Transportation Fuel Cell R&D Needs
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Overview

- Purpose: To provide automotive OEM perspective on topics considered worthy - and *not* worthy - of study in the DOE Fuel Cell Subprogram
- Categories described within DOE Fuel Cell Request for Information (RFI):

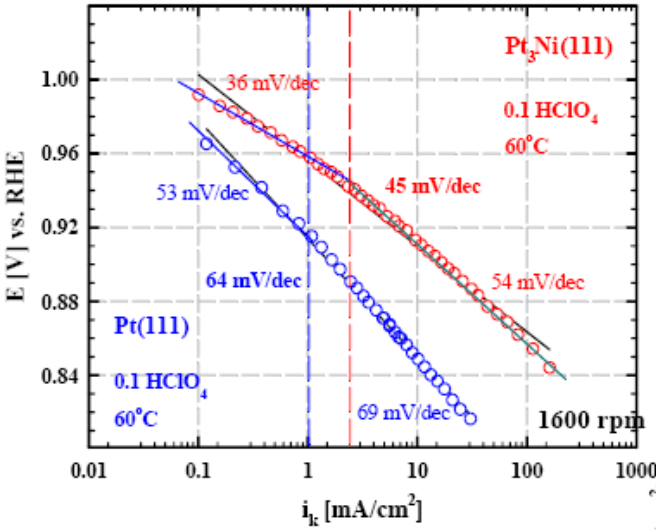
  - Catalysts
  - Catalyst layers
  - Water management
  - MEA optimization
  - Accelerated durability testing
  - Balance of plant
  - Impurity effects
  - Power plant demonstrations
  - Portable power systems
  - Inventive concepts
  - "Other areas":
    - Membranes
    - Plate materials and coatings
    - Seals

Overarching Themes

- Due to the influence of specific operating conditions, stack designs and system designs, and due to confidentiality boundaries, OEMs seek to use government projects to derive fundamental knowledge of component performance and degradation mechanisms.
- OEMs seek development of novel experimental or modeling tools that can be universally used for material/system characterization.
- OEMs seek high risk, high reward materials development (e.g. anhydrous proton conductors or non-PGM catalysts). Projects would be long shots, but would have a major impact if successful.

Catalysts: Topics for Study

- PGM cathode catalysts, mass activity > 0.44 A/mg$_{PGM}$
  - Core/shell
  - Structure-controlled PGM alloys
  - Enhanced activity through metal-support interactions
- Relating ORR activity to atomic-scale physical properties such as:
  - Surface structure
  - Location of alloying elements
  - Surface strain

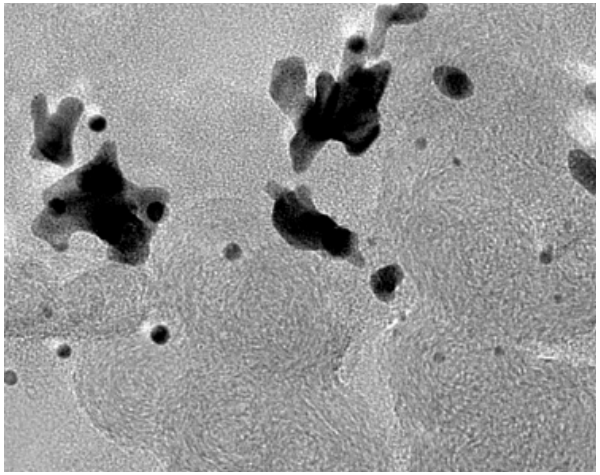


PAST ACCOMPLISHMENT: 9x activity increase for Pt_3Ni(III) versus Pt(III). Philip Ross, LBNL, 2006.

Catalysts: Topics for Study

- Fundamental studies of catalyst degradation mechanisms under automotive stresses.
  - Pt redistribution
  - Alloying element migration
  - Changes in ionomer interactions

PAST ACCOMPLISHMENT: TEM images showing Pt coarsening after extended V cycling. Karren More, ORNL, 2006.

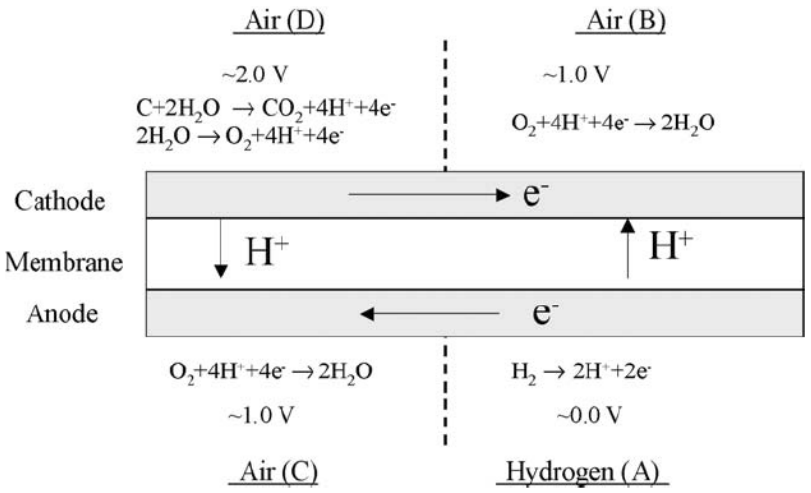


- High mass activity Pt catalysts on corrosion-resistant supports
  - High graphitized carbon
  - Non-carbon supports (e.g. 3M nanostructured thin films)

Catalysts: Topics for Study

- Durable non-PGM cathode catalysts
  - 300 A/cm3 at 0.8 $V_{IR\text{-}free}$
  - Fundamental studies of ORR mechanisms
  - Considered a “long shot”
- Development of hydrogen oxidation catalysts with low oxygen reduction activity
  - Lower half-cell potential
  - Lower corrosion

DEPICTION OF START/STOP STRESS:
Tang *et al.*, *J. Power Sources* **158** (2006) 1306.



Catalysts: Discouraged Topics

- Development of CO-resistant anodes for H_2 fueled automotive systems
  - *Exposure of anode to air during shutdown will clear CO*
- Catalysts using less expensive PGMs in excess (e.g. Pd, Ir, Ru)
  - *Catalysts will become expensive with commercialization*
- Cheaper ways of manufacturing PGMs
  - *Not a topic for government research*
- Pt recycling
  - *These efforts will be driven by economics*

Catalyst Layers: Topics for Study

- Measurements for H^+, O_2 transport modeling
  - Electrode protonic resistance, f(local T, RH)
  - Electrode O_2 diffusion coefficient
- Fundamental studies of ionomer structure
- Porosity distribution
  - Void space fraction, shape, size, connectivity
  - Porosity over range of humidity
- Mechanistic understanding of degradation
  - Carbon corrosion
  - Pt dissolution
- Studies of degradation mechanisms accelerated by low catalyst layer/PEM adhesion, catalyst layer defects, other interfacial phenomena

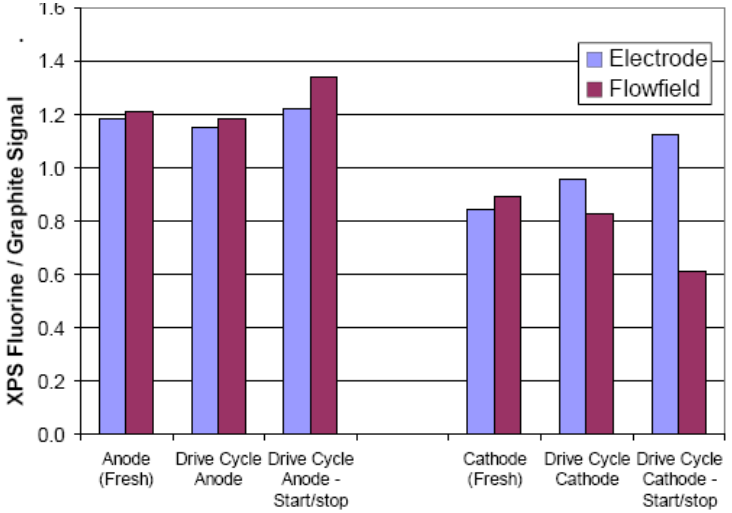
Water Management: Topics for Study

- Non-carbon GDLs with tailored thermal, mechanical and electrical properties.
- Fundamental study of performance, durability: “CCM” versus “GDE” fabrication routes.
- GDLs with increased water transport resistance (thickness / D_{eff}^{H2O}) and decreased O2 transport resistance (thickness / D_{eff}^{O2}).
- Measurement of key parameters for modeling:
  - GDL/catalyst layer interfacial resistance
  - In-situ GDL/catalyst layer adhesion
  - Directionally-specific thermal conductivity
- Models that predict degree of GDL intrusion/tenting

Water Management: Topics for Study

- Fundamental studies of GDL degradation mechanisms

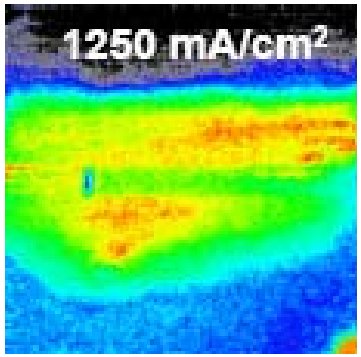
PAST ACCOMPLISHMENT: Elemental composition changes of GDLs after testing cycles. Changes in porosimetry, contact angle, MPL structure also noted. Rod Borup, LANL, 2007.



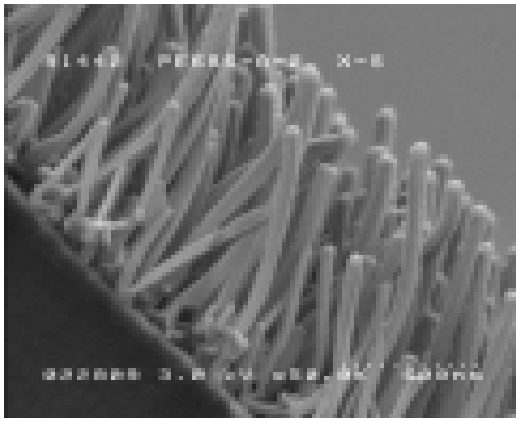
- Development of in-situ load sensing
- Test methods for ex-situ degradation of GDLs that is representative of in-situ degradation
  - Isolation of GDL degradation effects in subsequent in-situ tests

Water Management: Topics for Study

- Water transport fundamentals needed to improve water removal for MEAs with ultra-thin electrodes (e.g. 3M NSTF)



PAST ACCOMPLISHMENTS: Neutron imaging of liquid water in an operating fuel cell (left). Muhammad Arif, NIST, 2006. 3M NSTF catalyst support (right). Mark Debe, 3M, 2006.



- Characterization of hydration profiles across membranes using advanced methods
- Freeze effects on GDLs and plates
- Influence of liquid water on flow distribution and electrode degradation

Accelerated Durability Testing

- Discouraged: Proposal solicitations for development of stack level accelerated tests.
  - OEMs are responsible for establishing test cycles and for full system testing.
  - Relevant degradation tests should be covered in projects studying fundamental degradation mechanisms.
- Encouraged: Proposals for development of facilities in which to conduct accelerated tests defined within the Fuel Cell Roadmap. This includes MEA preparation with reference materials.

Balance of Plant Components

- Development of materials for low cost, compact, high performance membrane-based water vapor transport exchangers. Automotive stresses must be considered (e.g. low RH from cathode exhaust, flow transients).
- Low cost, low loss air bearings.
- Low cost, high efficiency motors
  - Pumps: low speed
  - Compressors: high speed
- Low cost, water/ice robust RH and pressure sensing.
- Low cost on-board diagnostic techniques for measuring humidification or indicating stack health.

Impurity Effects

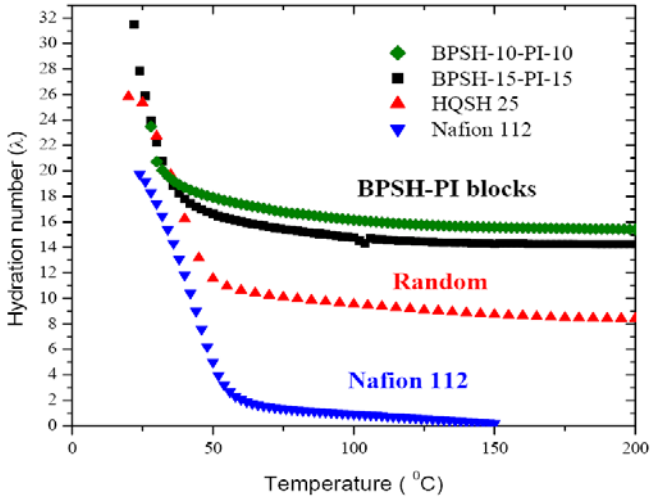
- Fundamental studies to evaluate the influence of the most probable contaminants from key polymers and elastomers in the fuel cell system.
- Increased focus on the impact of air-based contaminants.
  - Quantification of air pollution in urban areas.
  - Evaluate influence of likely contaminants on fuel cell cathode and determine acceptable contaminant levels.
  - Development of filter technology to remove contaminants down to levels acceptable to the stack.
- Continued support of Codes & Standards activities to establish a standard for fuel cell hydrogen.

OEM-Discouraged Topic Categories

- OEMs do not recommend proposal solicitations on MEA optimization. These studies are too dependent on soft good materials and cell design.
- Fuel cell power plant demonstrations.
- Durability and reliability of portable power systems.
- Inventive concepts.
  - Projects in this area have focused on novel stack designs and engineering solutions with little expected benefit to automotive fuel cells.

Membranes: Topics for Study

- Anhydrous proton conductors that operate at hot, dry conditions (>100ºC, < 20% RH) and are stable at low temperature (freeze, flooding).
- Membrane structure design to allow both:
  - Mechanical stability, reduced in-plane swelling
  - High through-plane proton conductivity



- Fundamental studies of membrane structure / property relationships to optimize performance and durability.

PAST ACCOMPLISHMENT: Optimization of membrane properties using multi-block copolymers . James McGrath, Virginia Tech, 2007.

Membranes: Topics for Study

- Cost effective methods for extrusion of low EW sulfonated polymer membranes. Membranes should be delivered in protonated form.
- Synthesis and stabilization of low pKa structures to enable high H^+ conductivity.
- Method development for measurement of water transport properties as f(T, RH, current density)
  - Diffusion coefficient
  - Electro-osmotic drag coefficient
  - Should relate properties to chemistry and include freeze
- Experimental and computation studies of degradation mechanisms of non-perfluorinated polyelectrolytes (e.g. sulfonated polyaromatics).

Membranes: Discouraged Topics

- Development of methods for measuring proton conductivity.
- Development of additives to improve Nafion conductivity.
- Ionomer recycling and recovery.
- Projects for development of novel ionomer structures that avoid evaluations of mechanical, thermal and chemical stability.
- Development of solid electrolytes for non-protonic ion transport (e.g. OH^-) that are not capable of limiting area specific resistance to < 30 $m\Omega*cm^2$ (non-freeze).

Plate Materials and Coatings: Topics for Study

- Development of stable hydrophilic (<20º contact angle) and hydrophobic (>120º) bipolar plate surface energies with a fundamental understanding of impact on PEMFC water management, performance and durability.
- Development of low-cost aluminum or carbon steel bipolar plates that meet DOE requirements.
- Quantum physics-based modeling of metal plate / GDL interfaces to obtain understanding of electron transfer mechanisms. Parameters should include:
  - GDL Type
  - Compression pressure
  - Coating layer thickness
  - Coating layer type
  - Surface roughness

Seals

- Encouraged: Fundamental work to develop seal materials which can meet requirements for:
  - Chemical stability
  - Thermal stability
  - Mechanical stability
  - Compression / compression set
  - Other criteria (very low electrical conductivity, very low gas permeation, etc.)
- Discouraged: Developing methods for manufacturing.

Cooling

- Fundamental studies related to novel coolant materials and integration into automotive fuel cell cooling systems. This includes using existing standard SAE practices for testing and benchmarking against conventional vehicle cooling.

Summary and General Considerations

- Automotive OEMs desire for DOE-funded researchers to study fundamentals:
  - Component performance
  - Component durability and degradation
  - Relationships between automotive stressors and resulting performance and degradation that can be used in modeling or for improved testing.
- Projects with material or component deliverables should be required to supply the DOE with samples or hardware for independent comparative evaluations.