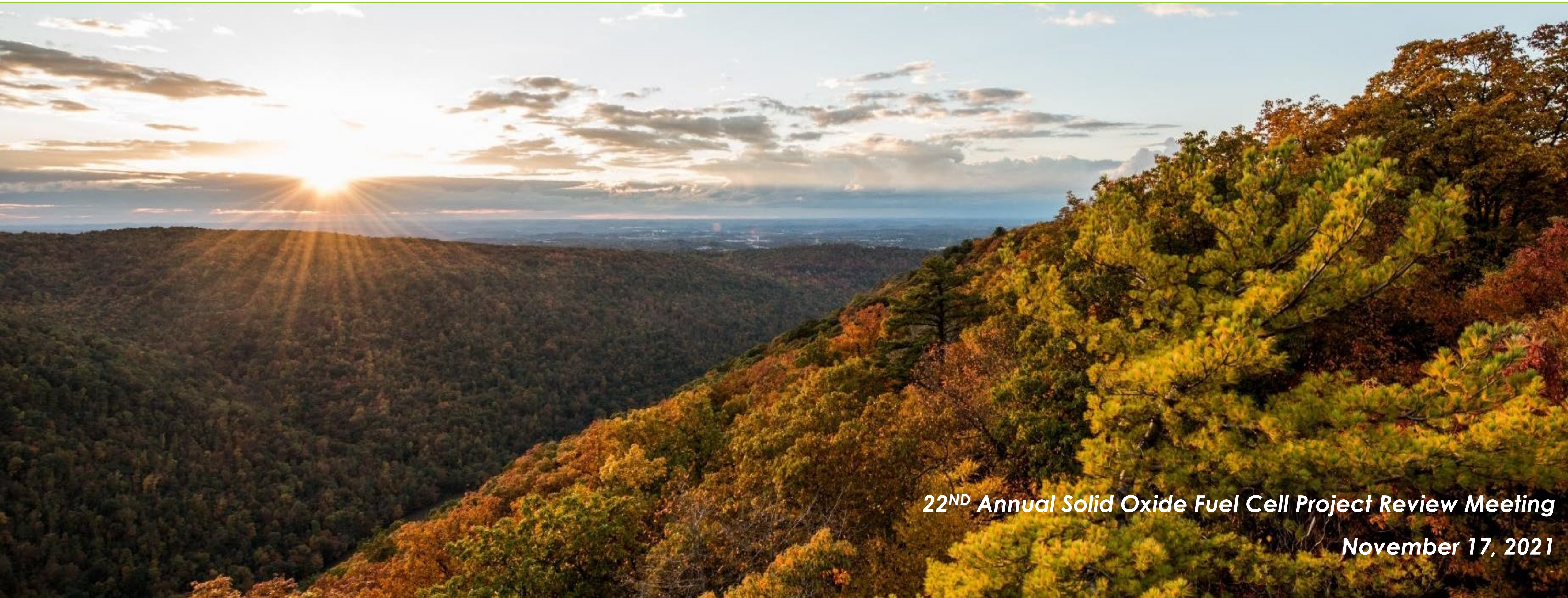
Solid-State Electrochemical Cell

R&D Progress at NETL

NATIONAL ENERGY TECHNOLOGY LABORATORY

Gregory A. Hackett, Ph.D.

Team Lead, NETL SSEC R&D

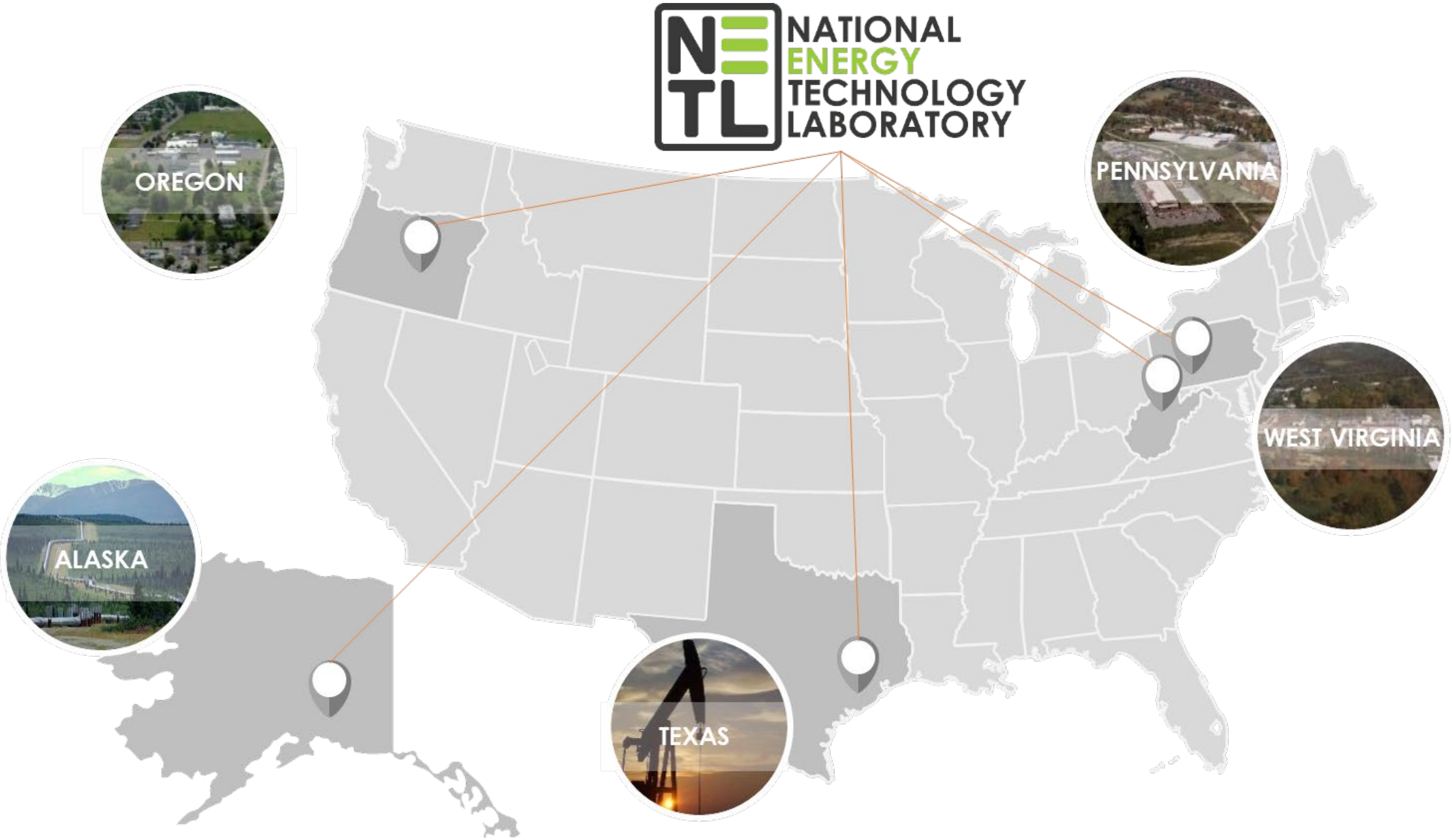


22ND Annual Solid Oxide Fuel Cell Project Review Meeting

November 17, 2021

Outline

- **Introduction**
- **Recent Progress Summary**
  - Cell and Stack Degradation Modeling and Simulation
  - Electrode Design and Engineering
  - Strategic Systems Analysis and Engineering
- **Summary of Other Efforts**
- **Wrap-Up**



NETL SSEC R&D Team

NETL (Federal Staff)

- Gregory Hackett, Team Lead (NETL)
- Harry Abernathy (NETL)
- Travis Shultz (NETL)
- Ron Breault (NETL)
- Rich Pineault (NETL)
- Yves Mantz (NETL)
- Yuhua Duan (NETL)
- Slava Romanov (NETL)
- Youhai Wen (NETL)
- Randy Gemmen (NETL)

West Virginia University

- Harry Finklea (Chemistry Emeritus)
- Ismail Celik (MAE Emeritus)
- David Mebane (MAE)
- Ed Sabolsky (MAE)
- Xueyan Song (MAE)
- Xingbo Liu (MAE)
- Yun Chen (WV Research Corp.)
- Bo Guan (WV Research Corp.)
- Jose Bohorquez (MAE, Student)
- Joshua Tenney (MAE, Student)

NETL (Site Support Team)

- Tom Kalapos (LRST)
- Billy Epting (LRST)
- Arun Iyengar (KeyLogic)
- Lynn Fan (LRST)
- Rick Addis (USSE2)
- Tianle Cheng (LRST)
- Youngseok Jee (LRST)
- Jian (Jay) Liu (LRST)
- Yueh-Lin Lee (LRST)
- Tao Yang (LRST)
- Yinkai Lei (LRST)
- Giuseppe Brunello (LRST)
- Hunter Mason (LRST)
- Yoosuf Picard (LRST)
- Kyle Buchheit (KeyLogic)
- Alex Noring (KeyLogic)
- Fei Xue (LRST)

TARGETED FOCUS:
Collaboration
Technology Transfer
Open-source tool development

Carnegie Mellon University

- Paul Salvador (MSE)
- Shawn Litster (MechE)
- Tony Rollett (MSE)
- Liz Holm (MSE)
- Hokon Kim (MSE, Grad Student)
- William Kent (MSE, Grad Student)

Clemson University

- Kyle Brinkman (MSE - Chair)
- Jack Duffy (MSE)

Georgia Southern University

- Hayri Sezer (Engineering)

Penn State University

- Long-Qing Chen (MSE)
- Yanzhou Ji (MSE, Student)

University of Wisconsin-Madison

- Dane Morgan (MSE)
- Ryan Jacobs (MSE)

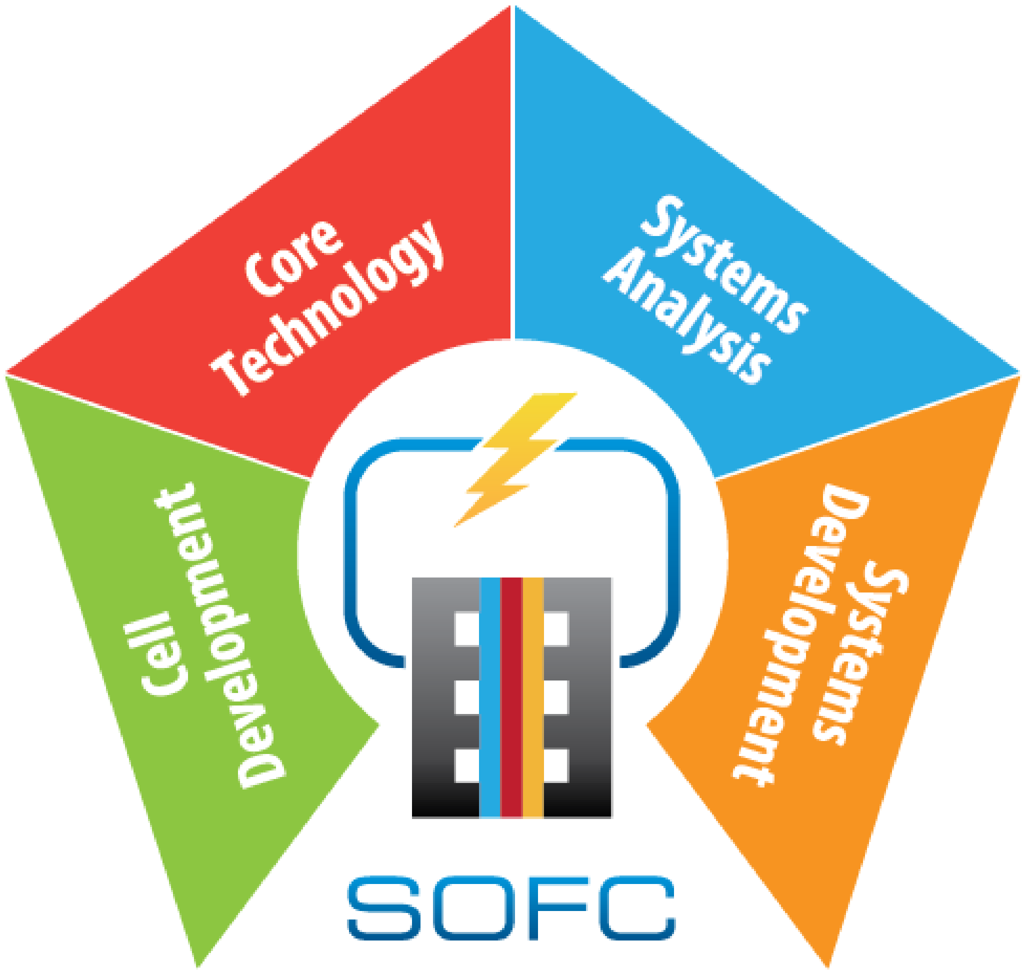
Wake Forest University

- Michael Gross (Chemistry)
- Sixbert Muhoza (Post-Doc)

Currently 50+ SOFC Team Members

Cell and Stack Degradation

Modeling and Simulation



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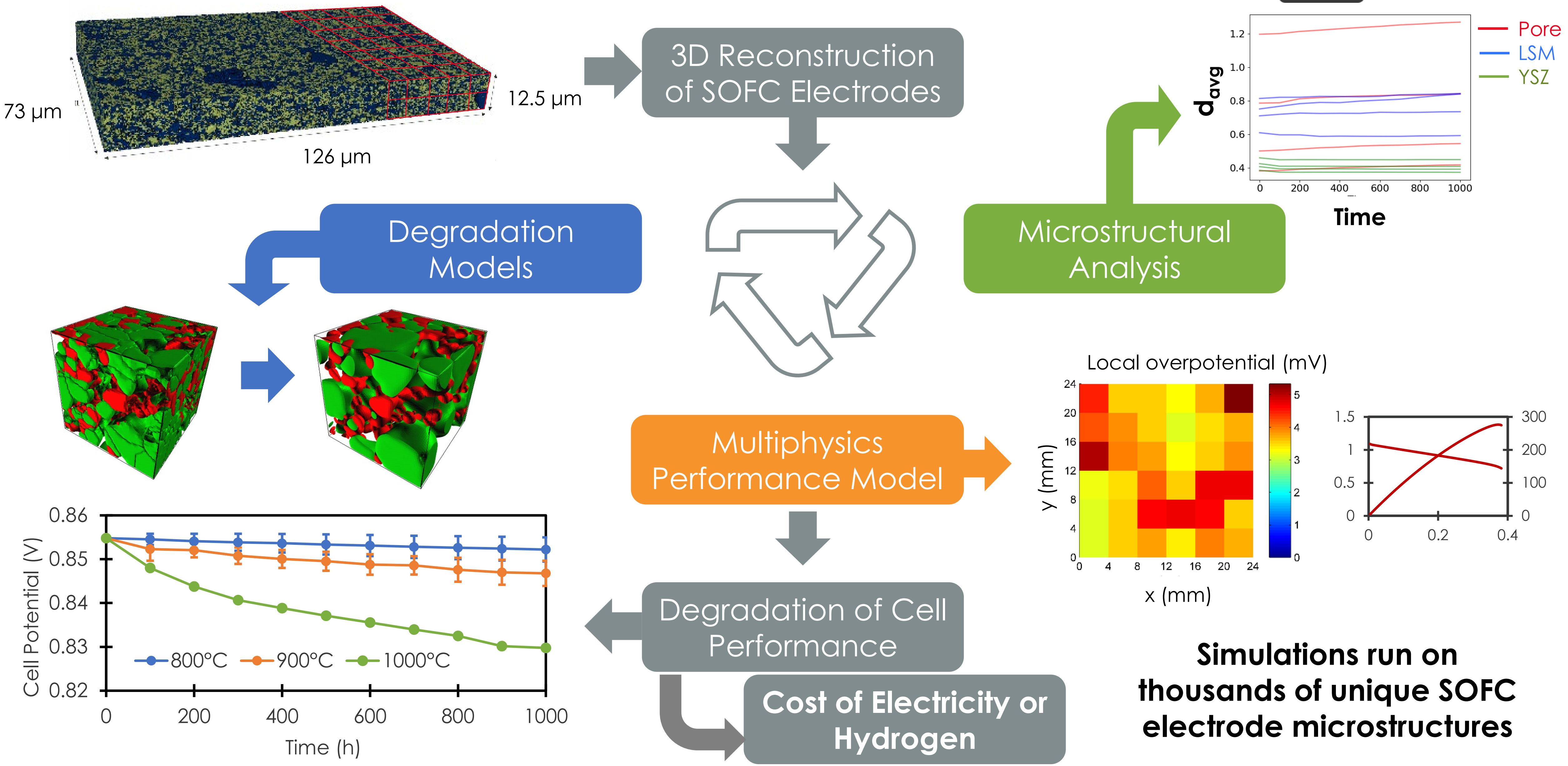
Integrated Cell Degradation Model



Coupling Advanced Techniques

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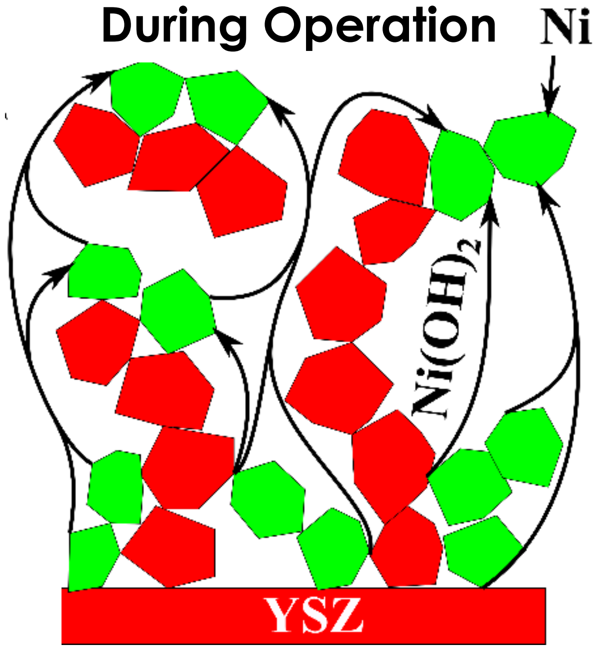
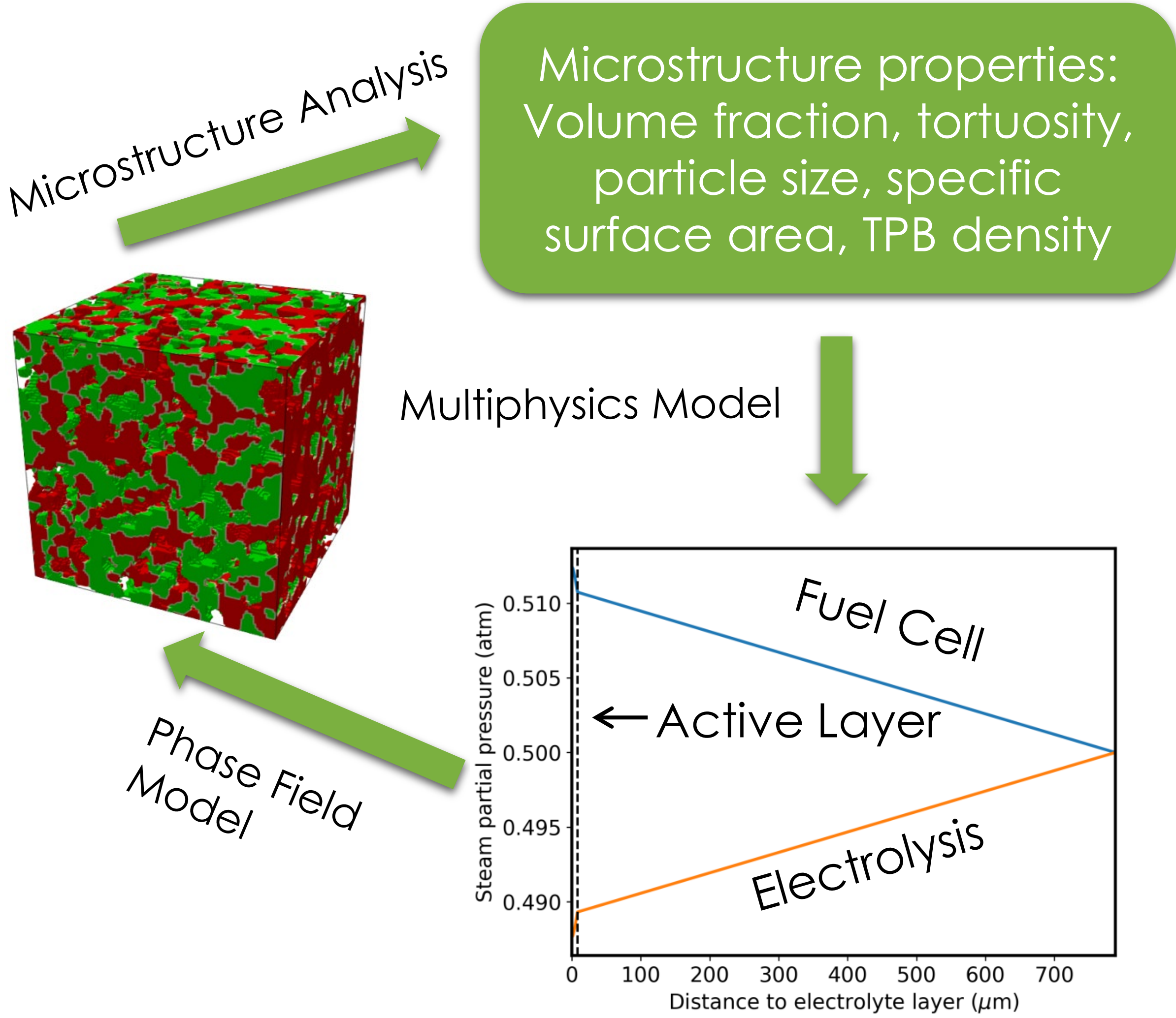
Microstructure Evolution in Ni-YSZ Electrodes under Operating Conditions

- Coupling the phase field model, microstructure analysis toolset, and multiphysics model for modeling the microstructure evolution

- Ni bulk diffusion, $Ni(OH)_2$ formation and diffusion through the pore phase and Ni-YSZ wettability change are incorporated in the model as the driving forces of the microstructure evolution





Lei et al, J. Power Sources, 345 (2017) 275-289; Lei et al, J. Power Sources, 482 (2021) 228971
Lei et al, Proceedings of TMS 2022, accepted.

Adapting Capability to R-SOC/SOEC Mode

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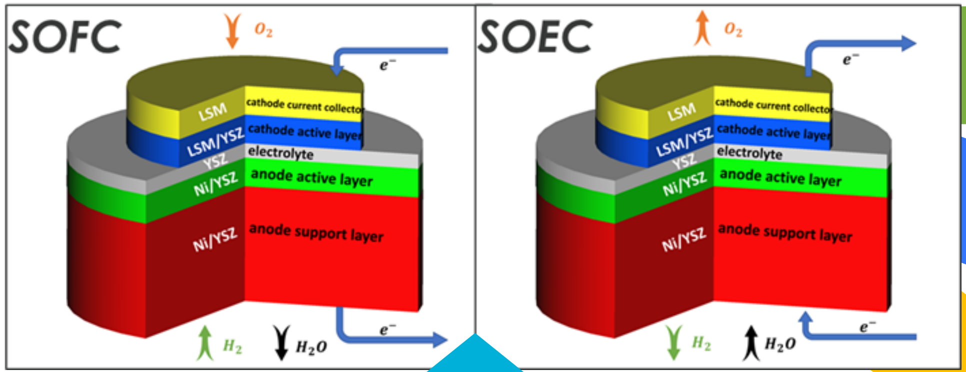
Multiphysics, ECR Characterization, Performance, Infiltration Modeling

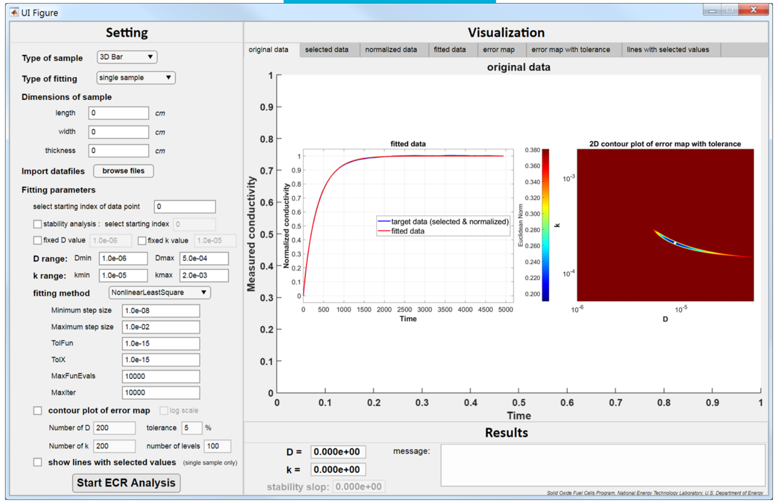


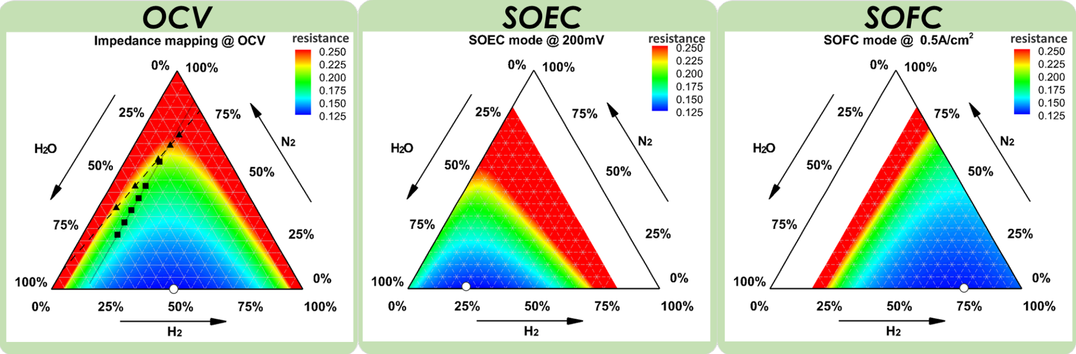
Reversible Mode

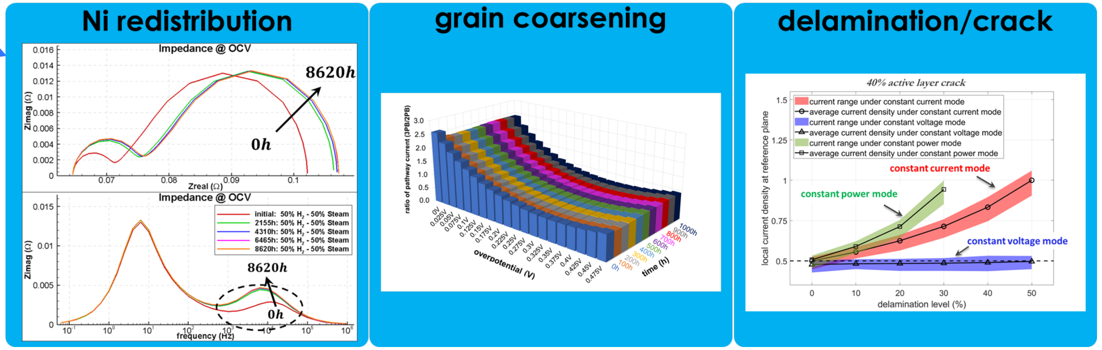
Performance Degradation

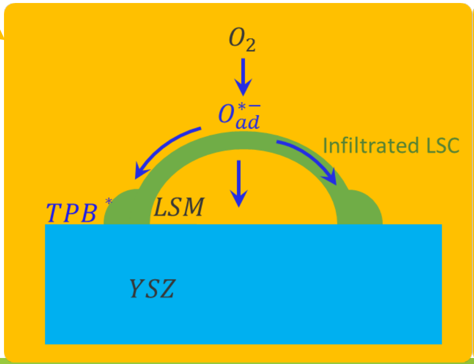
Nanoparticle Infiltration

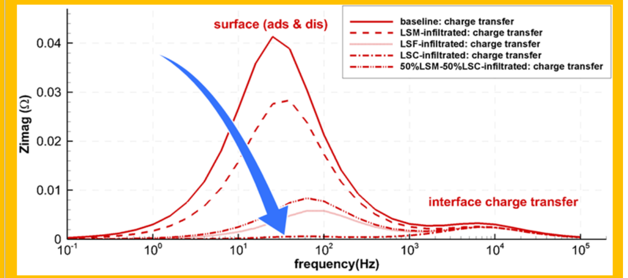
ECR Tool









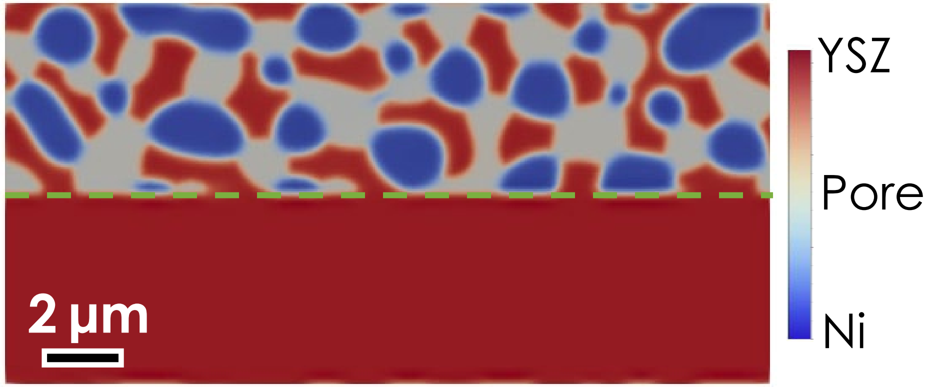


Incorporation of Additional Degradation Mode

Simulation of Mechanical Degradation Considering Microstructures

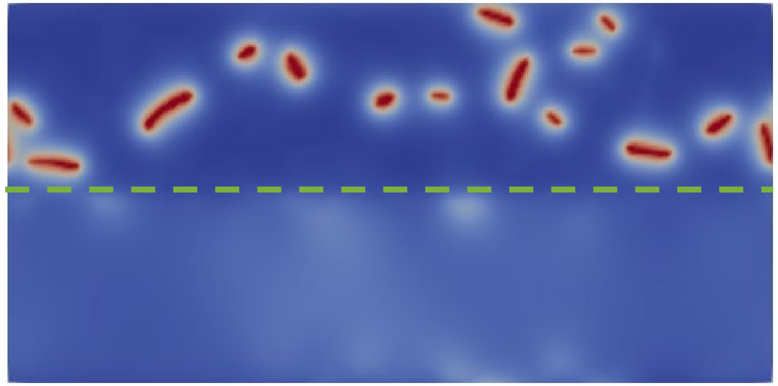
Expanded modeling capability of simulating crack growth considering SOC microstructures

Microstructure

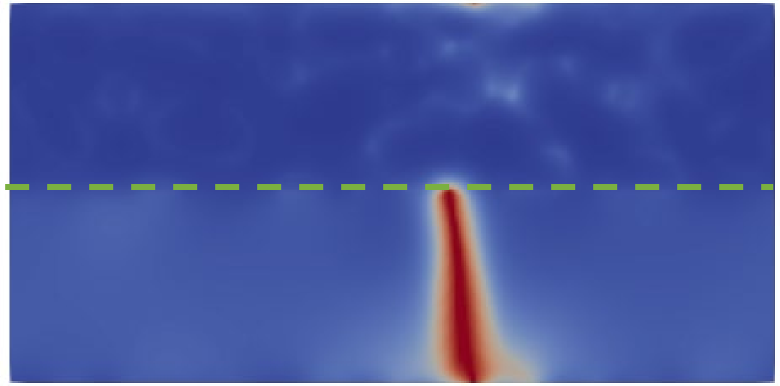


Interphase cracking and through cracking under thermal and redox cycling, respectively

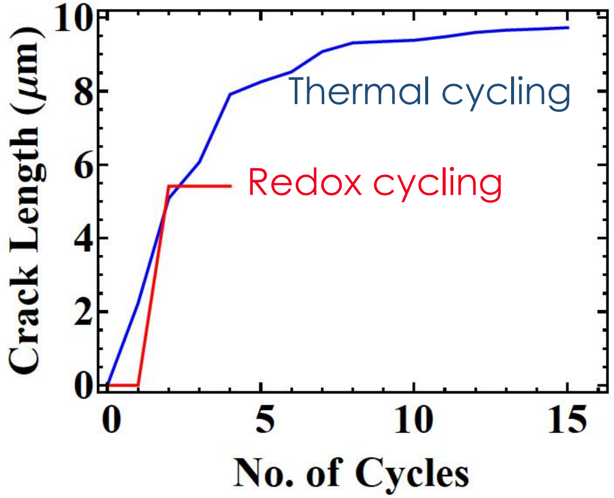
Thermal Cycling

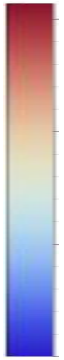


Redox Cycling



Crack Length vs # of Cycles





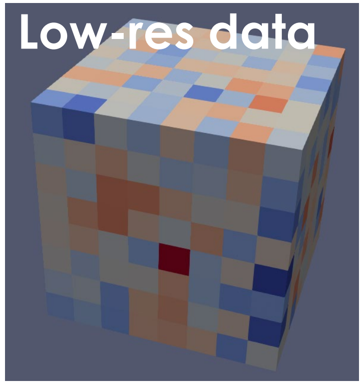
Machine Learning and Microstructure

Convolutional Neural Networks

Super-resolution

3D analysis

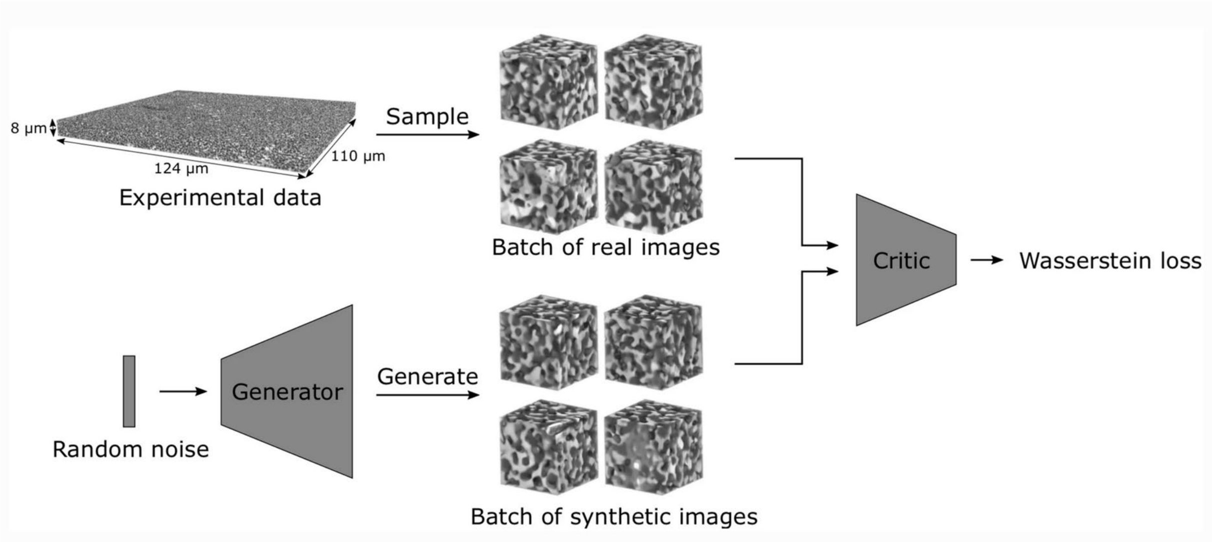
Properties	
Porosity	0.21
LSM/YSZ	0.8
Davg1	445
Davg2	610
Davg3	555
TPB	4.35
+ tortuosity, SA, etc	



Machine Learning Model

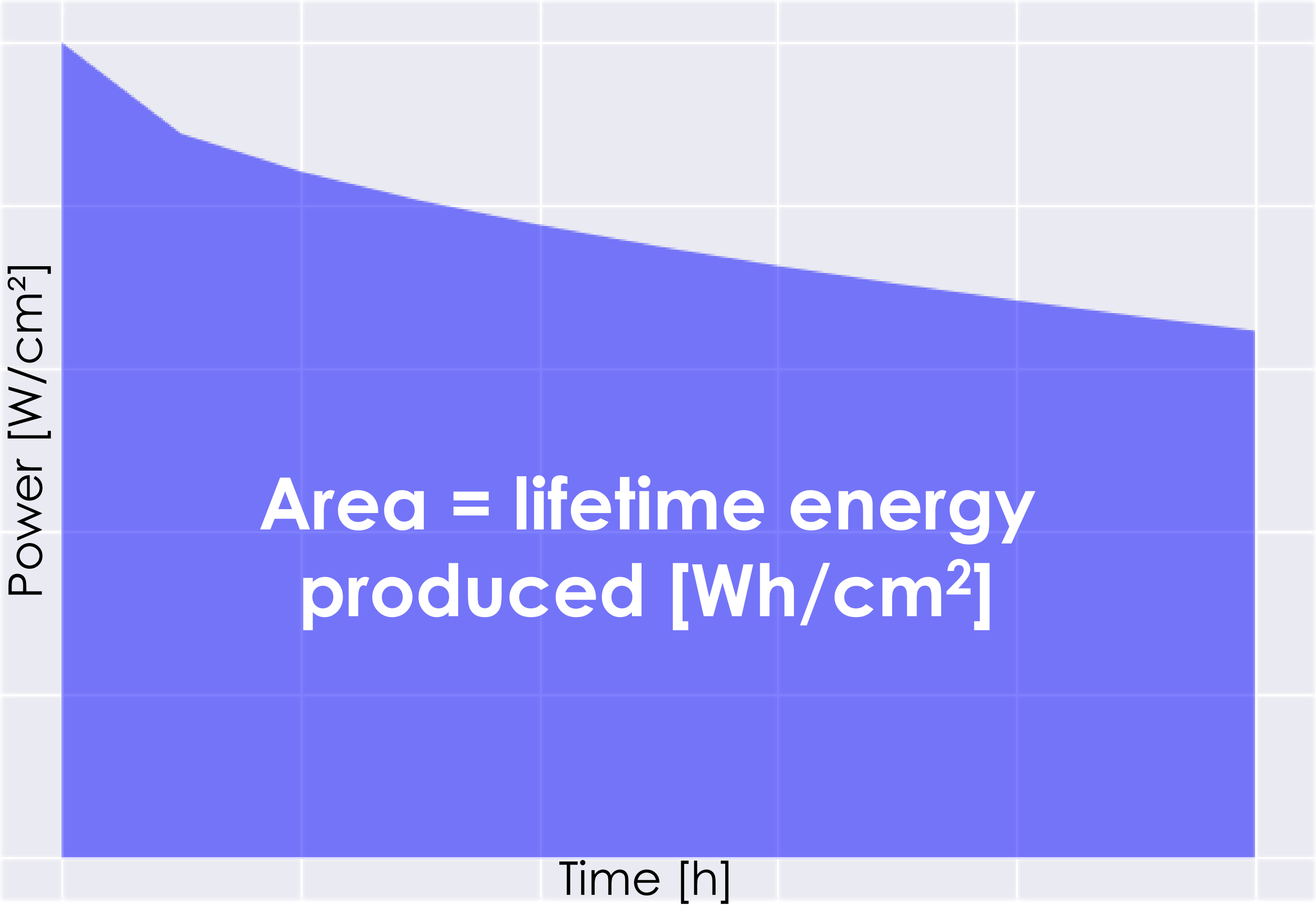
Properties	
Porosity	0.26
LSM/YSZ	0.86
Davg1	480
Davg2	660
Davg3	503
TPB	4.1
+ tortuosity, SA, etc	

Microstructure Generation



Tim Hsu et al., "Microstructure generation via generative adversarial network for heterogeneous, topologically complex 3d materials." *JOM* v73 pg 90 (2021)

Lifetime Energy as Figure of Merit



Voltage decay is important but misses whether electrode was a poor performer to begin with

Need a single figure-of-merit that captures both initial performance and stability

Lifetime energy production – at a given current density, up to a given time

Proxy for $/kWh, which is what a plant operator would care about

Cathode Feature Importance Ranking

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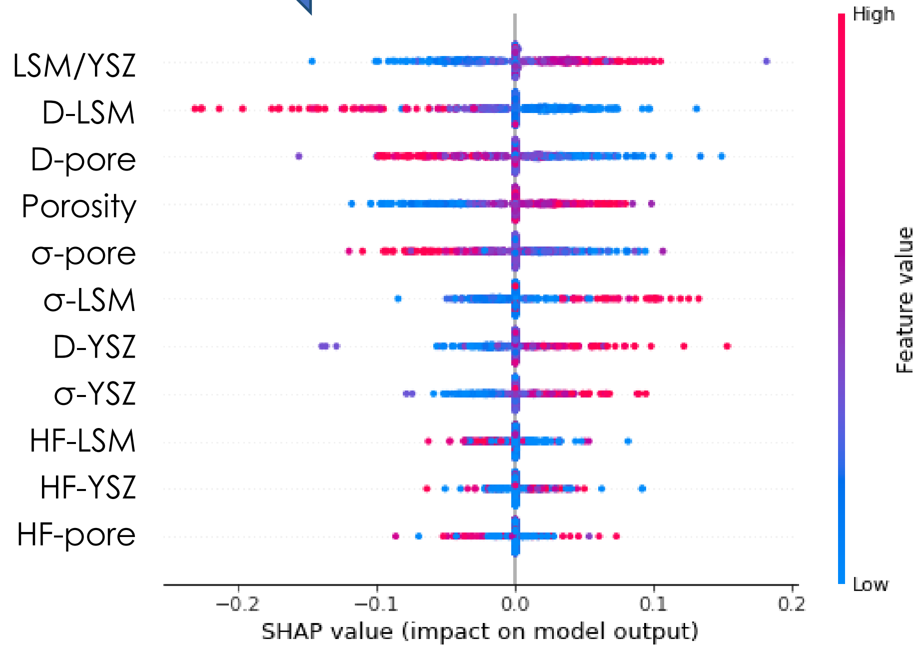
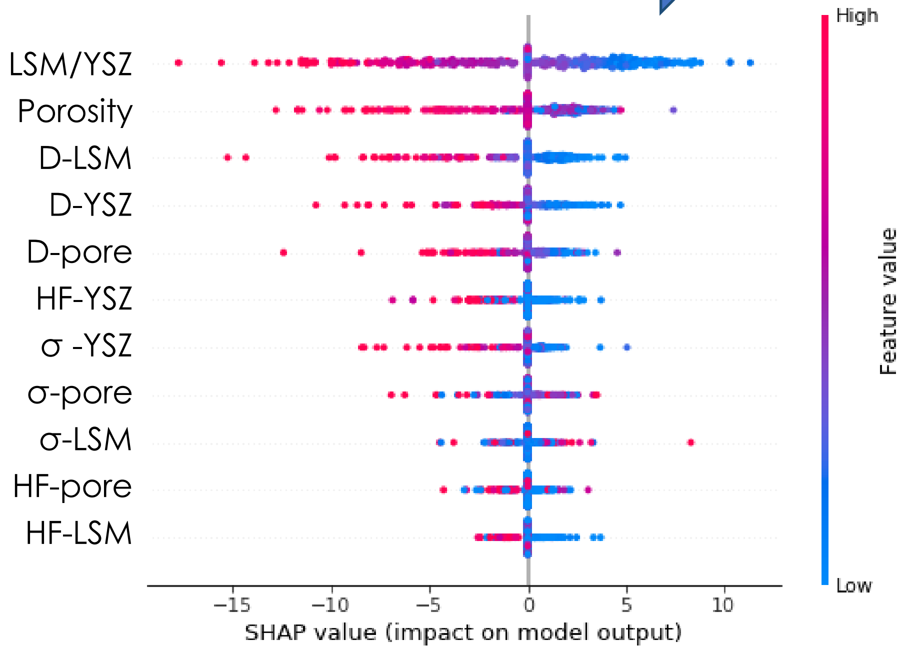
Impact on voltage decay [%/khr]

Lower is better



Impact on lifetime energy [Wh/cm^2]

Higher is better



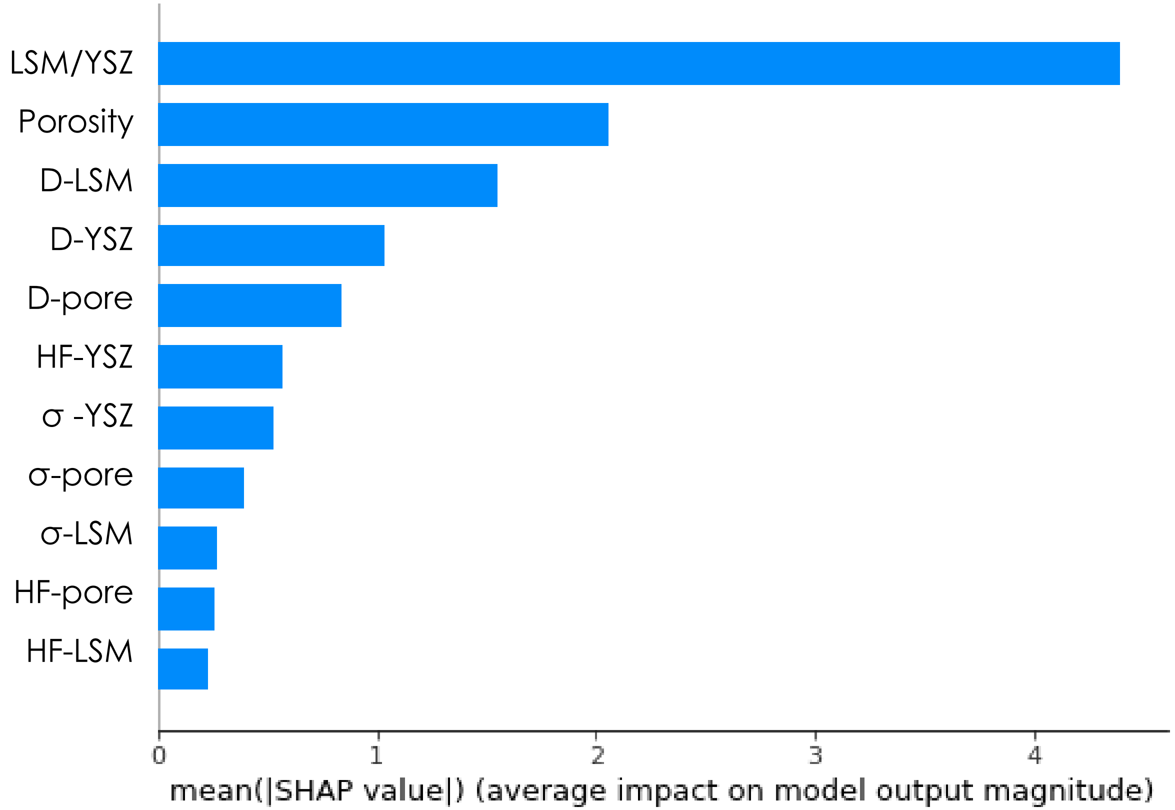
Small LSM particle sizes are bad for voltage decay, but net good for lifetime performance

Lower LSM/YSZ ratio is good for both metrics

Machine Learning Results of Analysis

Cathode (Air Electrode) Feature Importance Ranking

Each cathode feature's impact on lifetime energy produced at 400 mA/cm^2

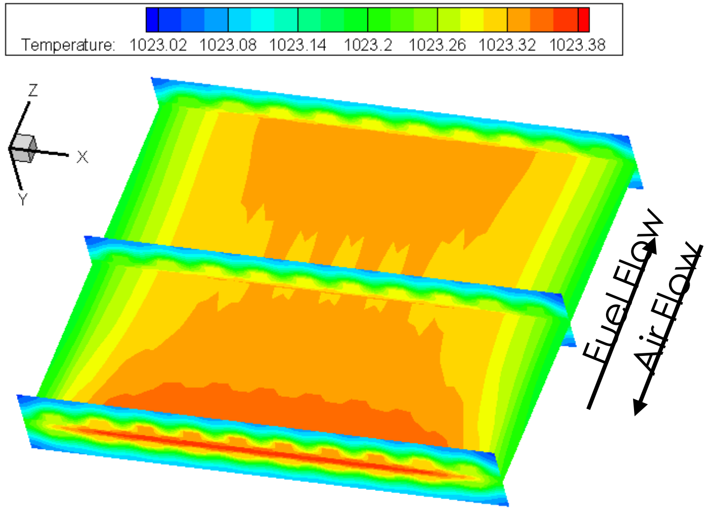


Low LSM/YSZ ratio, low porosity, and small solid particles are beneficial

Additional Progress

Too Much Progress is a Good Problem to Have…

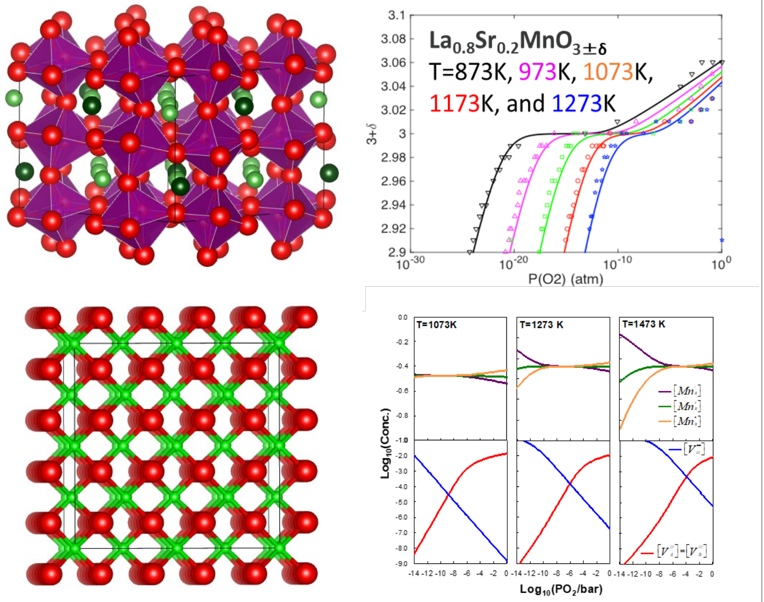
Large Cell Simulations



- DREAM SOFC Full 3D Planar
- Hydrogen/Hydrocarbon Fuels
- Contaminant Poisoning
- Impedance Analysis
- Electrolysis/r-SOC Operation

Sezer, et al., ***ECS Transactions*** 103(1):751 2021.
Sezer, et al., ***ECS Transactions*** 103(1):959 2021.

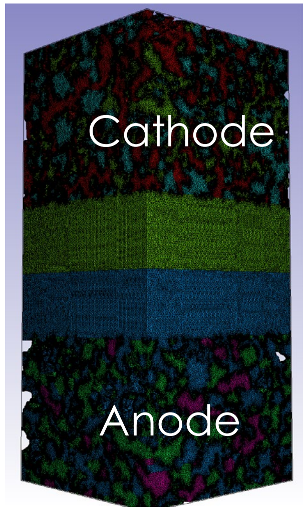
Defect Chemistry

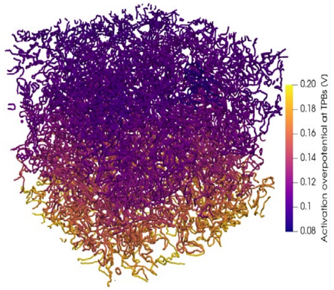


- Provides electronic and energetic insights
- Parameters integrated with phase field/reaction models

Lee, et al., ***Phys. Rev. Applied*** 8(4):044001 2017.
Lee, et al., ***Phys. Rev. Research*** 3:013121 2021.

EC Reaction Analysis





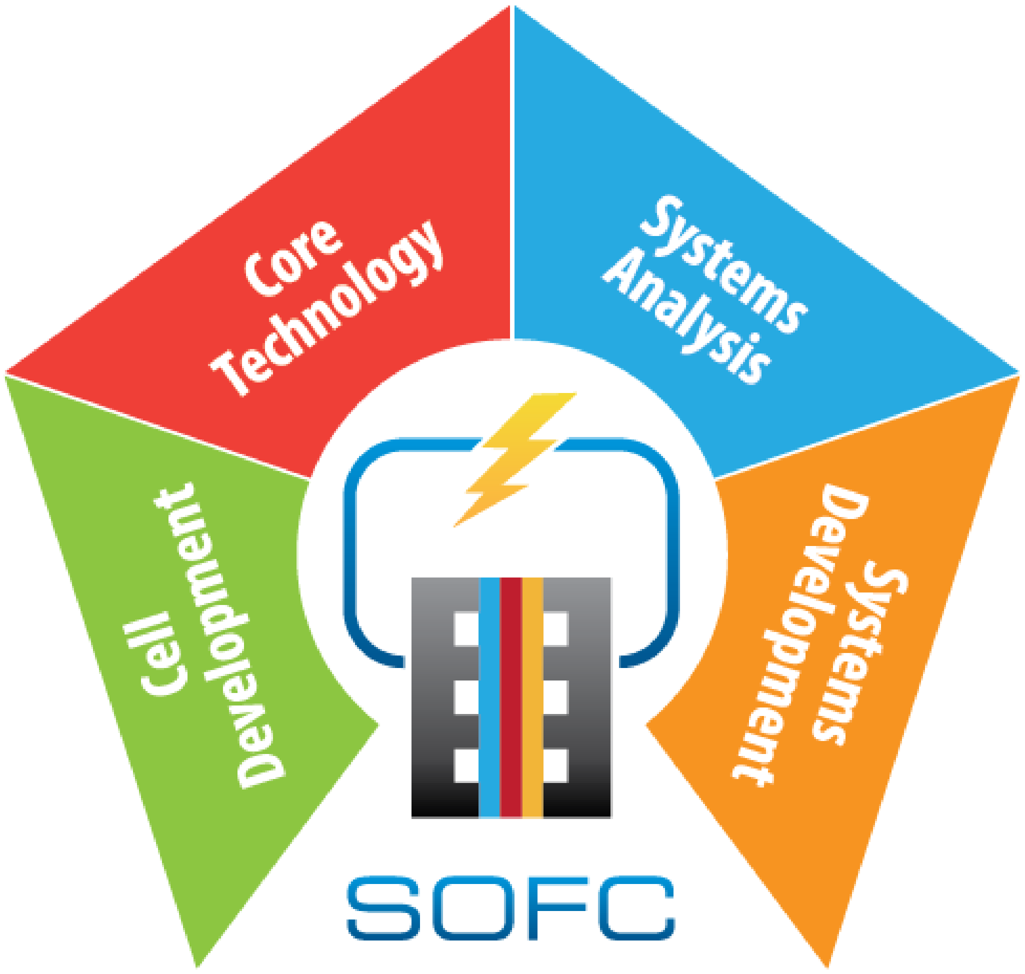
TPB Boundary Activity Map

- Developed ERMINE module in MOOSE
- Direct simulation of SOC physics in 3D microstructures
- Deeper look at heterogeneity, reaction distribution

Hsu, et al., ***MethodsX***, 7:100822 2020.
Hsu, et al., ***Electrochim. Acta*** 345:136191 2020.

Performance Enhancement & Degradation Mitigation

SOC Electrode Design and Engineering



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SOC Electrode Design and Engineering

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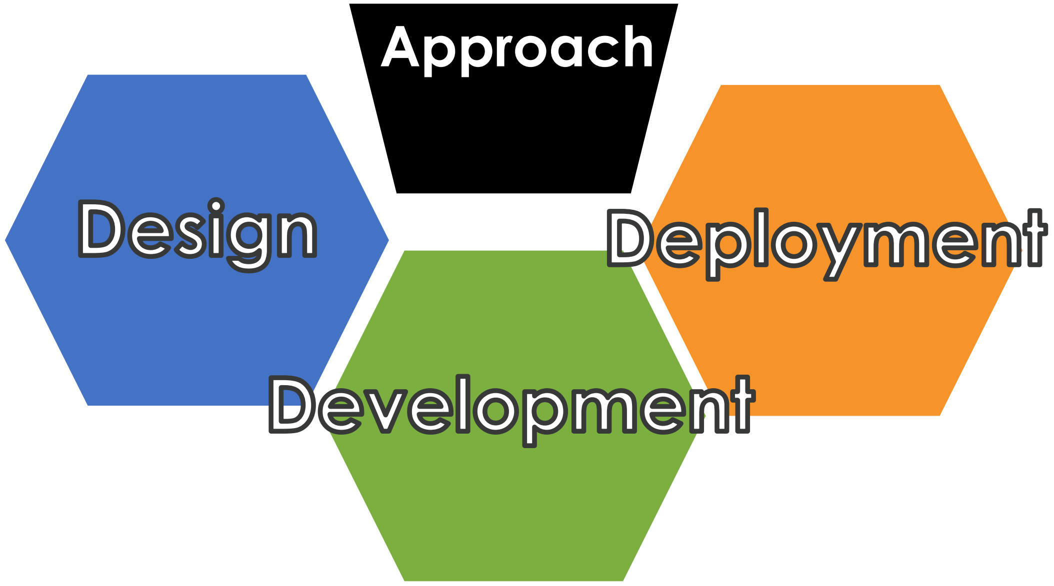
Designing, Developing, and Deploying Advanced Electrode Eng. Techniques

Objectives

- Enhancement of performance and longevity
- Materials engineering
- Microstructure engineering



Benefits

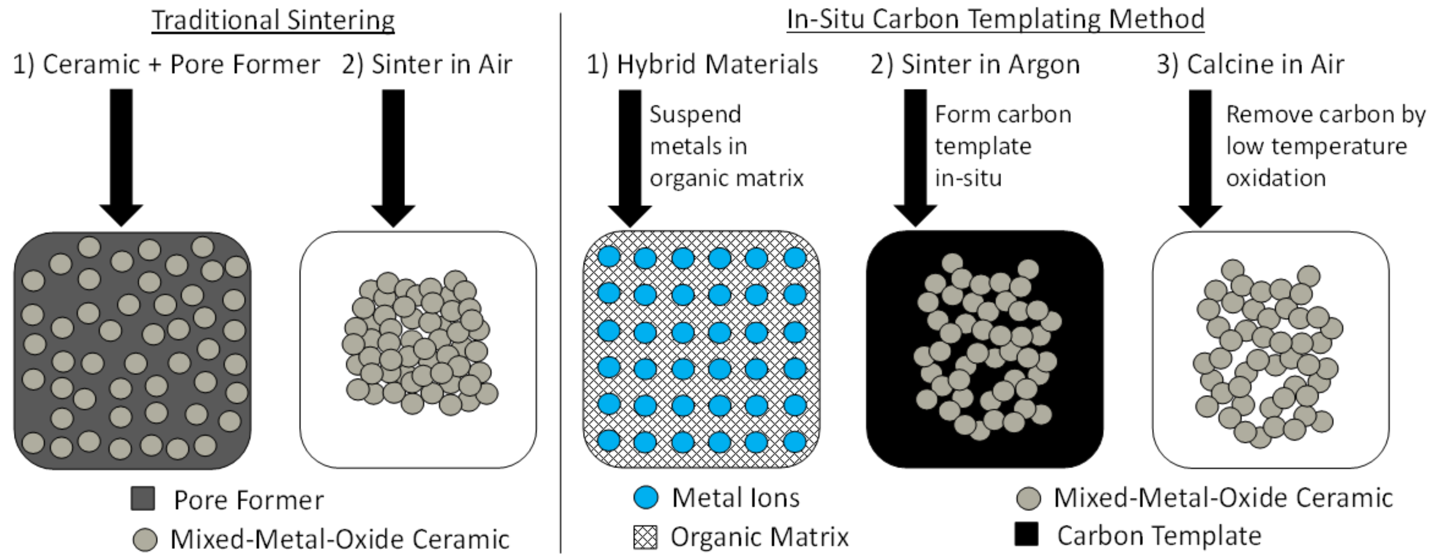
- Cell/stack cost reduction
- Cell overpotential reduction
- Thermo-chemical / thermo-mechanical stability increase
- Reduced cost-of-electricity and/or cost of hydrogen produced

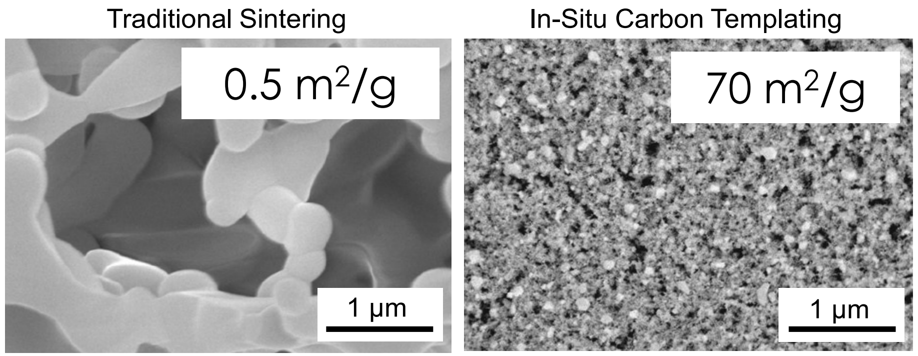
DESIGN of materials and nanostructures

DEVELOPMENT through tailored electrode construction

DEPLOYMENT in commercial SOC systems

Hybrid Materials-Assisted Templating



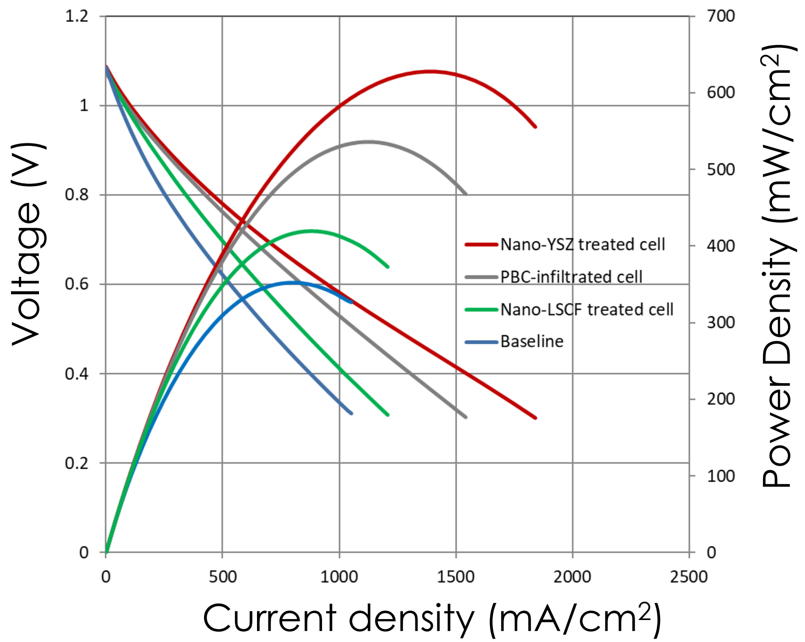


Traditional sintering | **In-situ carbon templating**

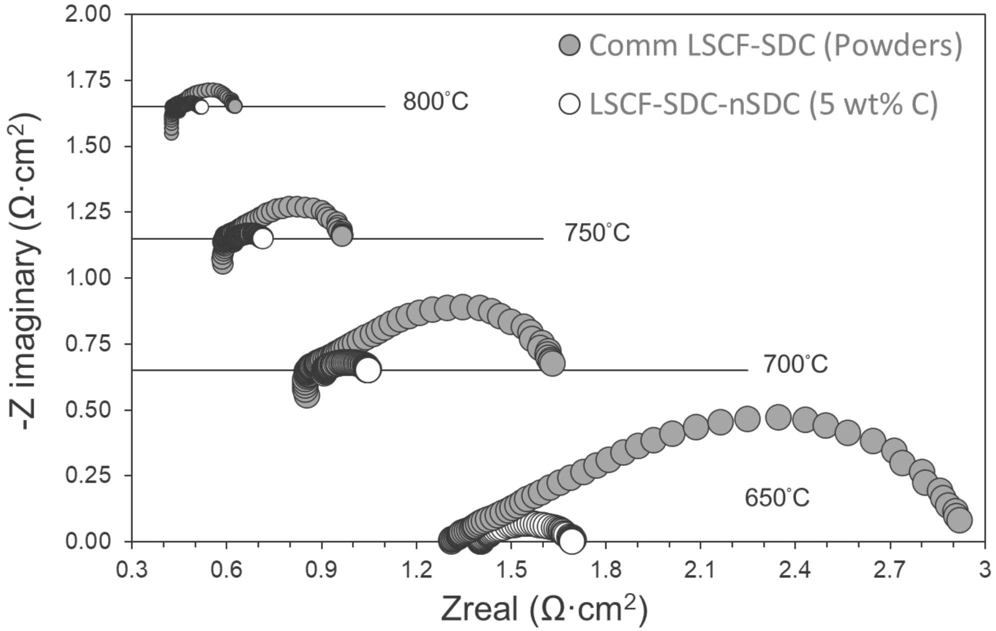
- **Hybrid Materials**: Metal and organic components mixed at atomic level
- **Sintering in inert atmosphere**: carbon template forms *in-situ* and remains during sintering; carbon is subsequently burned out at 700°C.

Infiltration of Nano-Structured Catalysts

- *In-situ* carbon templating method expanded to larger set of SOC materials
  - Reductions in $\mathbf{R_P}$ and $\mathbf{R_\Omega}$ possible by adding nano-size ionic conductors to backbone.
  - Protonic conducting oxide ($BaCe_{0.2}Zr_{0.7}Y_{0.1}O_{3-\delta}$) also formulated for IT-SOC applications



Previous results: Power curves of infiltrated **LSM/YSZ** baseline cells

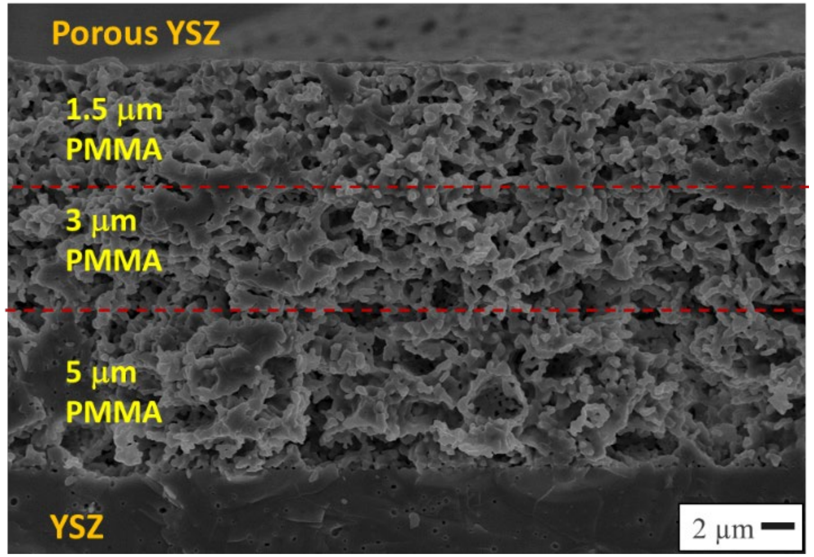


New Results: Decrease in polarization resistance of **LSCF/SDC** baseline cells when infiltrated with nano-SDC (nSDC)

Additive Manufacturing of SOC

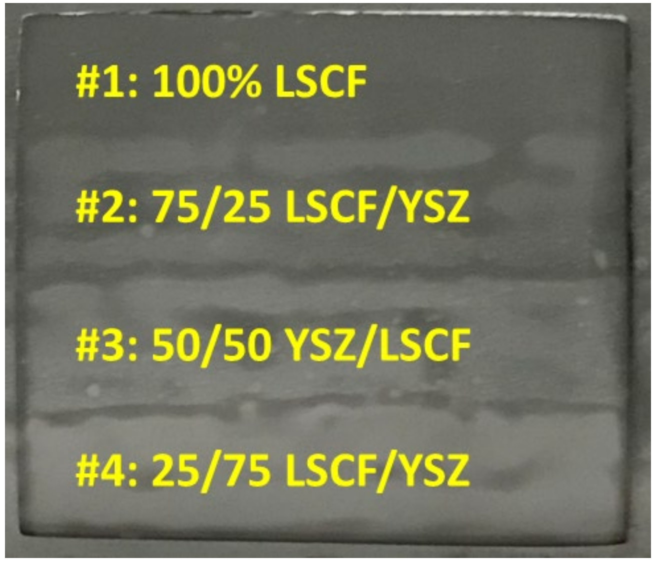
Functionally Graded Electrodes to Mitigate Degradation, Boost Performance

- Built automated layer-by-layer dip-coating and aerosol spray deposition systems to create 3D functionally graded electrode structures
  - Can vary **composition**, **particle size**, and **porosity** of composite electrode components
- Aerosol system has six inlet tubes (2 cleaning solutions, 4 electrode compositions)
  - Can change nozzle to change the width of deposited stripe
- Systems will be used to create optimized electrodes designed through simulations



YSZ backbone porosity varied in z-direction on YSZ substrate

Electrode composition varied from inlet to outlet on 5×5 cm^2 substrate (YSZ used for cost considerations during system development phase)



Atom Probe Studies of Degradation

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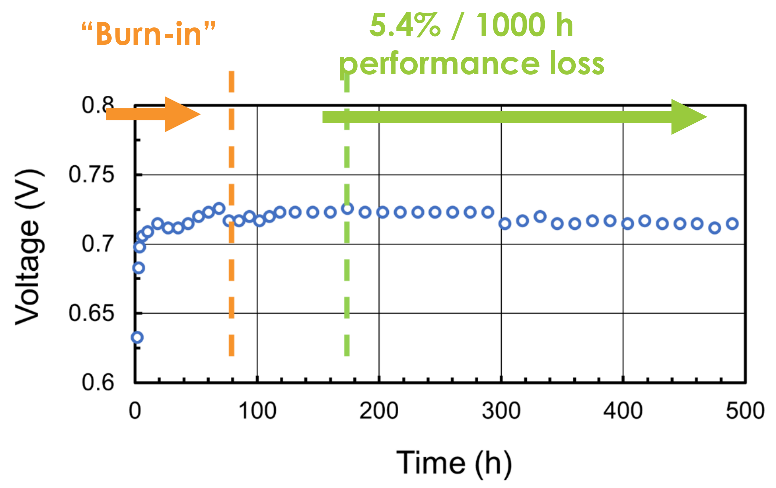
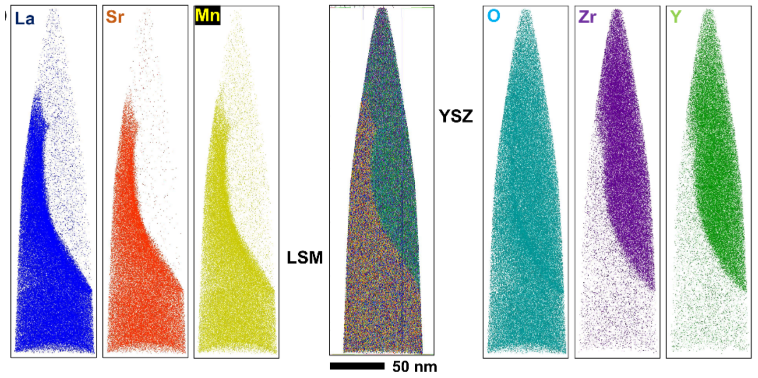
Advanced Characterization of Cation Interdiffusion across Interfaces

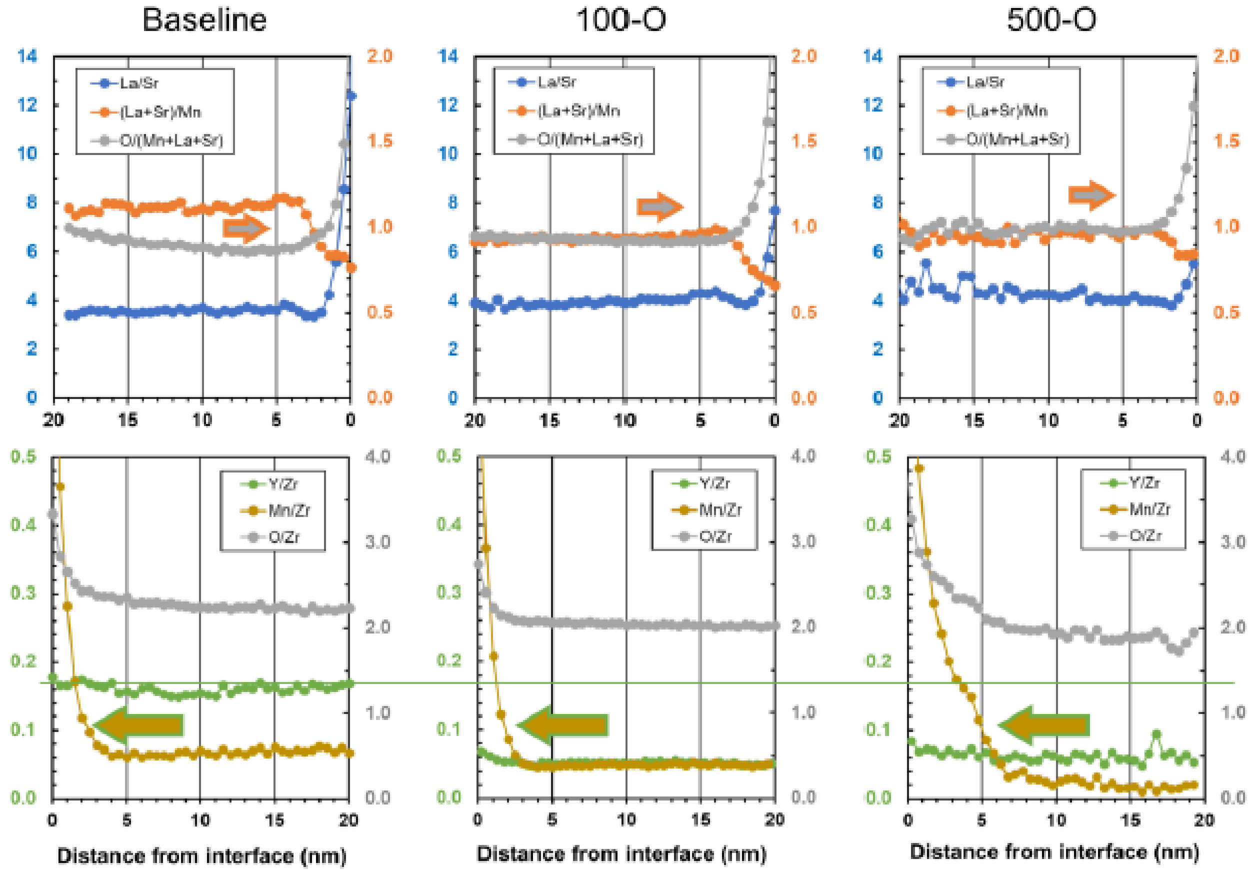
500-hour SOFC operation test: 0.75 A/cm², 800°C



Atom Probe Tomography (Cameca LEAP 4000X HR)



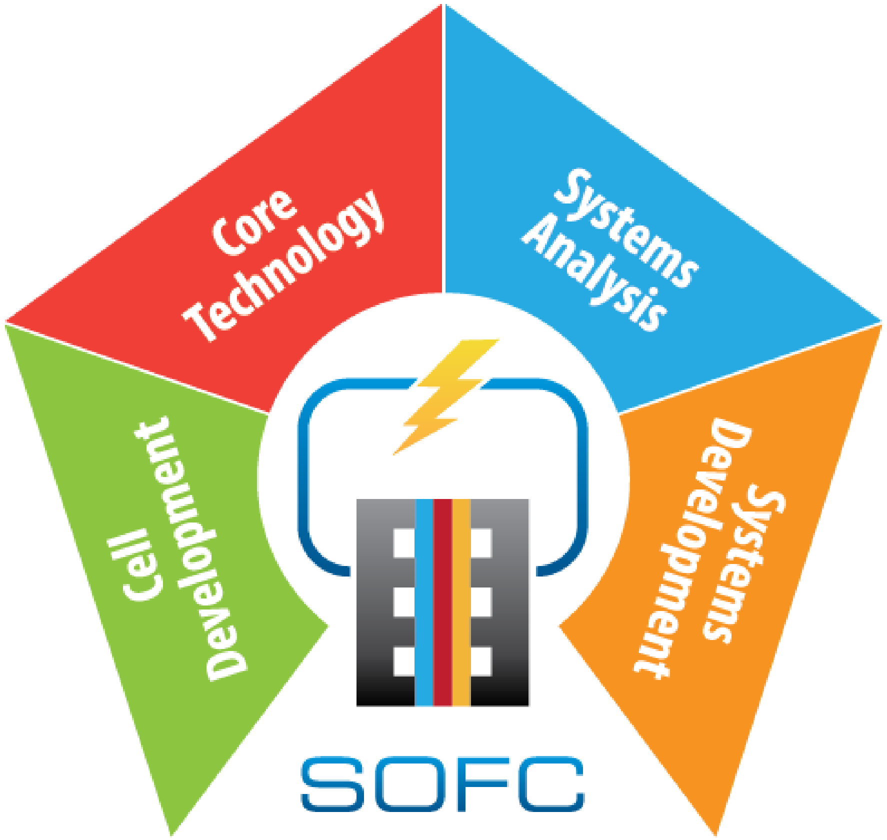
Change in cation ratios during LSM burn-in period different from longer term operation, showing impact of different driving forces



APT studies done in collaboration with J. D. Poplawsky at ORNL

Strategic Systems Analysis and Engineering

Pulling It All Together



Systems Analysis Recent Progress

Solid Oxide Cell and Stack Cost Production Study Expansion

Rationale

- A robust cell and stack production cost tool was developed previously
- In response to the SOFC Program's investment in SOEC technology, this tool will be expanded to include SOEC production and additional cell geometries

Approach

- Cell and stack cost production spreadsheet tool will include all necessary cost inputs
  - Raw materials, equipment, energy, etc.
- Tool will allow sensitivity studies to be conducted on SOFC and SOEC
  - Total production, materials costs, etc.
- Detailed guidance document/instructions being prepared to accompany tool

Outcome

- Spreadsheet tool and guidance document in preparation
- Scheduled completion March 2022, likely December 2021

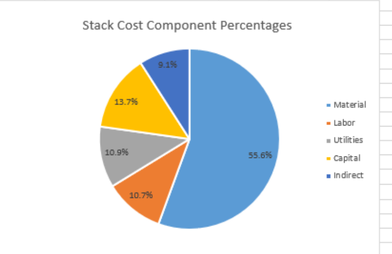
System Overview

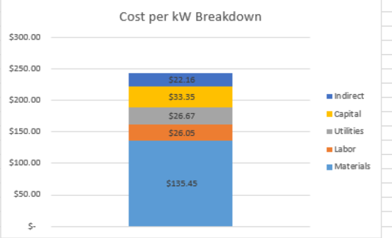
Stacks per year	20000	
Capacity per year	107.95	MW/year
Power Density	0.34	W/cm2
Stack Power	5.40	kW

Cost Basis
2019

Cost Summary

Group	Description	Annual Cost ($)	Cost per stack ($/stack)	Cost per kW ($/kW)	Percentages of Total: Individual	Percentages of Total: Group
Material	Cell Costs	$ 4,636,220	$ 231.81	$ 42.95	17.6%	55.6%
	Interconnect Costs	$ 9,986,239	$ 499.31	$ 92.51	38.0%	
	Total	$ 14,622,459	$ 731	$ 135.45		
Labor	Direct Labor	$ 2,812,320	$ 140.62	$ 26.05	10.7%	10.7%
Utilities	Electricity	$ 2,879,014	$ 143.95	$ 26.67	10.9%	10.9%
Capital	Equipment	$ 2,000,060	$ 100.00	$ 18.53	7.6%	13.7%
	Building	$ 1,600,048	$ 80.00	$ 14.82	6.1%	
	Total	$ 3,600,108	$ 180	$ 33.35		
Indirect	Cell Fabrication Maintenance	$ 70,002	$ 3.50	$ 0.65	0.27%	9.1%
	Cell Fabrication Consumables	$ 14,000	$ 0.70	$ 0.13	0.05%	
	Cell Fabrication QA/QC	$ 2,800	$ 0.14	$ 0.03	0.01%	
	Stack Assembly Consumables	$ 14,000	$ 0.70	$ 0.13	0.05%	
	Indirect labor	$ 562,464	$ 28.12	$ 5.21	2.1%	
	Overhead	$ 1,729,393	$ 86.47	$ 16.02	6.6%	
	Total	$ 2,392,660	$ 120	$ 22.16		
Total Production Cost		$ 26,306,561	$ 1,315	$ 243.69		
		Annual Cost ($)	Cost per stack ($/stack)	Cost per kW ($/kW)		





Cell Characteristics

Cell Voltage	0.85	V
Cell Current Density	0.4	A/cm²
Power Density	0.34	W/cm²
Cell Side Length	15	cm
Total Cell Area	225	cm²
Active Area Percentage	90%	
Active Area	202.5	cm²
Power per Cell	68.85	W

Stack Characteristics

Cells per Stack	80	
Cell to Cell Resistance	1.00E-04	Ohm-cm²
Stack Voltage Loss	3.16	mV
Ratio of average cell voltage to nomical cell	98.00%	
Stack Power	5.40	kW

Stack Production

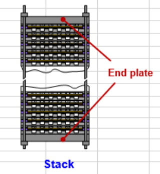
Stacks per year	20,000	
Capacity per year	107.95	MW/year

Yields

Tape Punching Yield	90%
Completed Cell Yield	97.7%

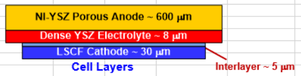
Total Stack Material Cost

$ 731.12



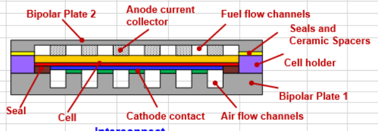
Cell Layers

Layer	Material	Thickness (u	Porosity	Density (g/cm3)	Weight per Cell (g	Weight w/ Losse	Cost per Cell	Cost per Stack
Cathode contact layer	LSCF	10	0%	6.30	1.28	1.31	$ 0.12	$ 9.50
Cathode current collector	LSCF	30	20%	6.30	3.06	3.13	$ 0.29	$ 22.81
Cathode active layer	LSM-YSZ	20	10%	6.50	2.37	2.43	$ 0.16	$ 12.98
Cathode interlayer	Gd/Sm	5	5%	7.90	0.76	0.78	$ 0.05	$ 4.00
Electrolyte	8YSZ	8	0%	6.10	0.99	1.01	$ 0.04	$ 3.46
Anode active layer	Ni-YSZ	25	10%	5.56	2.53	2.59	$ 0.10	$ 7.99
Anode support	Ni-YSZ	600	35%	5.56	48.79	55.49	$ 2.14	$ 171.06
								$ 231.81



Interconnect

Part	Material	Percent of Cell Area	Part Area + Scrap Area (cm2)	Thickness (mm)	Density (g/cm3)	Weight Required per Unit (kg)	Cost per Unit	Units per Stack	Cost per Stack
Frame	SS-441 Sheet	120%	270.00	1	6.81	0.18	$ 0.49	80	$ 39.36
Separater Plate	SS-441 Sheet	120%	270.00	1	6.81	0.18	$ 0.49	80	$ 39.36
Anode Flowfield	SS-411 Mesh	100%	225.00	0.5	1.70	0.02	$ 1.83	80	$ 146.36
Cathode Flowfield	SS-411 Mesh	100%	225.00	0.75	1.70	0.03	$ 2.74	80	$ 219.53
Spacers	Borosilicate glass	20%	45.00	1	2.23	0.01	$ 0.02	160	$ 3.44
End Plates	SS-441 Sheet	125%	281.25	50	6.81	9.58	$ 25.63	2	$ 51.26



Systems Analysis Recent Progress

Solid Oxide Cell Configuration Techno-Economic Analysis

Rationale

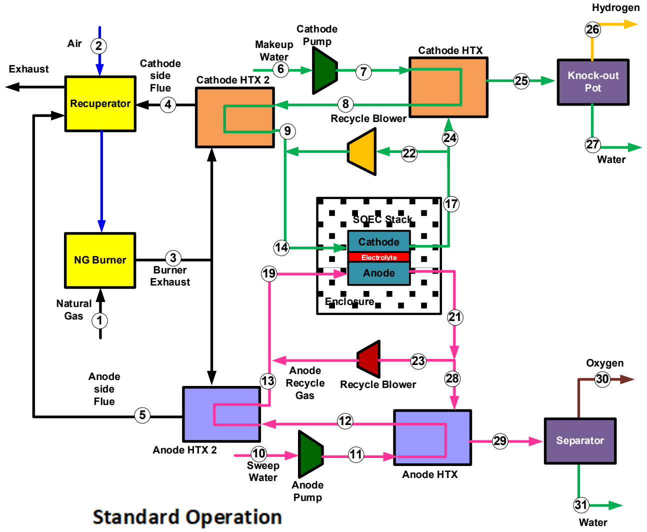
- In response to DOE interest, the SOFC Program has expanded its portfolio to include high-temperature solid-state electrolysis technology
- A detailed understanding of the merits/demerits of coupling SOFC/SOEC technology versus a single reversible SOC unit is needed as a basis for future analysis

Approach

- The analysis will consider the incorporation of reversible SOC and SOFC/SOEC paired equipment and details on the effects of integrated equipment in a hybridized energy system
  - E.g. capital cost of reversible SOC vs stability of separate SOFC/SOEC units will be a critical consideration

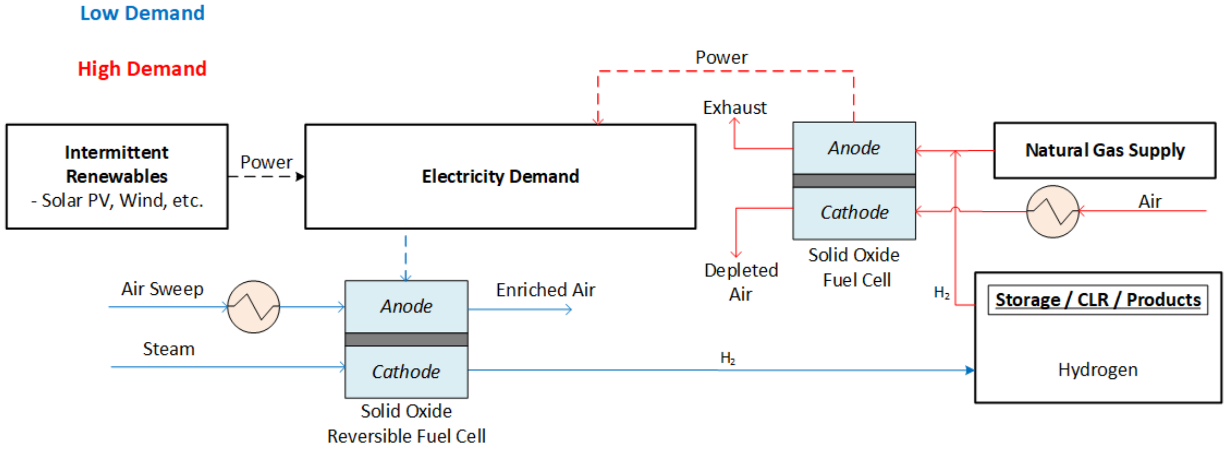
Outcome

- The analysis will provide critical information to serve as a foundation to inform the SOFC Program on targeted R&D needed for integrated energy systems with SOC technology(ies)
- Targeted guidance for future analysis scope
- Scheduled completion March 2022

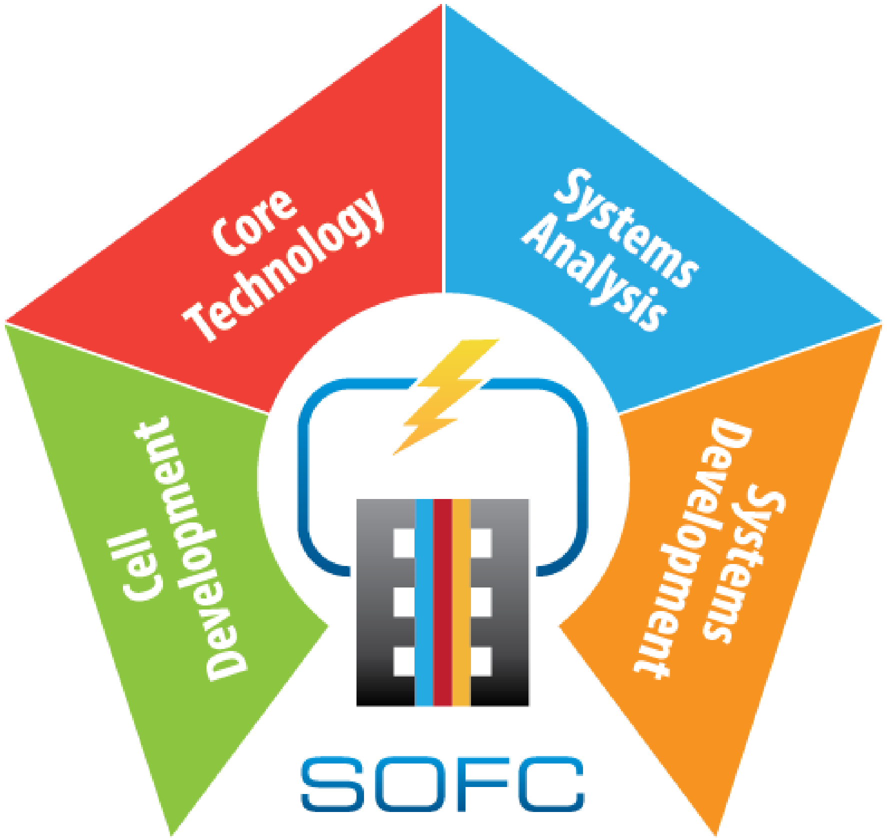


APPENDIX E – AREA OF INTEREST 5 : SOLID OXIDE ELECTROLYSIS CELL (SOEC) TECHNOLOGY DEVELOPMENT FOR HYDROGEN PRODUCTION

AOI Issue Date 01/15/2021
Submission Deadline for Full Applications 03/01/2021
DOE Share ($K) – 80% 1,000
Cost Share ($k) – 20% 250
Anticipated No. of Awards 8
Maximum Period of Performance 24 months (Single Phase/Single Budget Period)



Wrap-Up


Core Technology
Systems Analysis
Cell Development
Systems Development
SOFC

NETL Capability Overview

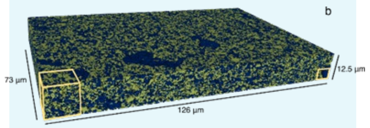
High Temperature Electrochemical Systems (SOFC / r-SOC / SOEC)

FECM-SOFC Program Goals and Objectives

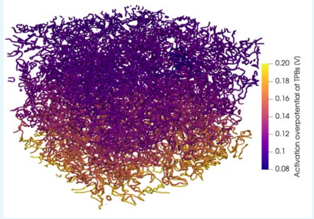
- Techno-Economic / Market Analysis
- Degradation Modeling
- Electrode Engineering

NETL Unique Capability and Achievements

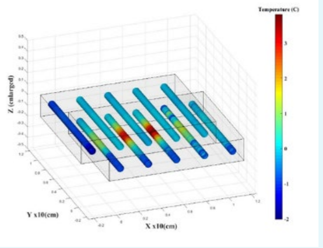
- Only team capable of modeling from atoms-to-COE
- Published high-resolution cell reconstruction datasets
- World leader in characterizing and simulating heterogeneity
- Advanced interface characterization - Atom Probe Tomography
- First using machine learning to create 40,000+ synthetic microstructures
- Able to provide targeted cell development feedback to industry
- In-situ high temp optical fiber sensor development (temp / gas comp)
- Experimental testing/electrode engineering/infiltration successes
- Extensive capability in strategic systems analysis and engineering



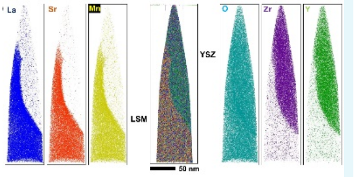
p-FIB Microstructure Reconstruction



TPB Boundary Activity Map

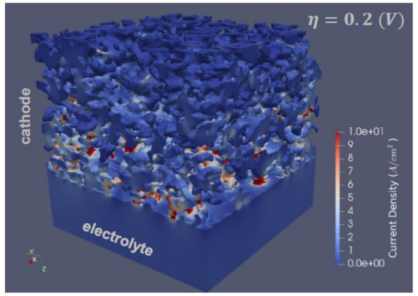


In-situ Sensor Temp Map

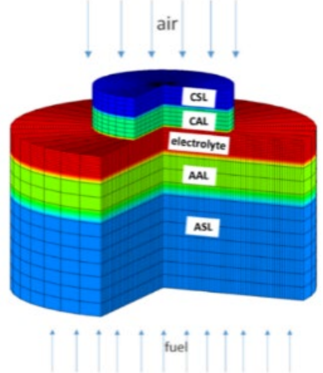


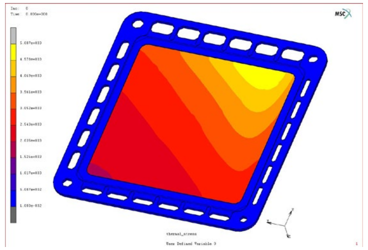
APT Composition Map

Modeling from the Atomistic Scale to the System Scale (w/ PNNL)

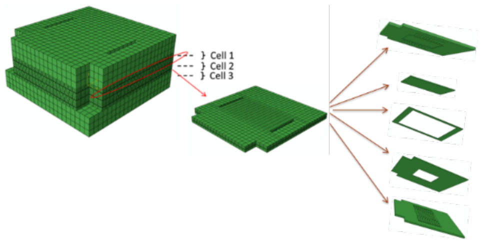


Electrode Sub-volumes



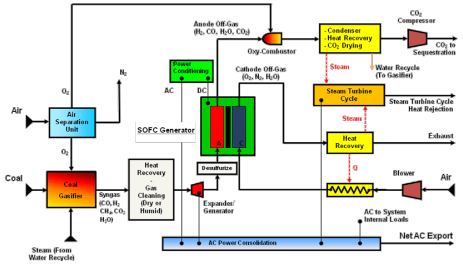


Single Cell



Multi-Cell Stack

PNNL SOFC-MP



SOC System

NETL — PNNL — NETL

Additional Efforts

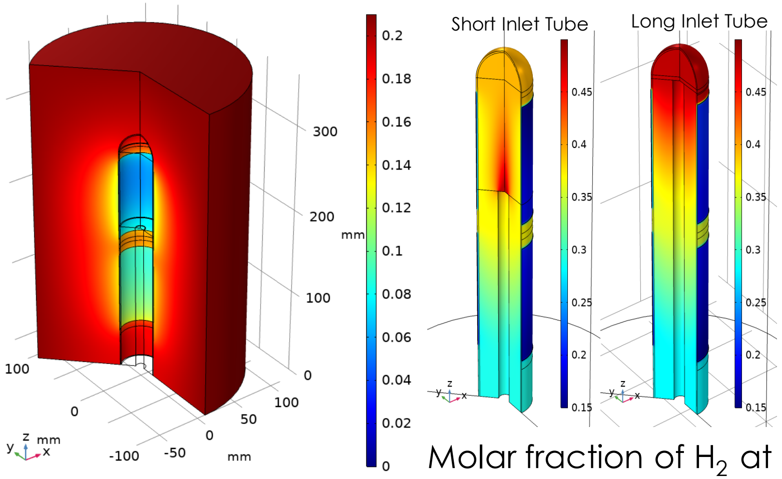
NATIONAL ENERGY TECHNOLOGY LABORATORY

Support of Other DOE/FECM/SOFC Program/HFTO Projects

Aris Energy Solutions, LLC

- System operational and producing power for the NETL site very soon!
- Please see presentation later today!
- Project: DE-FE31978

UNDEERC



Molar fraction of H_2 at 21% O_2 50% H_2 0.5 V

- Applying NETL capability to syngas fueled, tubular SOC
- Please see presentation from November 16
- Project: DE-FE31977

H_2NEW Laboratory Consortium (EERE/HFTO)

H2NEW

U.S. DEPARTMENT OF ENERGY

- Contributing expert guidance on modeling and characterizing SOC performance for new HFTO program

Final Announcement

- This will be Greg's final presentation as NETL Team Lead for SSEC R&D at these meetings
- NETL is in the process of transitioning the Team Lead role to Dr. Harry Abernathy
- Greg will continue to be involved in NETL Systems Analysis efforts and will continue to participate in these meetings in that role

Thank You!

VISIT US AT: **www.NETL.DOE.gov**

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