Development of Chromium and Sulfur Getter for SOFC Systems

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Project Team Introduction

- **Principal Investigator:**
  Prabhakar Singh, UTC Chair Professor, Materials Science and Engineering Department
- **Co- Principal Investigators:**
  Steven L. Suib, Board of Trustees Distinguished Professor, Chemistry & Chemical Engineering
  Boxun Hu, Research Assistant Professor

- **Participating Organization:**
  University of Connecticut
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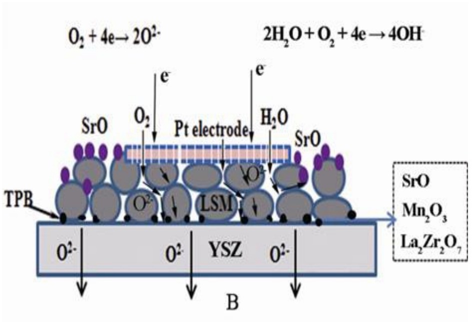
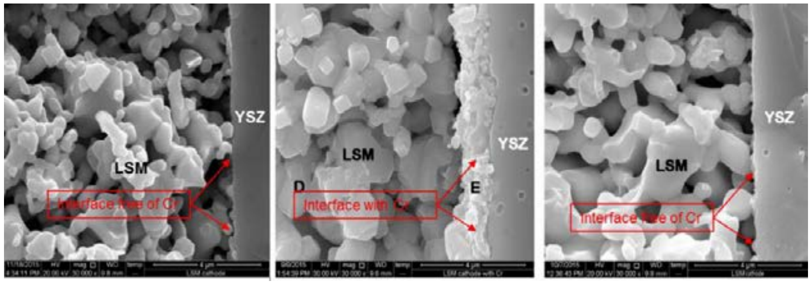
Background - SOFC

- Solid oxide fuel cell (SOFC) power generation system is an environmentally clean and efficient energy conversion technology that produces electricity and heat by electrochemical conversion of fuels at temperatures in the range of 600-1000^{0}C.
- The key advantages of SOFC are high efficiency, hybridization, modularity of construction, small CO_2 foot print per kWh of generated electricity and fuel flexibility
- Major impediment for large scale commercialization of the SOFC technology is the current inability of preserving long term performance and cost effectiveness of a SOFC power module for the operational period.
- The long term degradation of the SOFC is mainly due to the instability of the cell components and it remains an important subject in the SOFC development.
- The presence of water vapor in air has shown decrease in electrochemical performance by segregating the strontium oxide/hydroxides at the surface, oxide/hydroxides at the cathode-electrolyte interface and loss of effective interfacial contact area.





Background – Cr &S Impurities

- Cell degradation due to the presence of minor impurities (Cr vapor, SO_2) in the air stream has also been reported in the literature. Humidified air aggravates corrosion and oxidation of chromium containing alloys that leads to higher chromium vapor pressure compared to dry air.
- Cathode degradation arises from the gas phases such as CrO_3 and $CrO_2(OH)_2$ generated from the metallic interconnects, and balance of plant components, Na_2O, boron oxide/ hydroxide and $SiO_2/Si(OH)_4$ from seals and insulating materials and H_2O, CO_2, SOx/H_2S and particulate materials (PM) present in the ambient air stream. The current national ambient air quality standards (NAAQS) for SO_2 is described in the Table below.

Sulfur Dioxide (SO_2) Primary National Ambient Air Quality Standards

Pollutant	Type	Standard	Averaging Time	Regulatory Citation
SO_2	Primary	75 ppb	1-hour	40 C.F.R. 50.17a
SO_2	Secondary	0.5 ppm (1,300 µg /m³)	3-hour	40 C.F.R. 50.5a

Program Objectives

The overall objective of the proposed research program is to:

- **Develop and demonstrate the operation of engineered getter systems at technology readiness level (TRL)-5 for the capture of both, gaseous chromium and sulfur species present in the air stream entering the solid oxide fuel cells (SOFCs) power generation systems.**
- **Scale up the getter fabrication process to develop desired getter architecture for prototype stack integration and testing.**

The sub-objectives of the proposed program includes:

(a) **development and modification of chemical compositions and microstructure of getter coatings and supports using thermochemical calculation, process simulation and modeling technologies**

(b) synthesis of high surface area nano and meso architectures consisting of nanofiber and nanorod getter materials with micro channeled as well as porous coatings,

(c) develop in-operando monitoring of the chromium and sulfur breakthrough to predict the getter health and protect the SOFC stacks,

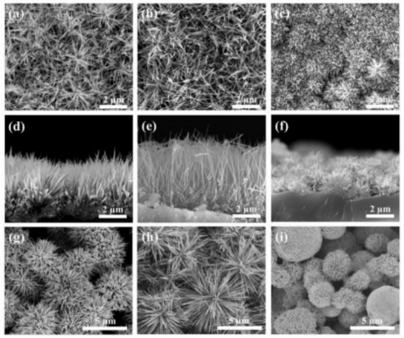
(d) scale up the getter fabrication processes and

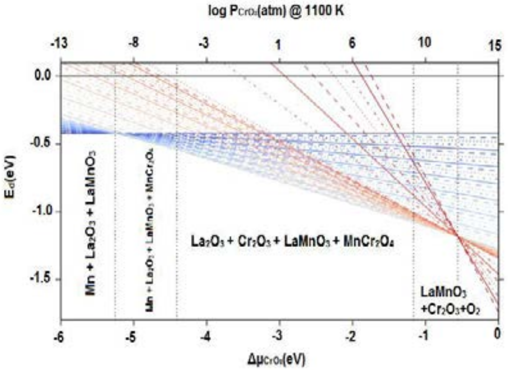
(e) test validate the getter at stack and system operating conditions to demonstrate the technology readiness level at TRL 5.

Technical approach

Development and demonstration of chromium and sulfur co-getter for SOFC system is proposed to advance the technology readiness level from TRL 2 to TRL 5.

- **Thermochemical calculations using HSC chemistry software and DFT**
- **Synthesis of advanced high surface area (nano and meso scale, nano-rod and nanofibers) powder materials**
- **synthesis process scale up**
- **Getter coating development**
- **Evaluation of the compatibility with the support under nominal operation conditions**
- **CFD analysis to optimize the getter design in order to maximize its utilization**
- **An *in-situ* sensor to monitor the getter degradation**



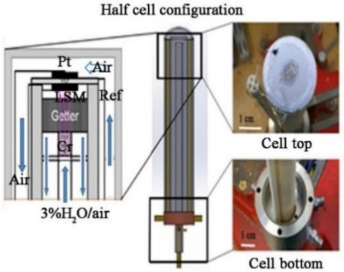


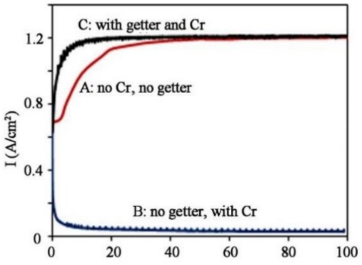
Technical approach

- Identification of getter materials and support
- synthesis procurement from commercial vendors
- Characterization of synthesized materials
- Test validation using in-operando and ex-situ techniques
- Scale up and technology transfer

The laboratory capabilities available for conducting the proposed research include:

(a)Fully instrumented chromium and sulfur evaporation and capture test facility (600-1000°C temperature range, up to 50% humidification)
(b)Symmetric half-cell test facility Cell test facility with integrated getter to perform electrochemical tests under simulated system conditions
(c)Extensive structural and chemical characterization facility
(d)Test facility for the operation of kWe class (1-5 kWe) SOFC stacks





Project Structure and Management

Development of Chromium and Sulfur Getter for SOFC Systems: Demonstration at TRL-5

Project Lead and PI
Professor Prabhakar Singh
Role: Manage the research program and have overall responsibility for program execution

Professor Steven Suib (Co-PI)
Role: Execution of high surface area materials synthesis and processing for coating materials

Dr. Boxun Hu
Role: Execution of experimental activities, test validation and technology transfer

Project schedule

	Start Date	End Date	Cost	Budget Period 1 10/1/2016-12/31/2016 Q1	Budget Period 2 01/1/2017-03/31/2017 Q2	Budget Period 3 04/1/2017-06/30/2017 Q3	Budget Period 4 07/1/2017-09/30/2017 Q4	Budget Period 5 10/1/2017-12/31/2017 Q5	Budget Period 6 01/1/2018-03/31/2018 Q6
Task 1.0 Project Management and Planning	10/1/2016	3/30/2018	62500						
Subtask 1.1 Project Management and Planning	10/1/2016	3/30/2018							
Subtask 1.2 Briefing and Report	10/1/2016	3/30/2018							
Milestones									
1.1 Established program priorities with DOE program manager									
Task 2.0 Identification of chromium and sulfur getter by "top-down" approach	11/1/2016	2/28/2018	187500						
Subtask 2.1 Exploration of material chemistry	11/1/2016	12/30/2017							
Sub-task 2.2 Materials synthesis process development	12/1/2016	2/28/2018							
Milestones									
2.1 Identified the materials chemistry									
2.2 Developed materials synthesis process for effective Cr and S getter									
Task 3.0 Getter development and scale up of high surface a with tailored porosity	1/1/2017	12/31/2017	125000						
Sub-task 3.1 Tailored porosity coating formulation	1/1/2017	9/30/2017							
Sub-task 3.2 Coating process scale up	3/1/2017	10/30/2017							
Sub-task 3.3 Coating characterization	4/1/2017	12/31/2017							
Milestones									
3.1 Optimized microstructure of the getter coatings									
3.2 Developed adherent porous coating on large scale substrates									
3.3 Surface and bulk characterization performed									
Task 4.0: Getter design optimization through computationa	1/1/2017	3/31/2018	62500						
Milestones									
4.1 Optimal parameters such as porosity and the thickness of coating materials achieved									
Task 5.0: Co-gettering testing and posttest characterizatio	4/1/2017	3/31/2018	93750						
Sub-task 5.1 Getter fabrication and scale up for testing in stacl	4/1/2017	3/31/2018							
Sub-task 5.2 Getter testing and performance evaluation	5/1/2017	3/31/2018							
Sub-task 5.3 Characterization of pre and posttest getter	5/1/2017	3/31/2018							
Milestones									
5.1 Symmetric and standard cells and getters fabricated									
5.2 Getters validated in "real world" atmosphere with no degradation for 200h									
5.3 Pre and posttested samples characterized									
Task 6.0 Sensor development and integration in getter for in-situ monitoring	7/1/2017	3/31/2018	93750						
Milestones									
6.1 Developed and integrated sensor in getter bed									

Project schedule

Milestone Title/Description	Planned Start Date	Planned Completion Date	Verification Method
Established program priorities with DOE program manager	10/1/2016	3/30218	Documentation
Briefing and Report	10/1/2016	3/30/2018	Documentation
Identified the materials chemistry	11/1/2016	12/30/2017	Thermodynamic and computational modeling
Developed materials synthesis process for effective Cr and S getter	12/1/2016	2/28/2018	Materials characterization methods
Optimized microstructure of the getter coatings	1/1/2017	9/30/2017	Morphological characterization
Developed adherent porous coating on large scale substrates	3/1/2017	10/30/2017	Morphological characterization
Surface and bulk characterization performed	4/1/2017	12/31/2017	SEM, TEM, Raman spectroscopy, FIB, FTIR
Optimal parameters such as porosity and the thickness of coating materials achieved	1/1/2017	3/31/2018	Computational fluid dynamics analysis
Symmetric and standard cells and getters fabricated	4/1/2017	3/31/2018	Documentation
Getters validated in "real world" atmosphere with no degradation for 200h	5/1/2017	3/31/2018	Electrochemical impedance analysis
Pre and post tested samples characterized	5/1/2017	3/31/2018	Materials characterization
Developed and integrated sensor in getter bed	7/1/2017	3/31/2018	Materials and electrochemical characterization

Project Budget

Overall Project Funding Profile

	Quarter 1 10/01/16-12/31/2016		Quarter 2 01/1/2017-03/31/2017		Quarter 3 04/1/2017-06/30/2017	
	Gov't Share	Cost Share	Gov't Share	Cost Share	Gov't Share	Cost Share
Prime Recipient Name	$52,087	$13,024	58,332	$14,583	$70,832	$17,708
Percentage	80%	20%	80%	20%	80%	20%

Quarter 4 07/1/2017-12/31/2017		Quarter 5 10/1/2017-12/31/2017		Quarter 6 01/1/2018-03/31/2018		Total Project	
Gov't Share	Cost Share	Gov't Share	Cost Share	Gov't Share	Cost Share	Government Share	Cost Share
$114,583	$28,645	$114,583	$28,645	$89,583	$22,395	$500,000	$125,000
80%	20%	80%	20%	80%	20%	80%	20%

Risk Management (Identification and mitigation)

Description of Risk	Probability (Low, Moderate, High)	Impact (Low, Moderate, High)	Risk Management Mitigation and Response Strategies
Technical/Scope Risks:			
Identify the Cr/S getter materials	Low	Moderate	Use additional literature and HSC based calculations
Development of HSA coating	Low	Moderate	Identify alternative approach to fabricate nano-coating materials
Co-gettering of Cr/S and cathode mitigation	Low	Low	Evaluate performance of cathode in presence of Cr/S and validate it by posttest analysis.
Computational getter design optimization	Low	Low	Update the existing computational model of getter and coating for optimization
Chromium sensor fabrication and validation	Low	Moderate	Identify and update the materials selection and collaborate with fabrication experts
Scale-up and performance testing	Low	Low	Collaborate with industrial partners for large scale fabrication of co-getters for SOFC stack
Resource Risks:			
Infrastructure, personnel and equipment resources	Low	Low	-Timely evaluation of the equipment will be performed to avoid hurdles during the program - Availability of alternative equipment facilities
Management Risks:			
Project management and planning	Low	Low	PI and DOE program manager will discuss the program priorities, deliverables and milestones
Schedule Risks:			
Project timeline	Low	Low	Weekly progress meeting will be held with the members involved in the program to ensure no programmatic hurdles exist.
Budgetary Risks:			
Funding profile changes	Low	Low	Budget recombination
Environmental, Safety, and Health Risks:			
Experiments involved in chromium evaporation	Low	Low	- Evaporated chromium is trapped is two water traps in a closed system. -Laboratory safety protocols are in place and enforced. -Chromium containing wastes will be handled and disposed using appropriate EHS procedure.
External Influences Risks:			
Delay in materials supply	Low	Low	Reschedule work plan

Technology Readiness Level /commercialization goals

Increase TRL to TRL-5

- Laboratory bench top validation
- Validation under system operating conditions
- Validation by SOFC manufacturers
- Scale up and Technology transfer

Acknowledgements

- Dr. Rin Burke for technical and programmatic discussion
- Dr. Jeff Stevenson for technical collaboration and testing of UConn getter at PNNL
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- Dr. Hossein Ghezel-Ayagh for technical discussion
- Dr. Lou Carrero of NUWC for technical discussion
- UConn for providing test facility

Thank You

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