22nd Annual Project Review Meeting

DE-FE0031972

Reversible SOFC-SOEC Stacks Based on Stable Rare-Earth Nickelate Oxygen Electrodes

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Dr. Wenyuan Li[4], Dr. Whitney Colella[5]

1 Saint-Gobain
2 Boston University
3 Worcester Polytechnic University
4 West Virginia University
5 Gaia Energy Research Institute

MAKING THE WORLD A BETTER HOME

SAINT-GOBAIN

DE-FE0031972: TECHNICAL STRENGTHS AND BACKGROUND

SAINT-GOBAIN & SOFC PROJECT SUMMARY

Worldwide Footprint

- 2020 Turnover **38 €bn**
- Operations in **67 COUNTRIES**
- Over **170,000 EMPLOYEES**

Innovative & Reliable Stack Technology

- All-ceramic stack **10+ year lifetime**
- Operational simplicity **Modular design**
- Recognized Supplier **Industrialization**

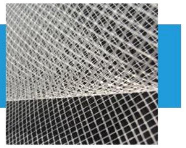
HIGH PERFORMANCE SOLUTIONS

ABRASIVES & COMPOSITE SYSTEMS

CERAMICS

LIFE SCIENCES

MOBILITY

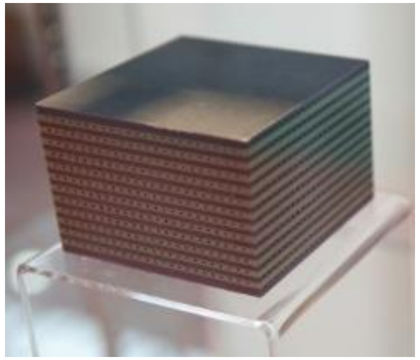


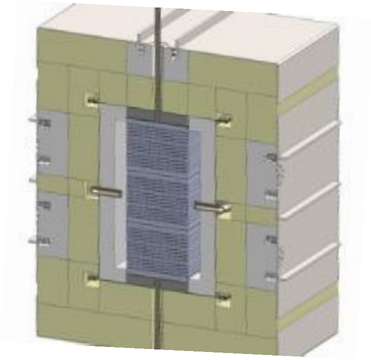
CONSTRUCTION INDUSTRY

REGIONAL BUSINESS

CERTAINTEED BUILDING MATERIALS

SAGE ELECTROCHROMIC GLASS





Culture of Innovation: 350 Years of Growth

One of the world's 100 most innovative **companies***

*Source: Thomson Reuters

History of Collaboration

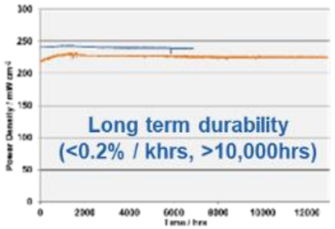
SOEC BACKGROUND: SUCCESSFUL EERE FUNDED SEEDLING PROJECT

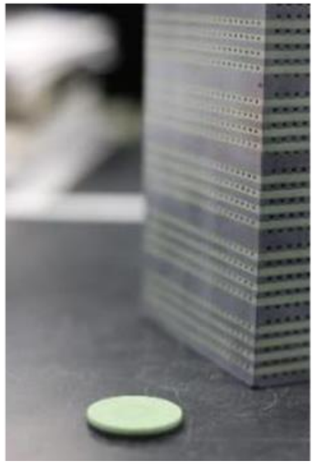
DE-EE0008377: DEVELOPMENT OF DURABLE MATERIALS FOR COST EFFECTIVE ADVANCED WATER SPLITTING

Leverage Strengths

Core Competencies

Businesses built around tailoring powder properties and scaling to production at industrial quantities

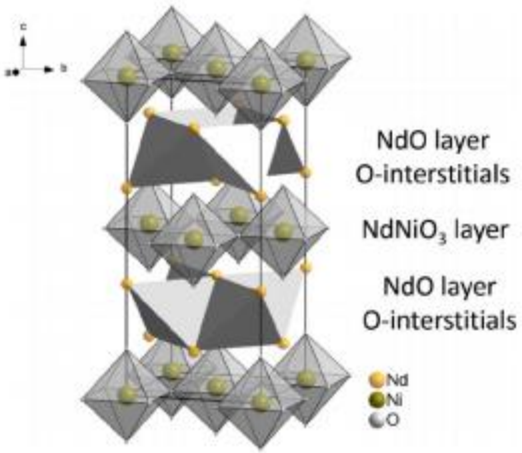




High Potential Material Set

Performance Potential of Nickelates (Ln_2NiO_4)

- Open alternating crystal structure provides a large number of oxygen interstitial sites
- Oxygen exchange and transport is greater than state-of-the-art perovskite oxides
- Potential to avoid degradation due to voids and cracks which typically form during operation



V.V. Kharton, et. al, J.Solid.State.Chem., 181, 1425-1433 (2008)

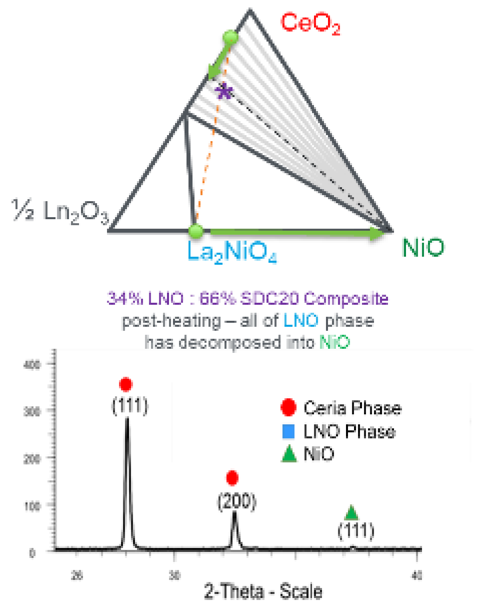
Issue To Be Solved

Material Decomposition

- Decomposition of nickelate phase when in contact with Ceria

$La_2NiO4 \rightarrow x\, LaO_{1.5} + 0.5x\, NiO$

Resulting Ceria Phase: $La_xSm_{0.2}Ce_{0.8-x}O_{2-\frac{0.2+x}{2}}$



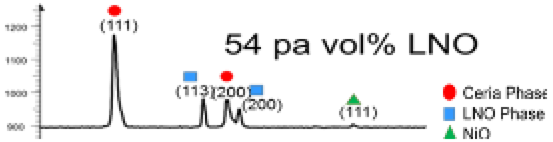
SAINT-GOBAIN

SOEC SEEDLING PROJECT MID-TERM RESULTS

IMPROVED PERFORMANCE AND STABILITY WHILE ENABLING LOW-COST BALANCE OF PLANT

Stabilization Achieved

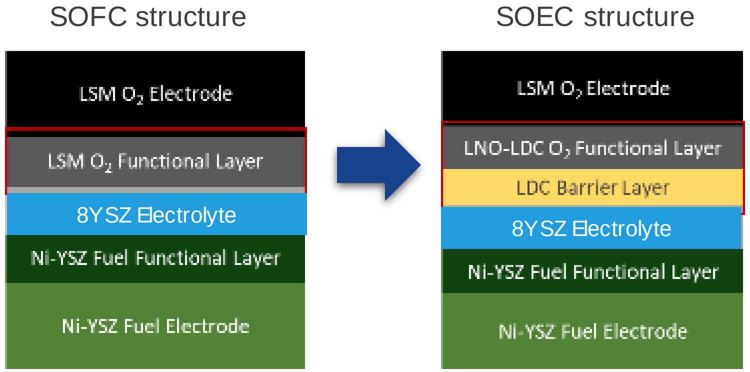
Stabilized LNO in presence of Ceria



La_2NiO_4 retention

Co-Sintering Developed

Incorporated nickleate within co-sintered cells

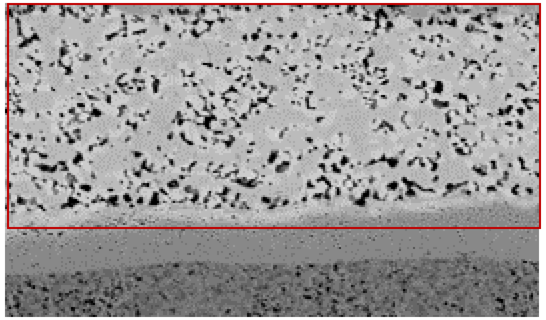


Microstructure achieved

Functional Layer

Barrier Layer

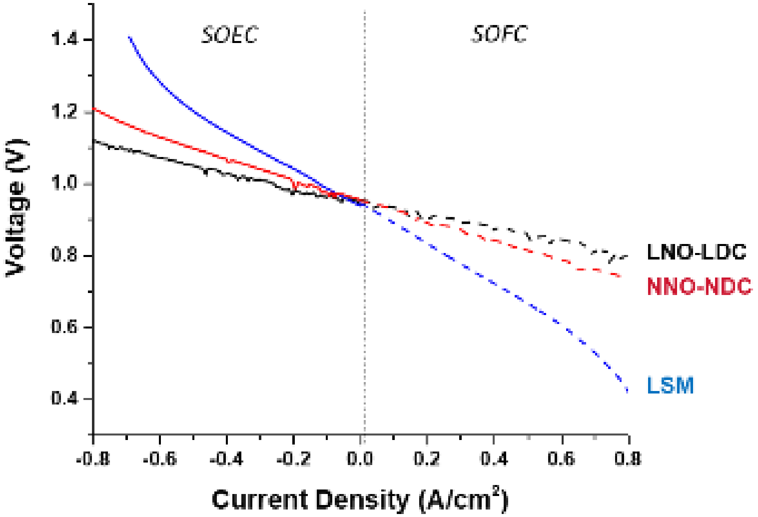
Electrolyte



SOEC Performance Enhancement

Performance Improvement

- LNO outperforms LSM electrode
- LNO Cell successfully co-sintered
- Independent of cell design (anode supported and co-sintered cells)



THIS PROJECT: INVESTIGATE OPERATIONAL & STACK DESIGN CONCERNS

DE-FE0031972: MOVE FROM BUTTON CELL TO STACK DESIGNS IN BOTH OPERATIONAL MODES

Stack designs can be grouped by the thickest layer of an individual cell and how they are connected into a stack

Stack Supported
- Air Electrode
- Electrolyte
- Fuel Electrode

Anode Supported
- Air Electrode
- Electrolyte
- Fuel Electrode

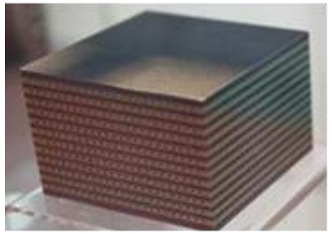
Electrolyte Supported
- Air Electrode
- Electrolyte
- Fuel Electrode

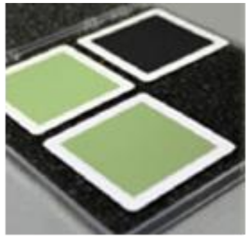
Metal Supported
- Air Electrode
- Electrolyte
- Fuel Electrode
- Metal

Ceramic Interconnect (Stack Supported)

Metal Interconnect (Anode Supported, Electrolyte Supported)

Integrated Interconnect (Metal Supported)





Commonalities to be studied

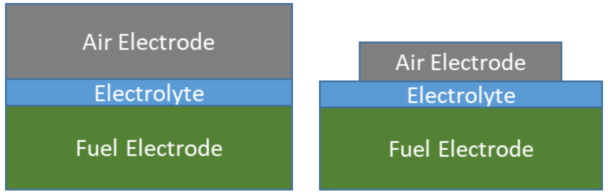
- Utilize the novel air electrode
- High humidity @ fuel electrode
- Interconnect Metal or Ceramic

CELL LEVEL DEVELOPMENTAL WORK

STACK AGNOSTIC SOLUTIONS FOR MODE SWITCHING ON THE AIR ELECTRODE

Cell Level

Oxygen Electrode Investigations (Nickelates)



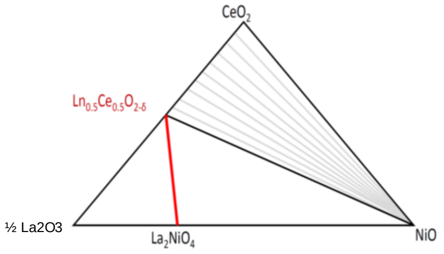
Stack Supported

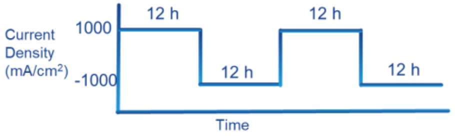
Anode Supported

Fuel Electrode Investigations (Nickel migration)

Investigate Composition-Performance-Stability relationship

- Operational mode switching between SOFC/SOEC
- Dopant type/concentration in barrier layer and active layers
- Microstructural/compositional changes due to chemical and electrochemical driven processes





Baseline
- Barrier SDC20
- Air electrode NNO/NDC50
- Directly out of Seedling

Quantify Electrode Performance

Stoichiometry Substitutions
- A-site
- B-site

S Gopalan

Calculated: Calphad (WPI)
- Stability calculations
- Conductivity (defect chemistry + mobility)
- TGA/conductivity

Y Zhong

Measured: Powder, Bars, Symmetric cells
- XRD
- DRT, IMP
- Microstructure
- Ionic conductivity bars
- EC Relaxation

S Gopalan

Effect of Impurities
- Experimental at WVU

Switch to better performing barrier layer from Seedling

Quantify Cell Performance

Button cells
- Barrier SDC20
- Paired down air electrodes

J Pietras

Microstructural
- Physical: porosity, etc
- Compositional: EDS, TEM, XRD

S Gopalan

Performance:
- DRT, IMP
- IV curves
- Operational conditions

S Gopalan

Button cell passing targeted performance

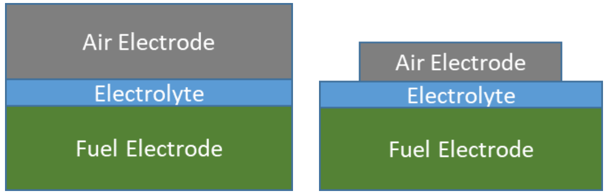
CELL LEVEL DEVELOPMENTAL WORK

NICKEL MIGRATION AS A FUNCTION OF CURRENT AND HUMIDITY

Cell Level

BOSTON UNIVERSITY · SAINT-GOBAIN · WPI

Oxygen Electrode Investigations (Nickelates)



Stack Supported

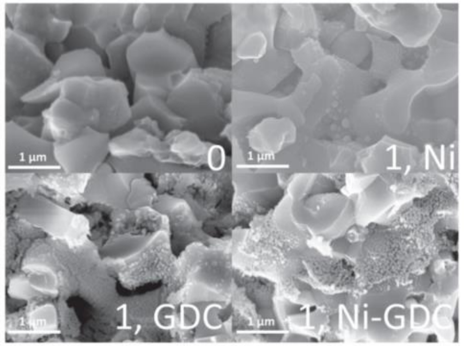
Anode Supported

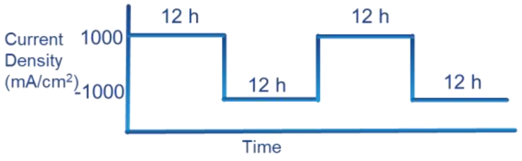
Fuel Electrode Investigations (Nickel migration)

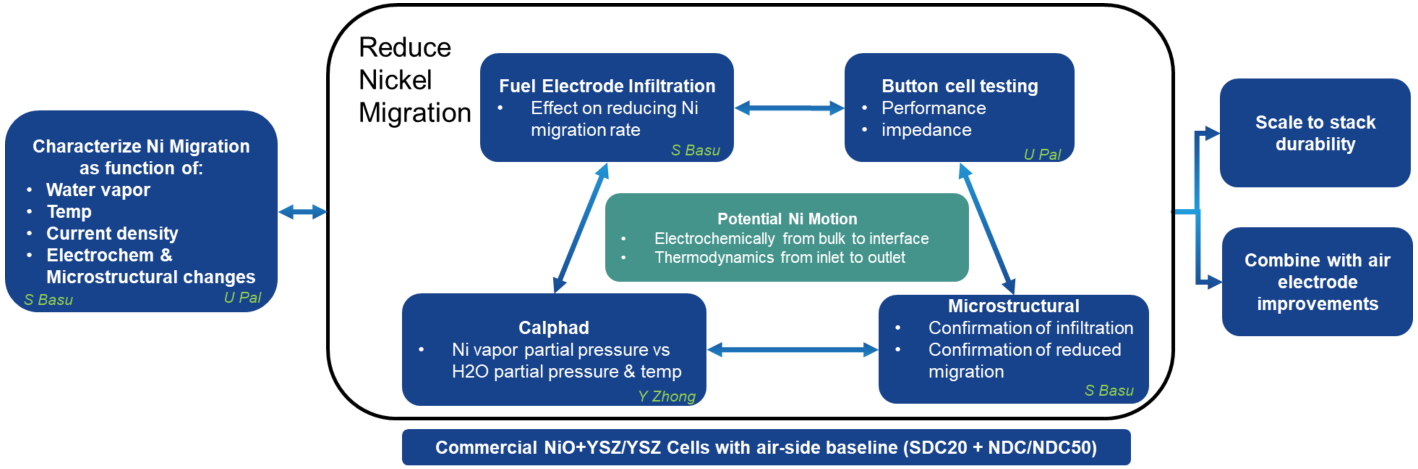
BOSTON UNIVERSITY · SAINT-GOBAIN · WPI

Mitigation of Ni migration

- Focus solutions on MIEC anode side infiltration
- Dynamic SOFC-SOEC mode switching
- A range of simulated fuel compositions & temperatures
- Microstructure and compositional evolution probed through SEM, TEM and SEM-FIB analysis
- Studies to be guided by CALPHAD







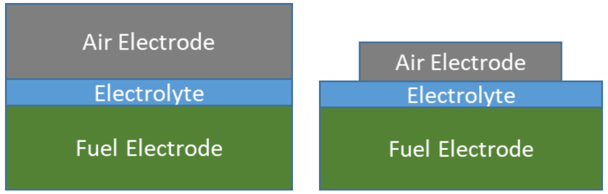
CHALLENGES OF CELL TO CELL CONNECTIONS WITHIN A STACK

INVESTIGATING EFFECT OF BOTH METALLIC AND CERAMIC BASED INTERCONNECTS

Cell Level

BOSTON UNIVERSITY · SAINT-GOBAIN · WPI

Oxygen Electrode (Nickelates)



Stack Supported

Anode Supported

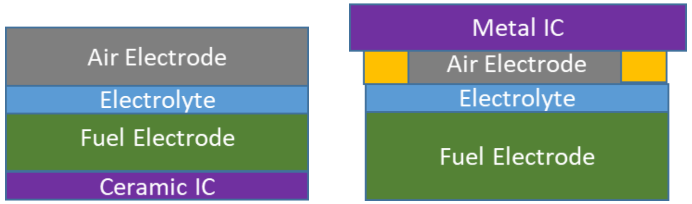
Fuel Electrode (Nickel migration)

BOSTON UNIVERSITY · SAINT-GOBAIN · WPI

Stack Level

WPI · West Virginia University

Nickelate – Cr interconnect interactions



Stack Supported

Anode Supported

Ceramic IC humidity interactions

West Virginia University · SAINT-GOBAIN

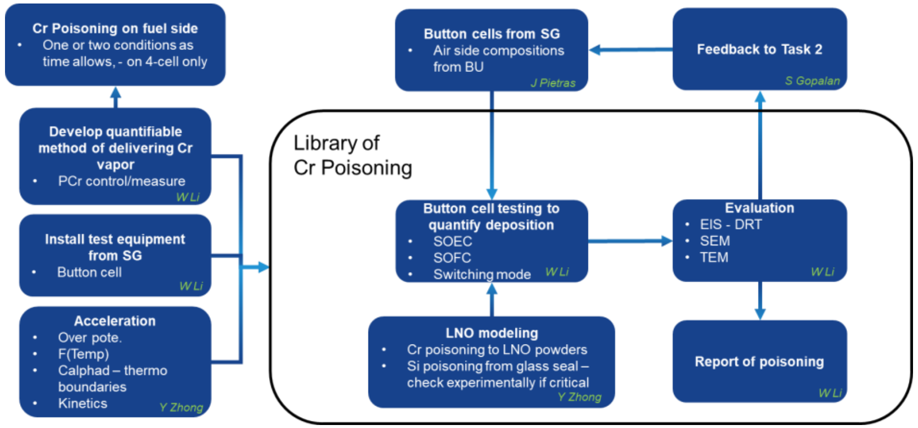
Reaction paths and kinetics of Chromium poisoning

- Electrochemical deposition identified in general but not well studied in nickelate systems

$$2CrO_3(g) + 6e^- \rightarrow Cr_2O_3(s) + 3O^{2-}$$

$$2CrO_2(OH)(g) + 6e^- \rightarrow Cr_2O_3(s) + 2H_2O + 3O^{2-}$$

- Determination of dominant reaction path as a function of operational state: SOFC, OCV, SOEC
- Utilization of EIS and microstructural observations along with Calphad simulation



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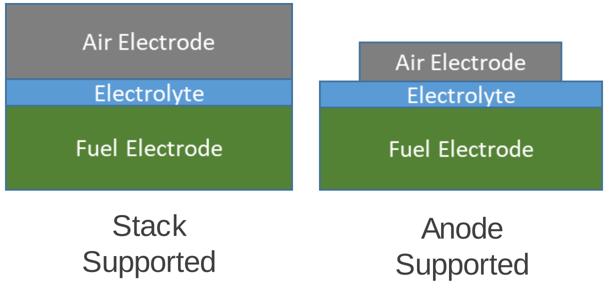
CHALLENGES OF CELL TO CELL CONNECTIONS WITHIN A STACK

INVESTIGATING EFFECT OF BOTH METALLIC AND CERAMIC BASED INTERCONNECTS

Cell Level

BOSTON UNIVERSITY   SAINT-GOBAIN   WPI

Oxygen Electrode (Nickelates)



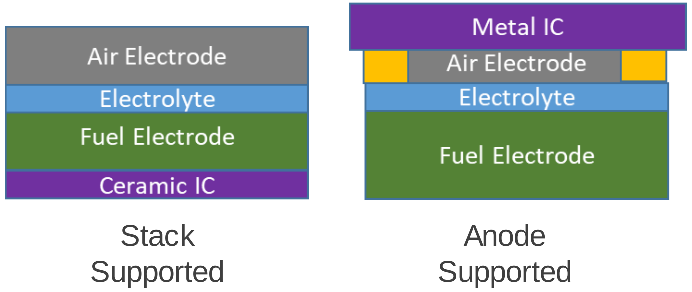
Fuel Electrode (Nickel migration)

BOSTON UNIVERSITY   SAINT-GOBAIN   WPI

Stack Level

WPI   West Virginia University

Nickelate – Cr interconnect interactions



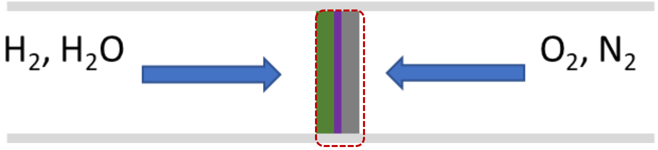
Ceramic IC humidity interactions

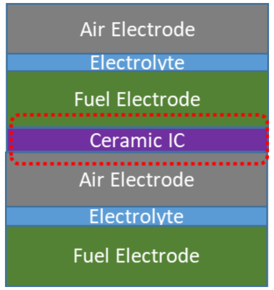
West Virginia University   SAINT-GOBAIN

Performance of Ceramic Interconnect

- Chemical stability and electrical conductivity
  - Upon change of P_{O2}, reaction with H_2 or steam
- Chemical expansion
  - Change of P_{O2}
- Cation diffusion under high current density
  - Induced cation/anion diffusion
- Mechanical stability in high steam concentration
- Conductivity experiments
- Microstructural and phase analysis

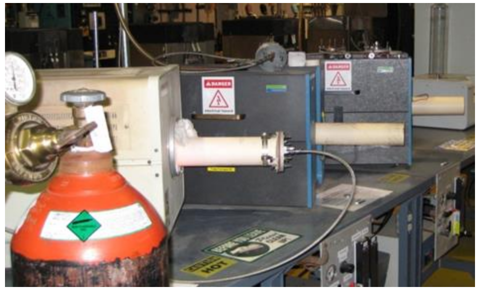
fuel electrode//interconnector//oxygen electrode





ENABLING STACK AGNOSTIC VOLUME PRODUCTION

LOW COST, HIGH VOLUME POWDER PRODUCTION CRITICAL FOR SOEC/SOFC ADOPTION



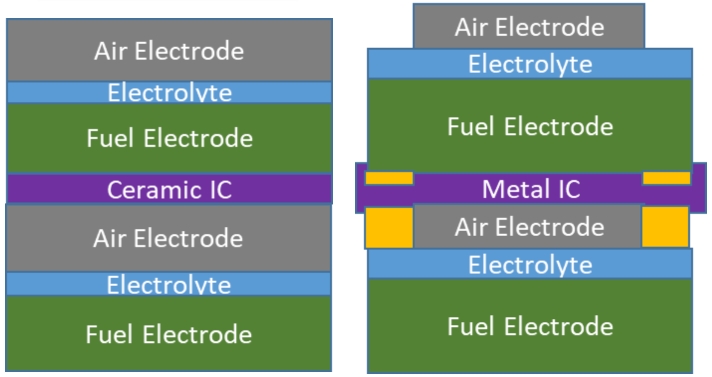
Powder Production

- Saint-Gobain Grains and Powders is a leading manufacturer of ceramic materials, ex. zirconia
  - Production plants include chemical and fusion based processes
  - Research equipment includes box, tube and rotary furnaces as well as extensive powder characterization tools

Scale Up

SAINT-GOBAIN WestVirginiaUniversity

Solution integration and stack testing



Stack Supported

Anode Supported

Techno-economic analysis

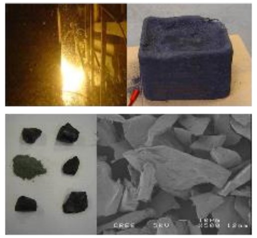
Gaia Energy Research Institute LLC (Gaia)
Energy, Environmental, and Engineering Research

WPI SAINT-GOBAIN

Cell and Stack Production at Saint-Gobain

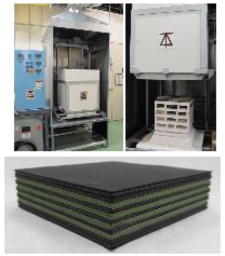
- Existing process was developed for the production of all-ceramic SOFC
- New materials will be incorporated into the existing process
- Co-sintering process to be optimized for new powders

Incoming Powder
Powders are formed processed to desired caraterisrics

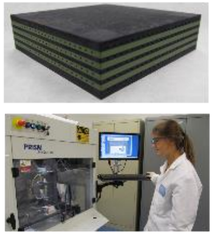


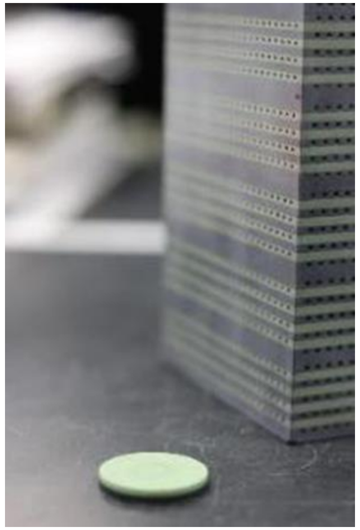
Sheet/Tape Casting
Powders are dispersed with binders and cast into sheets.

Assembly/Firing
Components are combined and sintered into cell/stacks



Finishing/Sealing
Final dimensions are achieved and glass seal is applied



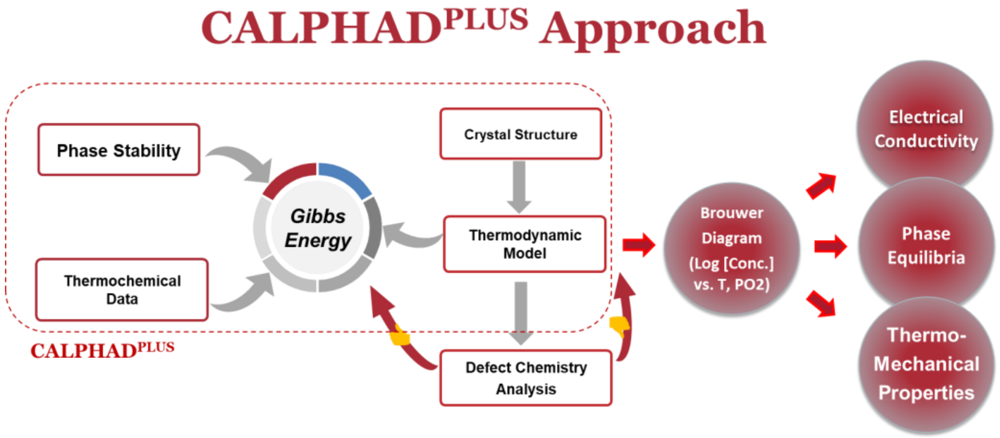


MULTI-LEVEL MODELING SUPPORTING THE PROGRAM

THERMODYNAMIC AND SYSTEM MODELING

Thermodynamic Calculations

WPI

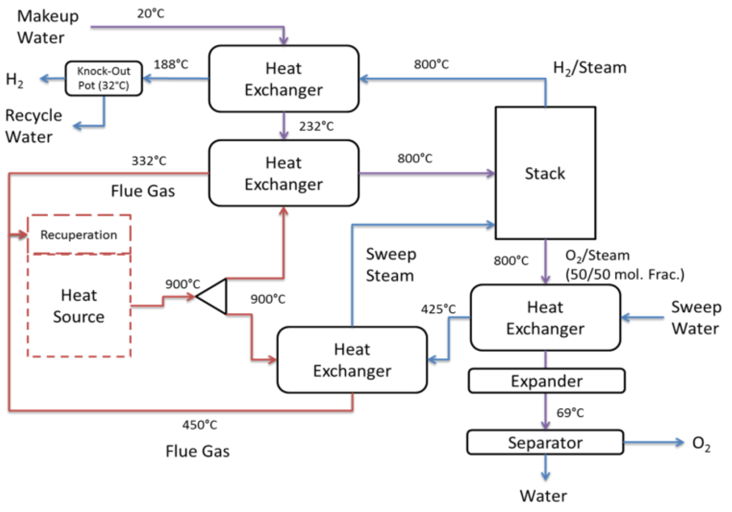


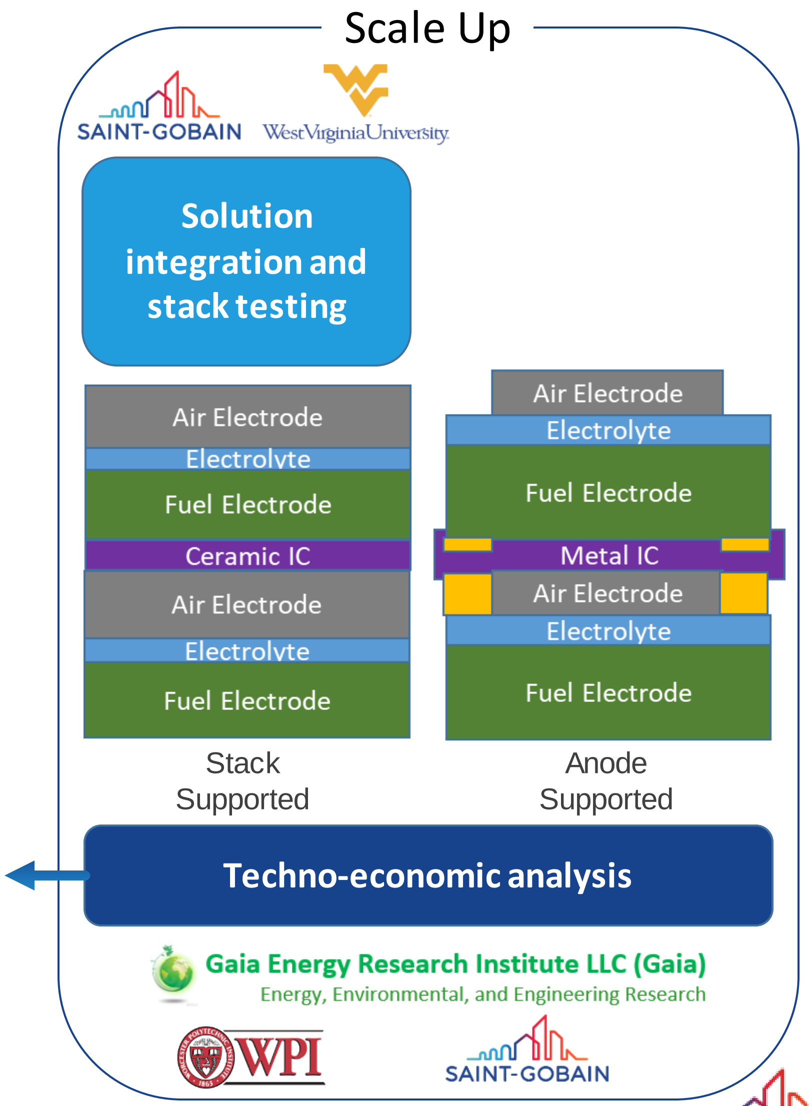
System Modeling

Gaia Energy Research Institute LLC (Gaia)
Energy, Environmental, and Engineering Research

<u>SOE System Cost Drivers</u>

- Stack power density
- System capital costs
- Electricity consumed per unit hydrogen produced
- Recovered heat





AMBITIOUS PROGRAM FOCUSED ON SCALING AND REVERSIBLE OPERATION

SOLUTIONS AT EACH LEVEL DESIGNED TO BE PORTABLE TO MANY SYSTEM CONFIGURATIONS

Cell Level

BOSTON UNIVERSITY · SAINT-GOBAIN · WPI

Oxygen Electrode (Nickelates)

Air Electrode
Electrolyte
Fuel Electrode

Stack Supported

Air Electrode
Electrolyte
Fuel Electrode

Anode Supported

Fuel Electrode (Nickel migration)

BOSTON UNIVERSITY · SAINT-GOBAIN · WPI

Stack Level

WPI · West Virginia University

Nickelate – Cr interconnect interactions

Air Electrode
Electrolyte
Fuel Electrode
Ceramic IC

Stack Supported

Metal IC
Air Electrode
Electrolyte
Fuel Electrode

Anode Supported

Ceramic IC humidity interactions

West Virginia University · SAINT-GOBAIN

Scale Up

SAINT-GOBAIN · West Virginia University

Solution integration and stack testing

Air Electrode
Electrolyte
Fuel Electrode
Ceramic IC
Air Electrode
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Stack Supported

Air Electrode
Electrolyte
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Anode Supported

Techno-economic analysis

Gaia Energy Research Institute LLC (Gaia)
Energy, Environmental, and Engineering Research

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REVERSIBLE SOFC-SOEC STACKS BASED ON STABLE RARE-EARTH NICKELATE OXYGEN ELECTRODES: DE-FE0031972

Objectives to be reached during this project

1. Establish state-of-the-art oxygen electrode materials
2. Stabilize Ni-YSZ hydrogen electrode against Ni migration
3. Quantify the effect of cell & stack design on durability – then improve it
4. Develop and quantify cost-effective and scalable manufacturing

Diverse and experienced team assembled

SAINT-GOBAIN

BOSTON UNIVERSITY

West Virginia University

WPI

Gaia Energy Research Institute LLC (Gaia)
Energy, Environmental, and Engineering Research

Program started in H2 2021

Grant Program Activity	Budget Federal	Budget Non-Federal	Budget Total
Budget Period 1	$799,199	$199,800	$998,999
Budget Period 2	$798,971	$199,745	$998,716
Budget Period 3	$792,500	$198,125	$990,625
Totals	**$2,390,670**	**$597,670**	**$2,988,340**

Acknowledgement

NATIONAL ENERGY TECHNOLOGY LABORATORY