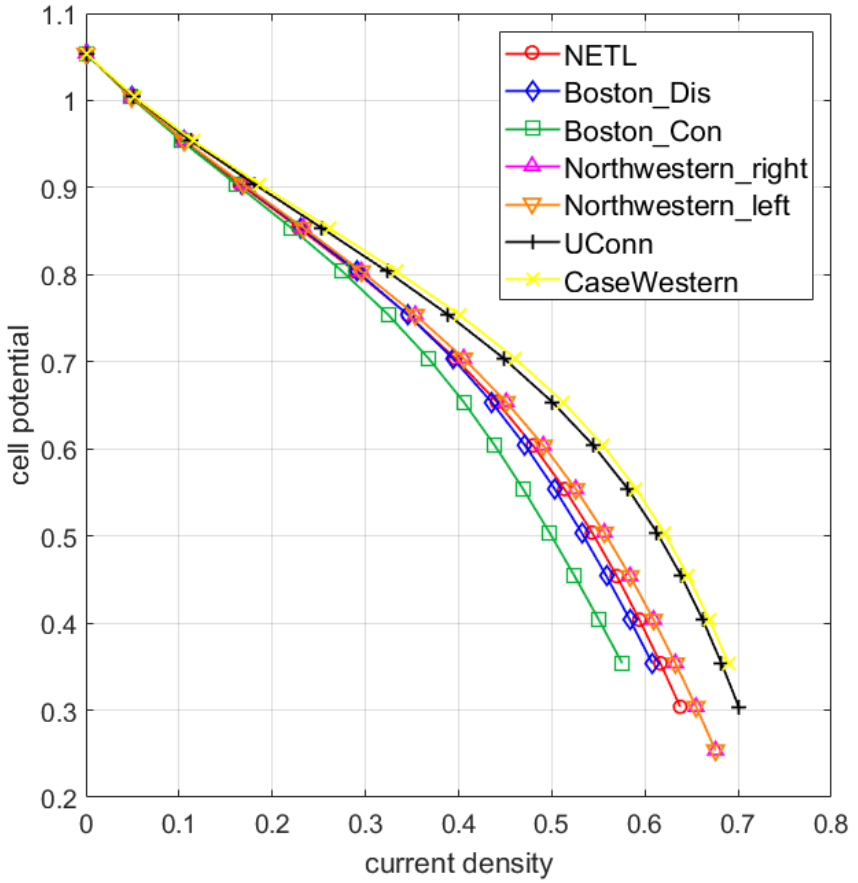
Polarization Curves

Based on Calibrated Butler-Volmer Electrode Kinetics

High Supply Case (air)



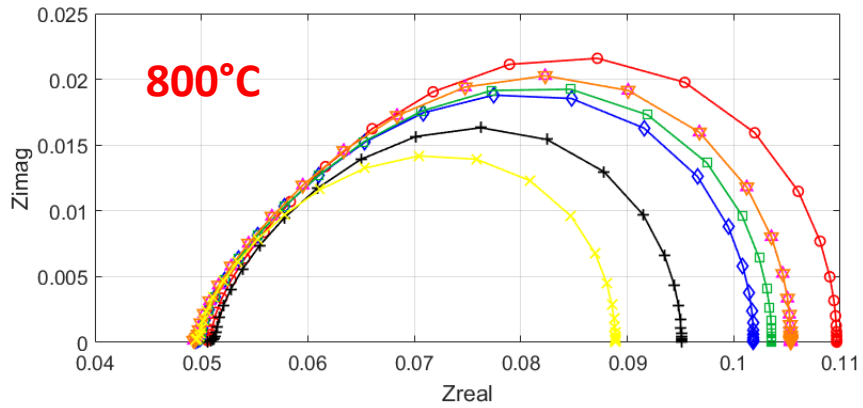
Low Air Supply Case (1/8 air)

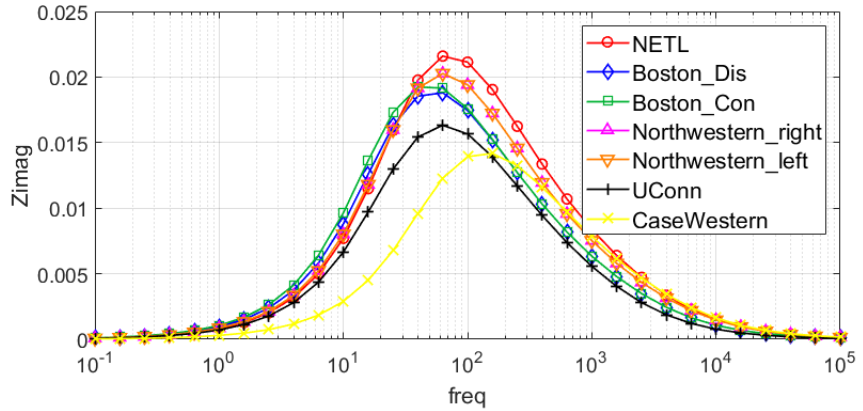


Impedance Simulations

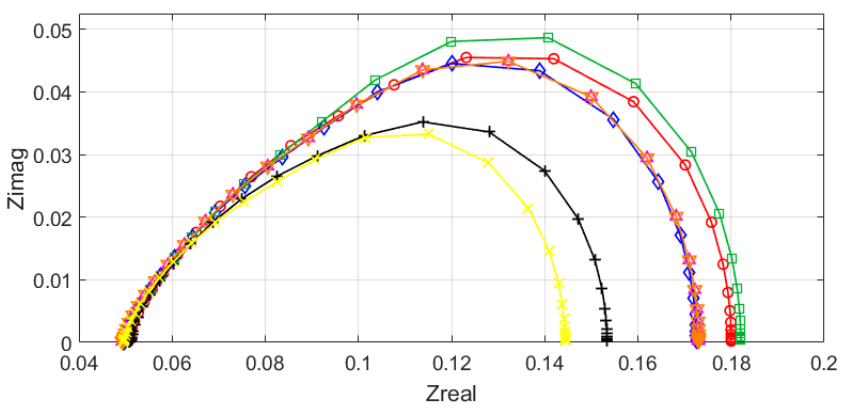
± 20% Variation in Simulated Polarization Resistance

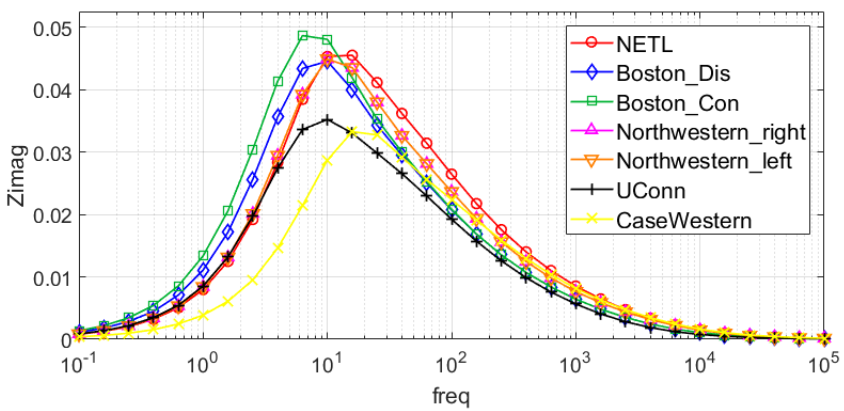
High Supply Case (air)





Low Air Supply Case (1/8 air)



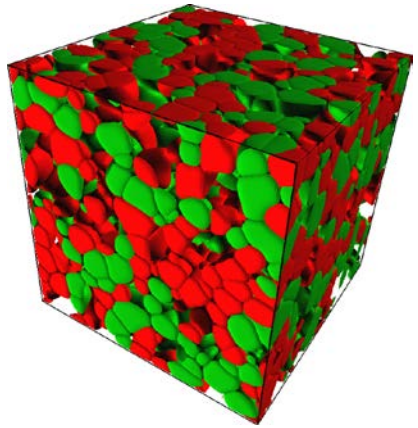


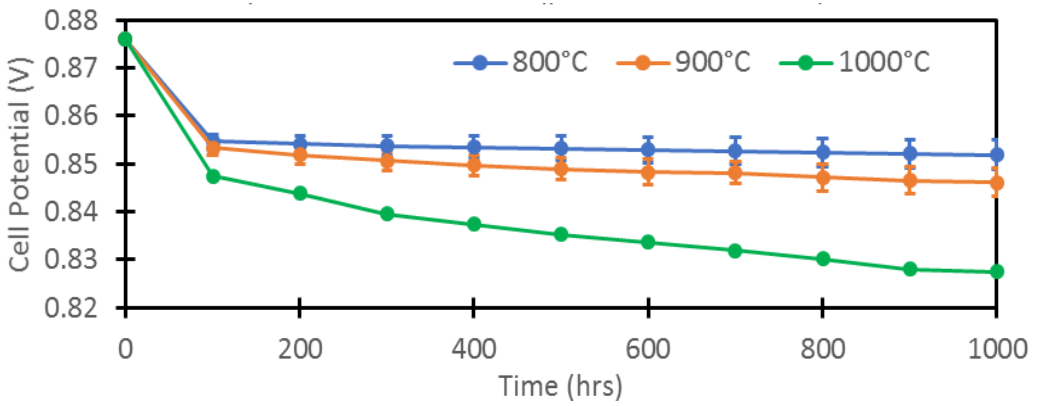
Triple phase boundary density variance impacts simulated performances

Expansion of Coarsening Study

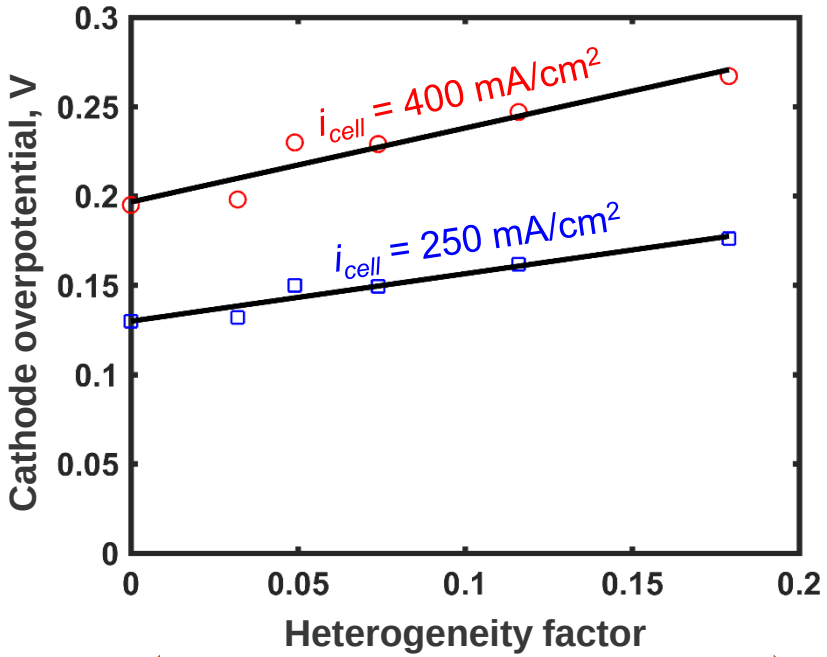
Coarsening Simulation of ~45,000 Different SOFC Button Cells

- **Synthetic microstructures created using Dream3D**
  - Vary phase fraction, particle size, particle size distribution, heterogeneity
- **Cells run through phase field coarsening model and the multiphysics performance model (underway)**
- **Balance performance with degradation rate**





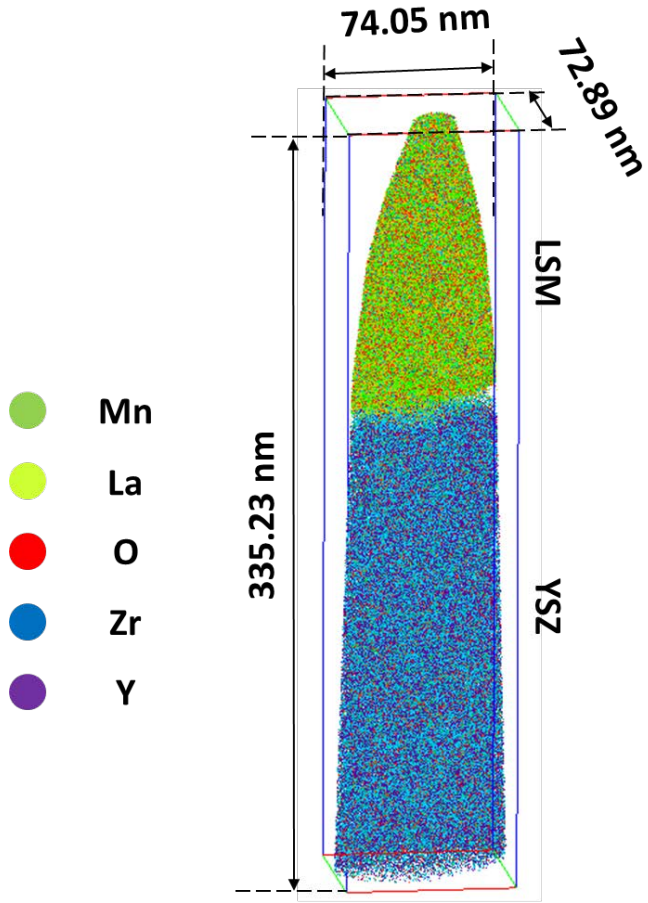
Performance degradation due to coarsening



Well-mixed — Poorly-mixed

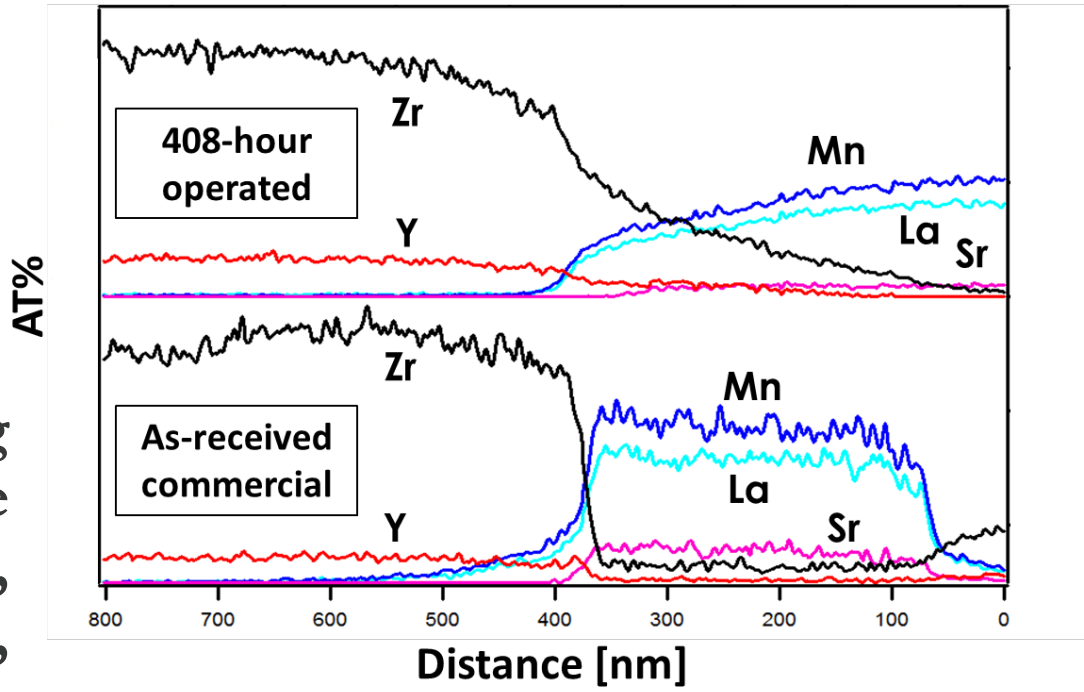
Expansion of Interfacial Characterization

Quantification of Interfacial Diffusion between Cell Components



APT reconstruction of LSM thin film deposited on YSZ

- Interfacial composition changes impacts reaction kinetics and condutivity around, through interface
- Probing cathode/electrolyte interface using TEM, atom probe tomography, and XPS depth profiling



EDS line scan across the electrode/electrolyte interface

NETL SOFC Predictive Modeling Tool

Conclusions

- **How can SOFC technology deployment be accelerated?**
  - Performance and durability enhancement greatly reduces cost
  - Need a thorough understanding of what causes performance loss and durability issues
    - Intrinsic/extrinsic degradation modes are being investigated at the microscale and the results are being passed up multiple scales to system level
    - **Understanding how materials properties (particle size distribution, etc.) change the cost-of-electricity can lead to optimization studies from the micro- to the system scale**
  - Detailed, comprehensive modeling tool can extend lifetime of operating SOFC systems by providing real-time feedback, greatly reducing operation costs
    - Real-time impedance analysis, sensor data
    - Course corrective actions
    - Planned shutdowns with sufficient advanced notice

Degradation Mitigation

Electrode Engineering

Enabling SOFC Technology through R&D at NETL

Electrode Engineering – Enhances Performance and Increases Reliability

COMMERCIALIZATION
Technology available for implementation in SOFC production line

DEMONSTRATION
Technology implemented and tested at SOFC stack (kW) scale

SYSTEM TESTING
Evaluate technology on several commercial developer cells

DEVELOPMENT
Patents obtained

DISCOVERY
Proof of Concept

Concept to Market Readiness

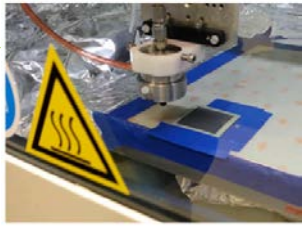
2019 — *Licensing to SOFC commercial developer*

TRL **7-8**

Atrex Cells

2017-18 — *Direct collaboration with Atrex Energy to scale up technology*

TRL **6**



Demonstration at Lab Scale

2012-16 — *Demonstration on commercially relevant scale*

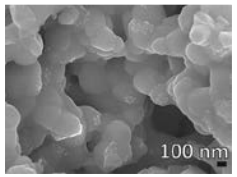
TRL **4-5**

Sonotek Sonic Spray Coater used for technology scale-up

2009-12 — *Technology validated on SOFC button cells (several W) scale*

TRL **2-3**

2009 — *Electrode infiltration technique evaluated*



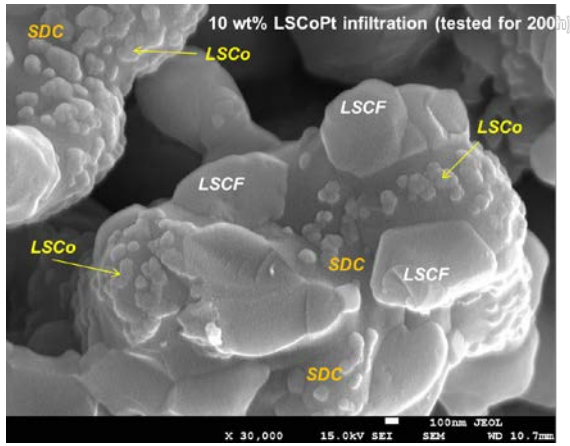
Infiltrated Cathode

Electrode Engineering

Electrode Infiltration Capabilities

Industrial Scale Electrode Infiltration Technology

- **NETL has developed and patented a single-step cathode infiltration technique that can be utilized by commercial SOFC manufacturers to improve their cell performance and durability**
  - Proven performance gains of
    - 10% peak power increase
    - 33% reduction is degradation rate
    - 200% lifetime increase
  - Low-cost ($0.006/cm^2)
  - Scalable
  - Ready for technology transfer
    - Collaboration with industry
    - NDAs executed
  - Ready for any cell geometry



Secretary Perry inserting an SOFC (Atrex Energy) into the Sono-Tek Spray Coater

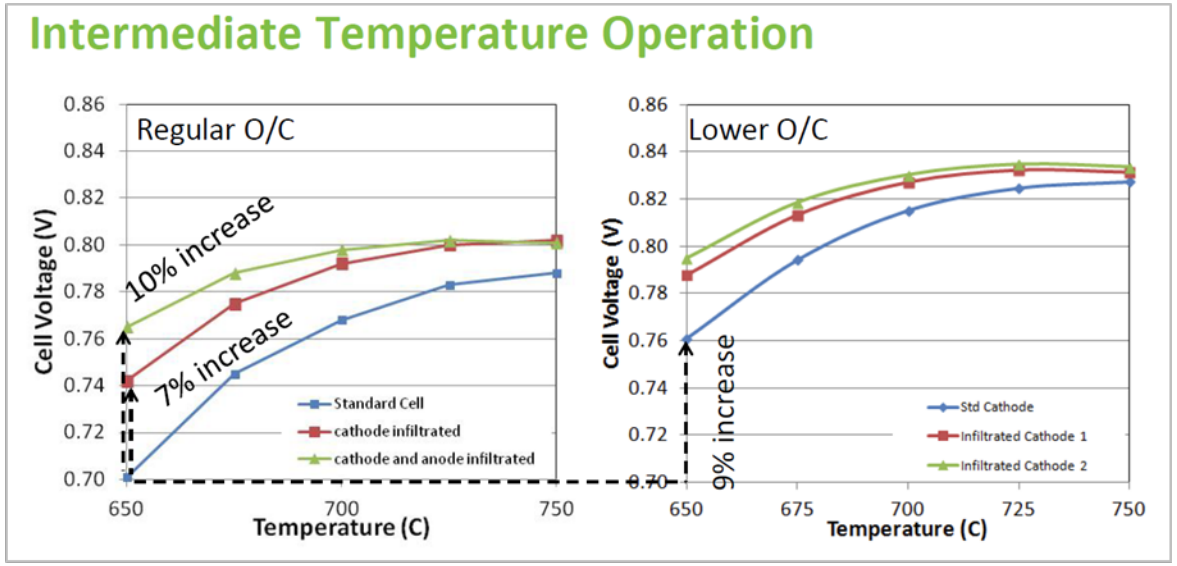
K.Gerdes, S. Lee, R. Dowd, "Methods of forming catalyst layer by single step infiltration," (US Prov. Patent Appl. No. 62191548 (2015)).
K. Gerdes, S. Lee, "Functionally grading of cathode infiltration for spatial control of activity," (US Appl. No. 14/804,492, PCT Appl.No. is 62/026,876 (2015))

Degradation Mitigation

SOFC Electrode Engineering

Collaboration with SOFC Commercial Developers

- **NETL has been working under a Technology Commercialization Fund Award for FY17/18 to scale up the single-step infiltration technology to commercially relevant scales**
  - Industry Partner: Atrex Energy
  - Results so far:
    - 7-10% cell voltage increased by application of spray infiltration with PSCo electrocatalyst
    - Performance enhancement more remarkable at lower temperatures

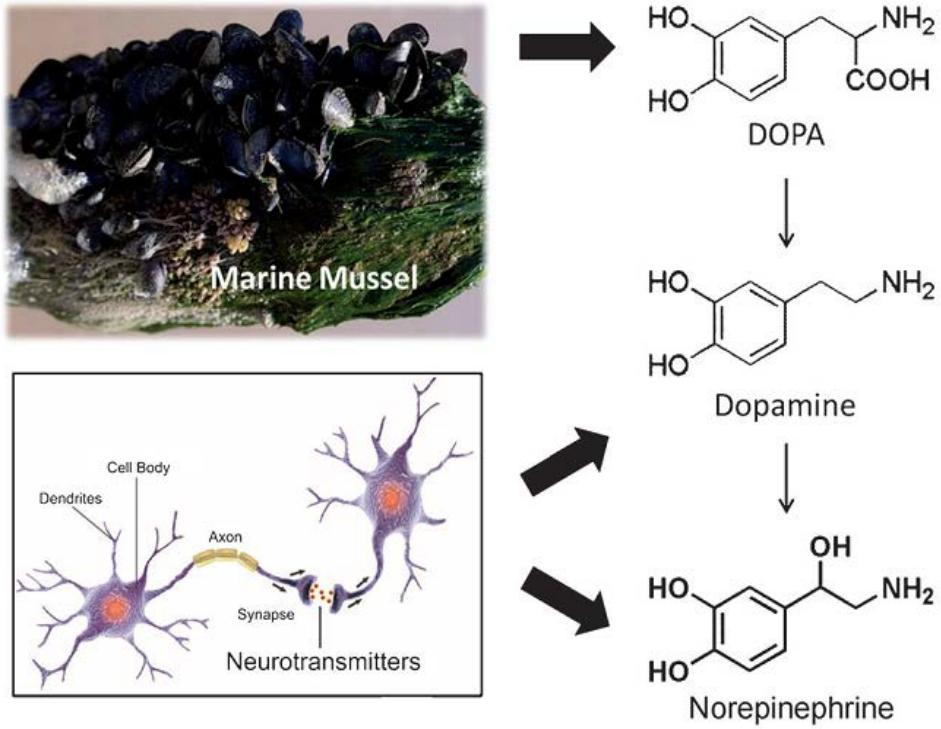


Chengxiang (Shawn) Ji (Atrex Energy, Inc.), 2017 18th annual SOFC Project Review Meeting (Pittsburgh, PA) (Courtesy of Atrex Energy)

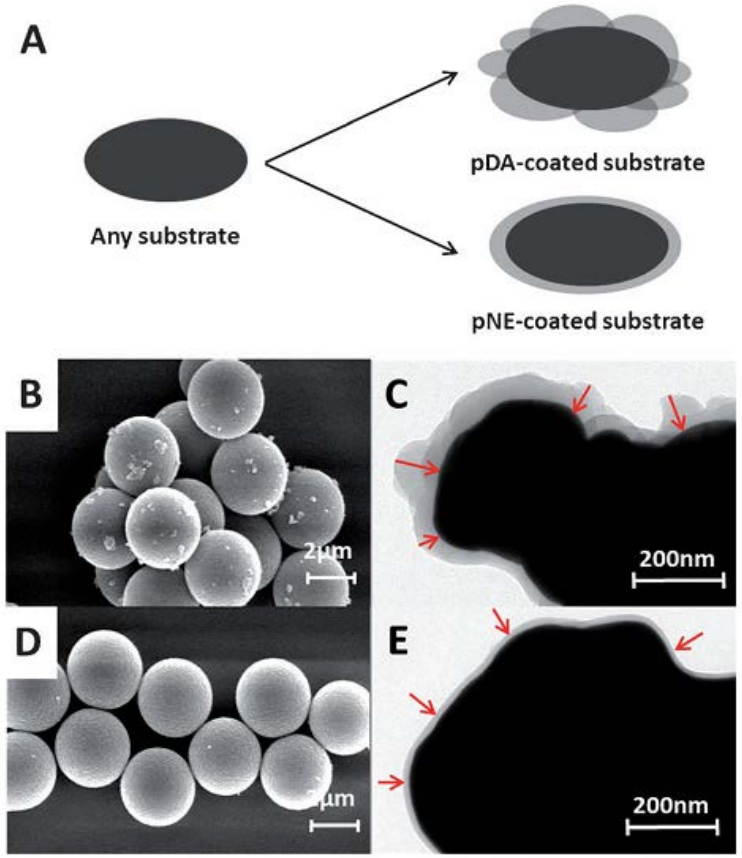
Patent "Method of Forming Catalyst Layer by Single Step Infiltration," US Patent No. 9960428 (2018).

Anode Infiltration Technique Exploration

- Bio-surfactant (e.g. polydopamine /polyepinephrine) application to improve infiltration of dense anode microstructures in collaboration with West Virginia University

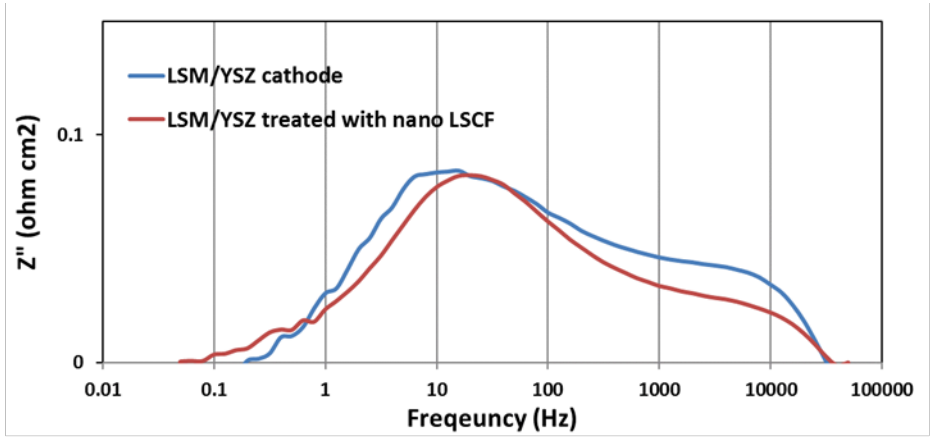


- Initiated collaboration with an SOFC commercial developer

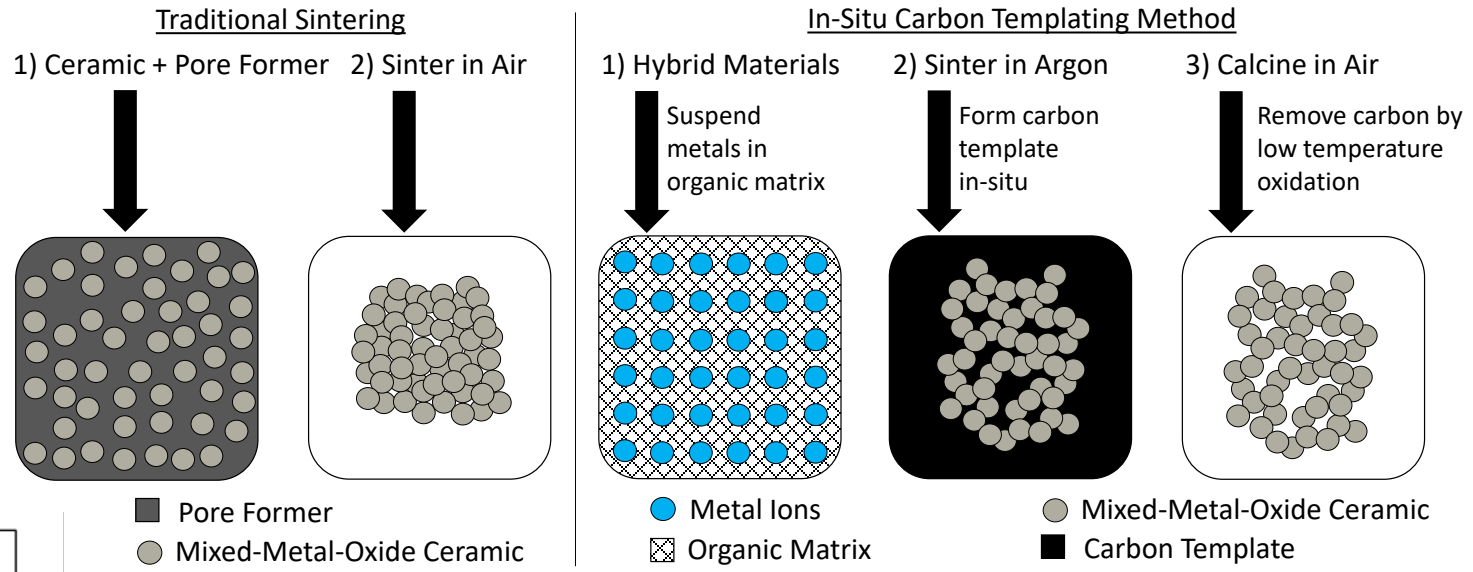


Advanced Materials Development

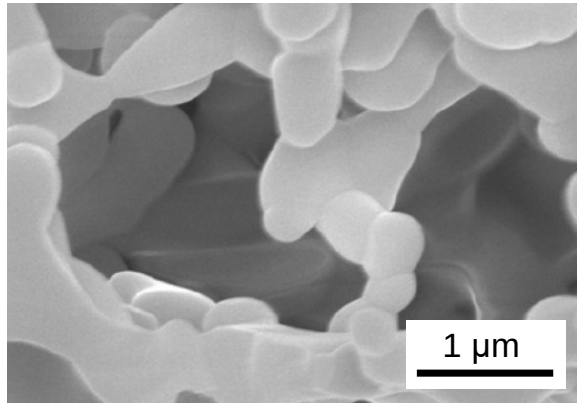
- In-situ carbon templating for high surface area electrodes
  - Collaboration with Wake Forest University
  - Professor Michael Gross



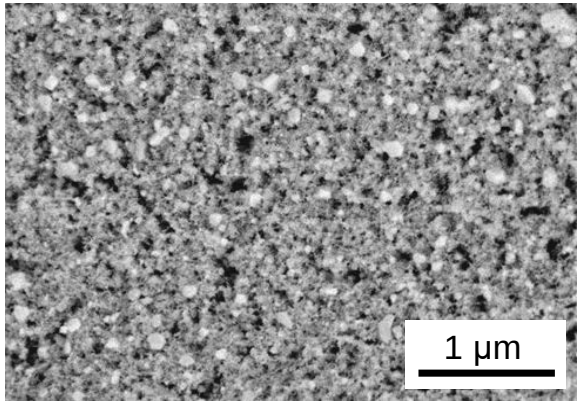
Bode plot of LSM/YSZ treated with nano-LSCF



Traditional Sintering

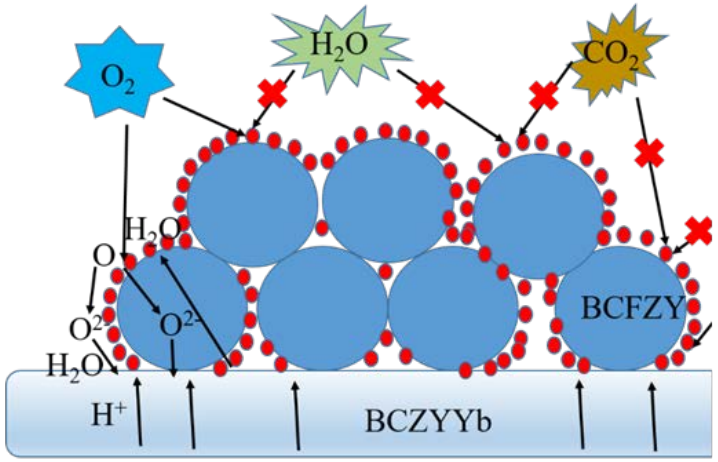


In-Situ Carbon Templating

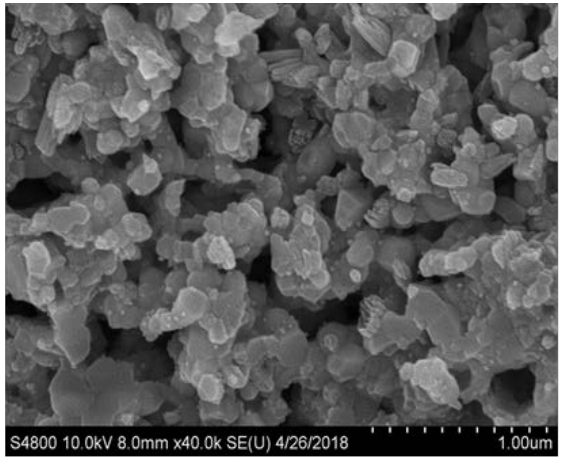


Advanced Materials Development

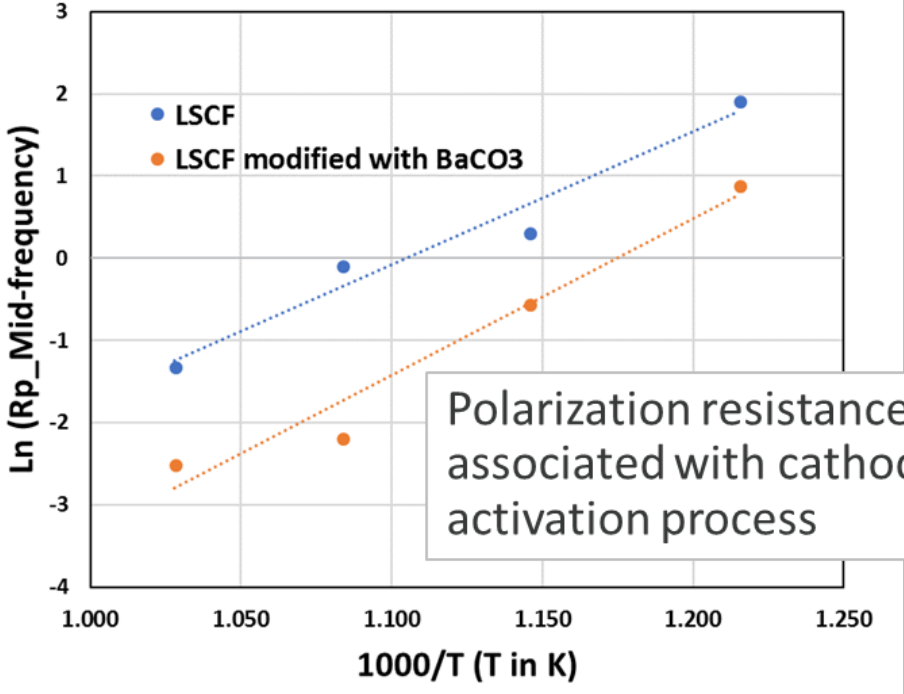
- **Electrode engineering of proton conducting electrodes for intermediate temperature SOFC operation**
  - Collaboration with Clemson University
  - Professor Kyle Brinkman



Cathode infiltration in Proton SOFCs



LSCF electrode infiltrated with $BaCO_3$



Polarization resistance (R_p) associated with cathode activation process

Poster Session

Please stop by to see our posters!

Poster Session 6:30-8:00 PM

Exhibit Halls B&C

FE074-p (Electrode Engineering)

FE075-p (Cell and Stack Degradation Modeling)

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