Rationally Designed Catalyst Layers for PEMFC Performance Optimization

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Overview

Timeline

- Project start date: April, 2013
- Project end date: March, 2016
- Percentage complete: 0%

Barriers

- Barriers addressed
  - A. Electrode performance
  - B. Cost
  - C. Durability

Budget

- Total project funding:
  - DOE: $3,480 K
  - Contractor share: $865 K
- Funding received in FY12
  - $0 K
- Funding expected for FY13
  - $ 843 K

Partners

- Johnson Matthey Fuel Cells
  - Jonathan Sharman, Alex Martinez, and Graham Hards
- United Technologies Research Center
  - Mike Perry and Zhiwei Yang
- University of Texas at Austin
  - Paulo Ferreira
- Indiana University Purdue University Indianapolis
  - Jian Xie
- Project lead: Argonne National Laboratory
  - Debbie Myers

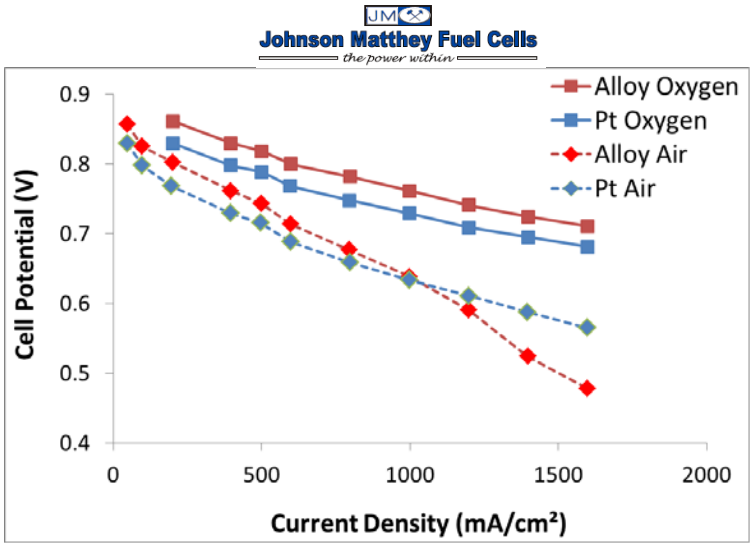
Roles of Team Members

- Johnson Matthey Fuel Cells
  - Provide state of the art catalysts and CCMs, fabricate CCMs using new ink compositions/techniques, and scale-up the CCMs for large cells and short stacks
- United Technologies Research Center
  - Integrate JMFC CCMs with state-of-the art cell fixture and fabrication procedure, test and perform diagnostics on cells, and fabricate and test a short stack based on these CCMs
- University of Texas at Austin
  - Pre- and post-test electron microscopy characterization of catalysts, electrodes, and CCMs
- Indiana University Purdue University Indianapolis
  - Functionalize carbon blacks, develop ink compositions, perform ultra-small angle X-ray scattering and cryogenic transmission electron microscopy analysis of catalyst/ionomer inks, develop ink solvent removal processes, perform porosimetry measurements on the catalyst layer, test small-scale CCMs
- Argonne National Laboratory
  - Project management
  - Modeling of optimum catalyst layer structure, ink formulations, agglomerate size analysis, conductivity and electrochemical analysis of electrode layers, small fuel cell testing, characterization of microstructure formed using X-ray and microscopy techniques, and assessment of the cost and manufacturability of the technology and process

Relevance

- **Objectives**
  - The goal of this project is to realize the ORR mass activity benefits of advanced Pt alloy cathode electrocatalysts, observed on oxygen and at low current densities and in rotating-disk electrode measurements, in MEAs and stacks operating at high current densities and on air

- **Impact**
  - Meeting this objective will enable MEAs to achieve DOE 2017 Technical Targets for
    - Performance
      - >300 mA/cm^2 at 800 mV
      - >1000 mW/cm^2 at rated power
    - Cost: \$5-9/kW$_e$ catalyst, <\$30 kW$_e$ system
    - Durability with cycling 5,000 hours (≤80°C) and 2,000 hours (>80°C)
      - ≤40% loss of initial catalytic mass activity at 900 mV on O_2; <30 mV loss at 0.8 A/cm²



Example of lack of performance benefit of a Pt alloy over Pt when operating at > 1000 mA/cm² on air (cathode loading 0.2 mg Pt/cm², 80°C, 50/50 kPa gauge)

Approach

- Determine the agglomerate, particle, and pore structure of the state-of-the-art Pt alloy/C-based electrodes
  - The advanced Pt alloy is a state-of-the-art de-alloyed Pt/Ni catalyst developed in the on-going General Motors-led project (FC087). The key catalyst characteristics and metrics are:
    - Catalyst deposited as nanoparticles onto conventional carbon black supports, identical to those used for standard Pt/C reference catalysts.
    - Catalyst deposition chemistry is proven and via methods scalable to commercial levels
    - Nominal initial atomic composition prior to de-alloying is $Pt_{25}Ni_{75}$
    - Mass activity (O_2 @0.9 V) is >0.60 A/mg Pt (exceeds DOE 2017 target)
    - Mass activity loss after 30,000 - 0.60 to 1.0 V cycles is <40% (exceeds DOE kinetic stability target)
- Use this information to determine the performance-limiting property of the current electrode
- Rationally design the catalyst layer/MEA structure guided by computational modeling
- Study the dispersion of Pt alloy/C catalyst aggregates and the PFSA ionomer particles in liquid media and the agglomeration of these aggregates/particles during the evaporation process
- Develop a solvent removal process that maintains the dispersion and agglomerate structure of the ink
- Develop the catalyst support morphology, surface functionality, and catalyst ink composition to optimize the performance of the cathode, guided by the modeling results

Approach

Project timeline

April 1, 2013

Project Schedule	Year 1				Year 2				Year 3			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Task 1. Characterization of electrode layer structure, nanoparticle structure, and electrode properties												
1.1 Structural and morphological characterization												
1.2 Microscopic characterization of catalysts and MEAs												
1.3 Conductivity and ECA characterization												
Task 2. Characterization of ink structure and properties												
2.1 Characterization of baseline Pt/C and Pt/alloy inks												
2.2 Characterization of Pt alloy/C and Pt alloy/FCB inks												
Task 3. Computational modeling												
3.1 Mapping of Electrode Structures												
3.2 Kinetic Monte Carlo Algorithm												
3.3 Model Application												
3.4 Optimum Modeled Structures												
Task 4. Development of Pt alloy/C-PFSA dispersions												
4.1 Ink composition/solvent system development												
4.2 Development of functionalized/modified carbon black support for Pt and Pt alloys catalysts												
Task 5. Development of solvent removal and MEA fabrication processes												
5.1 Solvent removal												
5.2 Small-scale membrane-electrode assembly fabrication and testing												
Task 6. Catalyst preparation, membrane-electrode assembly fabrication, testing, and characterization												
6.1 Catalyst preparation												
6.2 CCM fabrication and testing using baseline materials												
6.3 CCM fabrication, characterization, and testing on selected new layers using Baseline Pt/Pt alloy catalysts or analogues on functionalized carbon Black												
6.4 Alternative MEA fabrication												
6.5 MEA testing and degradation mode identification												
Task 7. Short-stack fabrication, assembly, and evaluation												
7.1 MEA scale-up												
7.2 Stack testing												
Task 8. Cost assessment												

Approach: *Milestones, Go/No-Go Decision Point, Project Deliverable*

- FY13 Milestone
  - Benchmark performance of advanced alloy-based catalyst relative to DOE 2017 target of 0.44 A/mg Pt @ 0.9 V, 300 mA/cm²@0.8 V, and 1,000 mW/cm² @ rated power (MEA performance) and identify sources of performance losses on air and at >1 A/cm² to improve performance by 10% - 09/13
    - Work in progress
- Go/No-Go Decision Point
  - Go/No-Go Decision Point (Y2-Q3): Demonstration of 50% improved air performance for advanced Pt alloy catalyst in an MEA versus existing state-of-the-art JMFC cathode catalyst materials and formulations
- Project Deliverable
  - Electrode performance, durability, and a short stack for testing at DOE approved site

Proposed Future Work for FY13

- Identify the sources of the performance loss of cathodes based on an advanced cathode catalyst
- Establish the correlations between agglomerate structure in the advanced cathode catalyst inks and electrode layer structure, as determined using, for example, X-ray and microscopic techniques
- Determine the effects of ink composition (e.g., catalyst to ionomer ratio) on electrode properties and performance and on the effect of catalyst type (i.e., advanced alloy versus Pt of similar particle size)
- Develop a method and an algorithm to map electrode structure from imaging data

Summary

Relevance: To realize the ORR mass activity benefits of advanced Pt alloy cathode electrocatalysts observed at low current densities and on oxygen and in rotating-disk electrode measurements in MEAs and stacks operating at high current densities and on air to enable MEAs to achieve the DOE 2017 performance targets.

Approach: (1) Determine the agglomerate, particle, and pore structure of the state-of-the-art Pt alloy/C-based electrodes (de-alloyed Pt/Ni catalyst from project FC087); determine the performance-limiting property of the current electrode; (2) Rationally design the catalyst layer composition and structure, guided by computational modeling, and develop catalyst support morphology, surface functionality, catalyst ink composition, and solvent removal processes to achieve this structure

Accomplishments: Project anticipated start date of April 1, 2013; The advanced cathode catalyst to be studied in this project has been identified. It has oxygen reduction activity and kinetic stability in an MEA that exceeds DOE 2017 target and has been scaled up by Johnson Matthey Fuel Cells.

Collaboration: Project team of JMFC, UTRC, UT-Austin, and IUPUI

Future work: (1) Identify the sources of the performance loss of cathodes based on an advanced cathode catalyst; (2) Establish the correlations between agglomerate structure in the advanced cathode catalyst inks and electrode layer structure, as determined using, for example, X-ray and microscopic techniques; (3) Determine the effects of ink composition (e.g., catalyst to ionomer ratio) on electrode properties and performance and on the effect of catalyst type (i.e., advanced alloy versus Pt of similar particle size); (4) Develop a method and an algorithm to map electrode structure from imaging data

Collaborations and acknowledgments

- Project team (subs) within DOE H_2 Program
  - Johnson Matthey Fuel Cells
  - United Technologies Research Center
  - University of Texas at Austin
  - Indiana University Purdue University Indianapolis

- General Motors
  - In-kind contributor

Thanks!

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