

# Improved Fuel Cell Cathode Catalysts Using Combinatorial Methods

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NuVant Systems Inc.  
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**Project ID #  
FCP10**

# Overview

## Timeline

- **Start date: 7/21/2004**
- **End date:7/13/2006**
- **Percent complete 38%**

## Budget

- **Total project funding**
  - **DOE share:\$650,000**
  - **Contractor share:\$70,558**
- **Funding received in**  
**FY04:\$216,666**  
**FY05: \$73,763**

## Barriers

- **Barriers addressed**
  - **Catalyst Cost**
  - **Electrode performance**

## Partners

- **T. E. Mallouk, Penn State**
- **E. S. Smotkin, UPR**

# Objectives

## Project objectives

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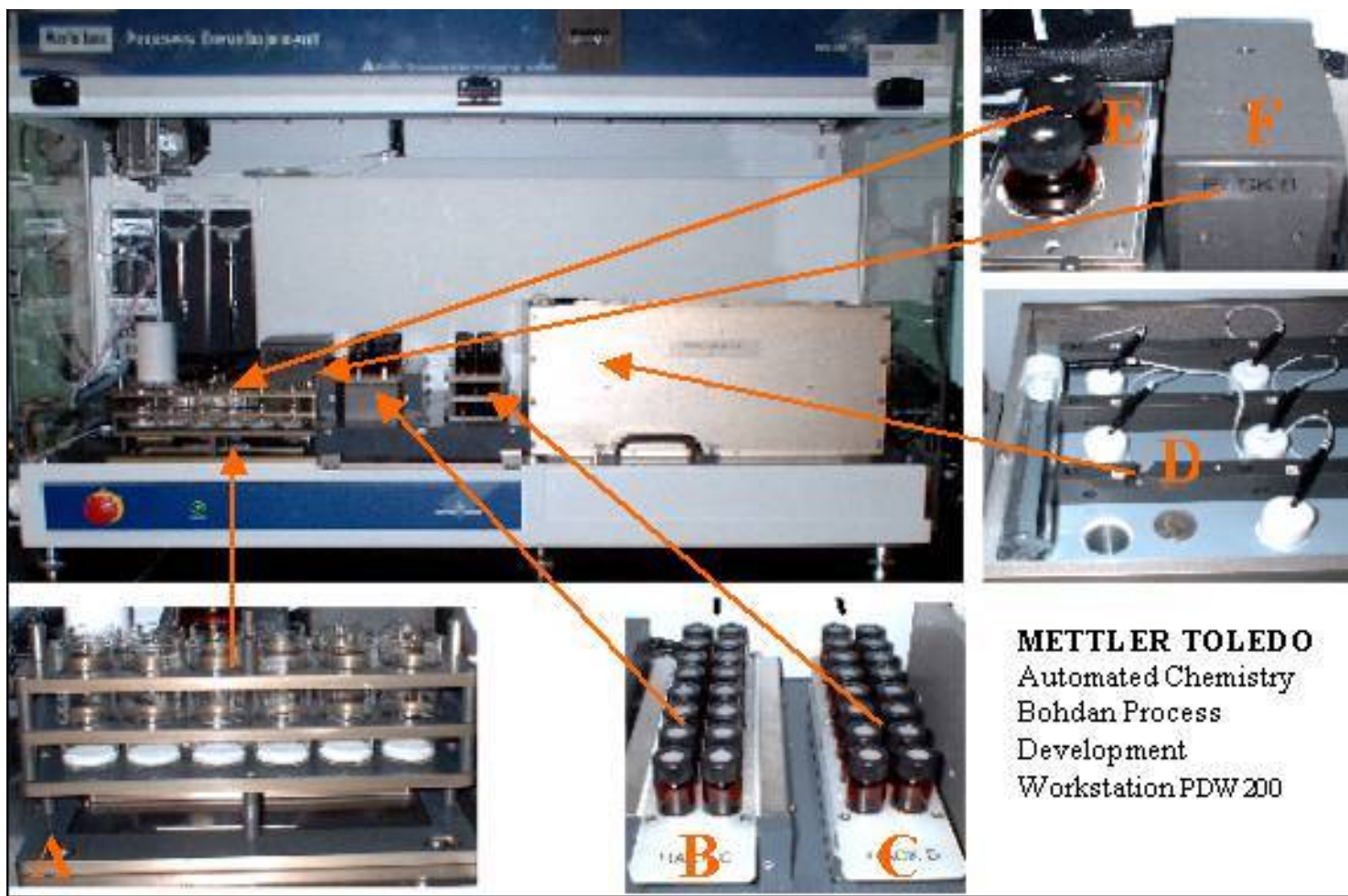
**Assist DOE in the discovery of a PEMFC cathode catalyst with an order-of magnitude improvement over state-of-art catalysts to decrease the cathode cost and improve cathode performance.**

- **To establish high throughput discovery methodology**
  - **To address issues concerning materials and operations**
  - **Upgrade electronics and software for the high throughput systems**
  - **Upgrade array fuel cell flow field design**
  - **To perform the control experiment on the array fuel cell**
- **Optimize operating conditions for the high throughput synthesis of catalysts on a synthesis/analysis working station**
- **To set metrics and baseline data for the array fuel cells by ranking five commercial catalysts**
- **To optimize synthetic route for the size-controlled synthesis**

# Approach

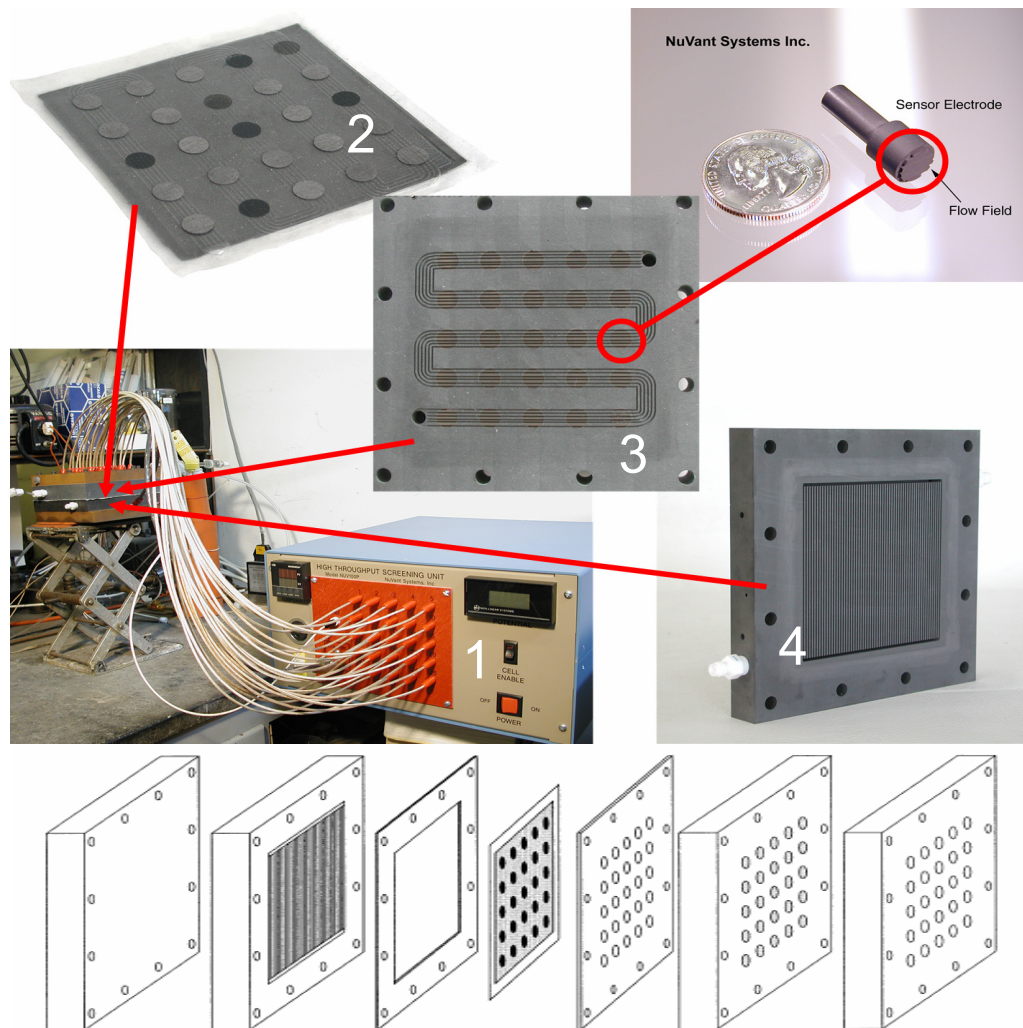
- Development of revolutionary cathode catalysts for the PEMFC through an integrated discovery program
  - Efficient factorial search strategies
  - High throughput synthesis using customized process control robotics
  - High throughput focus screening
  - Development of synthetic routes
- Demonstration of revolutionary catalysts in a single cell
- Development of heuristic rules for catalyst discovery

# High throughput synthesis work station



**A. Array vacuum filtration device; B. Metal ion solution array; C. Reducing agents array; D. 12 Vessel reaction array with controlled T, headspace and stirring; E. Acid and Base solutions for pH adjustment; F. Inert atmosphere chamber for sensitive reagents**

# NUV100P high throughput screening system



## Components:

- (1) 25-channel potentiostat
- (2) Array MEA
- (3) Serpentine flow field
- (4) Counter electrode flow field

**Progress: (1) Increased allowable operating T of flow fields from 50°C to 80°C; (2) Increased catalyst spot channel current from 200 mA to 480 mA; (3) Software upgrades.**

# Conditions for control experiments

## Loadings:

Sample 1: 2.02 mg cm<sup>-2</sup>, JM 20 wt%Pt/C

Sample 2: 2.01 mg cm<sup>-2</sup>, JM 20 wt%Pt/C

Sample 3: 2.05 mg cm<sup>-2</sup>, JM 20 wt%Pt/C

Sample 4: 2.02 mg cm<sup>-2</sup>, JM 20 wt%Pt/C

Sample 5: 2.03 mg cm<sup>-2</sup>, JM 20 wt%Pt/C

Counter electrode: 2 mg cm<sup>-2</sup> JM 20 wt%Pt/C

## Operating conditions:

Cell temperature: 60 °C

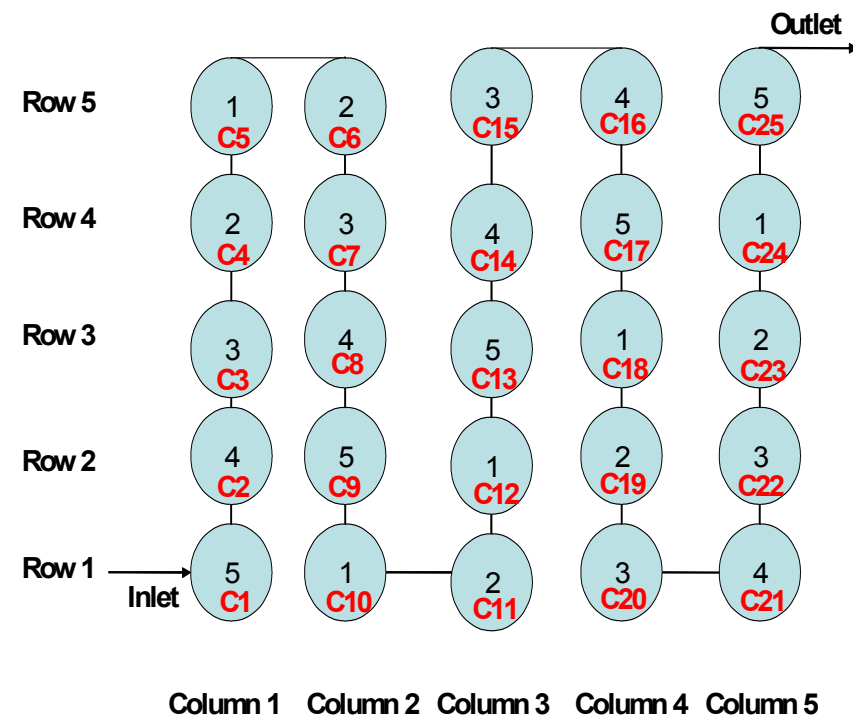
Oxygen/air side: 1000 SCCM O<sub>2</sub>/air with sparger 60 °C and tube 60 °C

Hydrogen side: 200 SCCM with sparger 65 °C and tube 65 °C

## Measurement

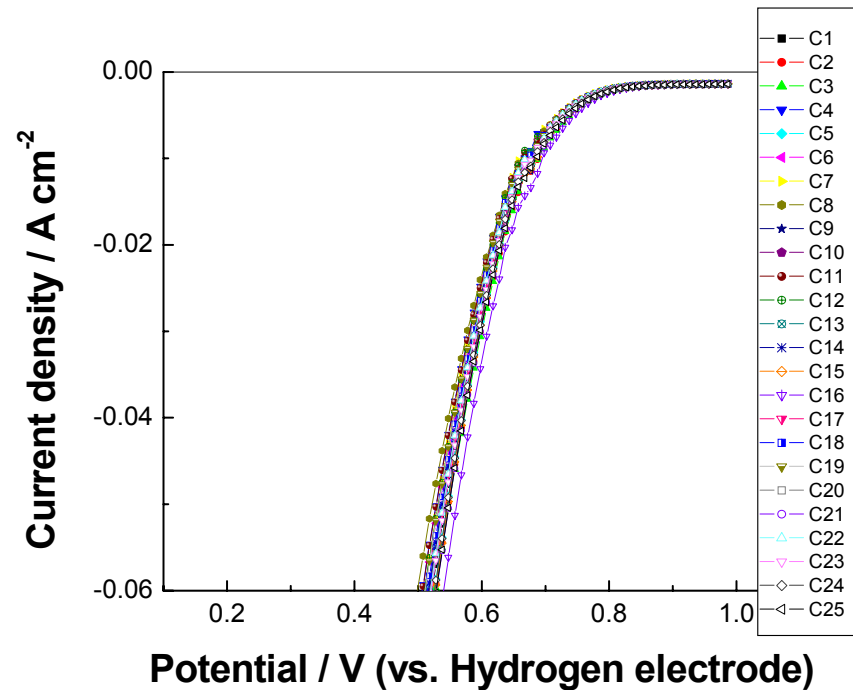
Scanning potential from 1.0 to 0.60 V at 10 mV s<sup>-1</sup>

## Sample maps (Latin square design)

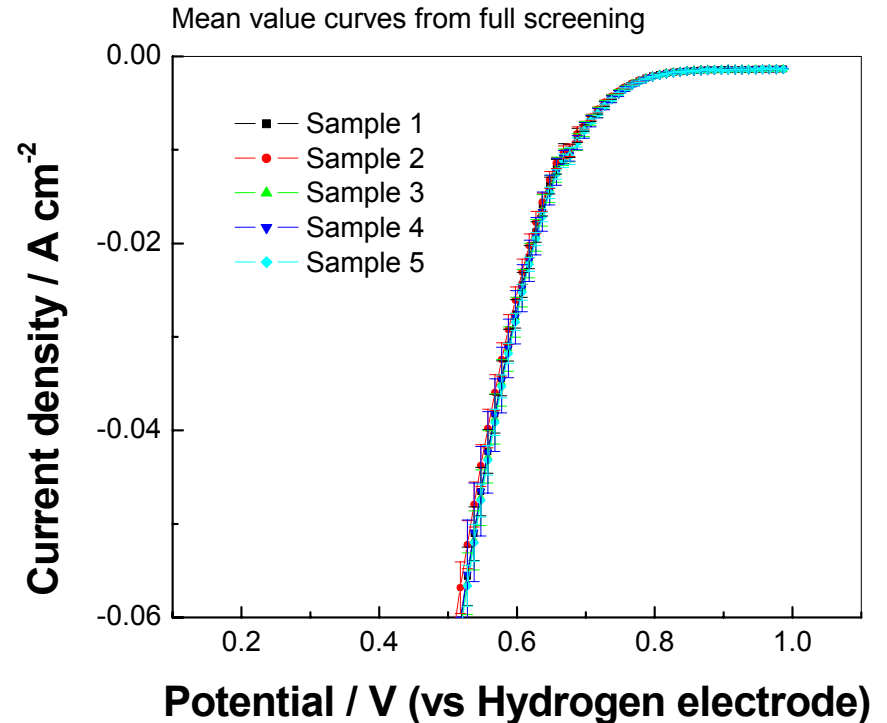


# Data for H<sub>2</sub>-Air control experiment

(a) Polarization curves obtained at 25 spots with identical catalyst



(b) Mean value curves for sample 1-5

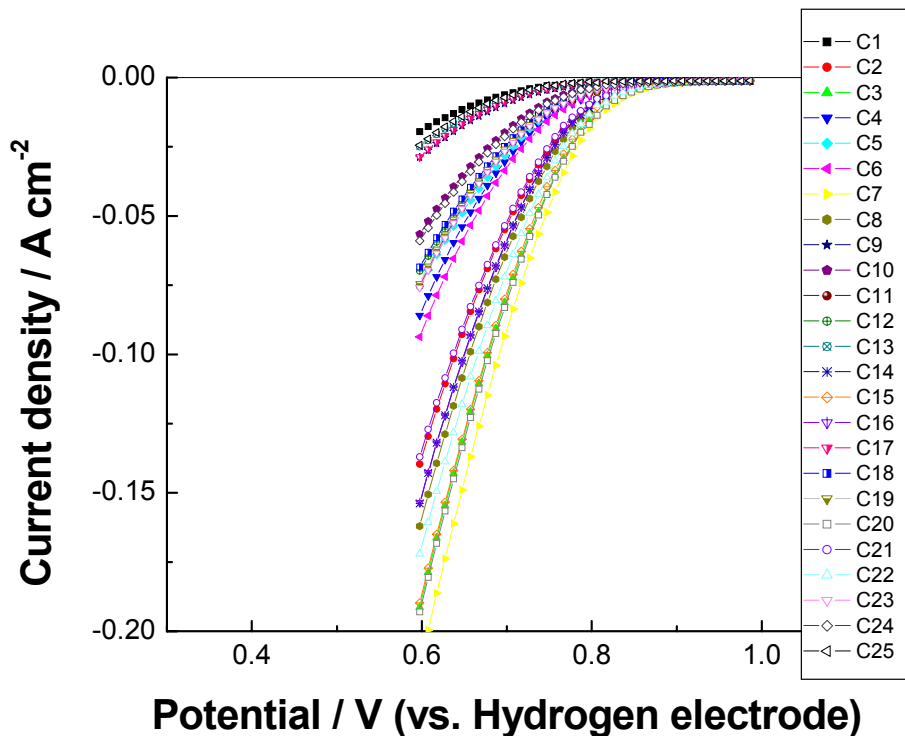


- **Good uniformity is obtained at 25 spots in the control experiments.**
- **The mean value curves for five samples are very close.**
- **Difference of 10 % in the activity can be distinguished at 0.80 V where the reaction is in kinetic control.**

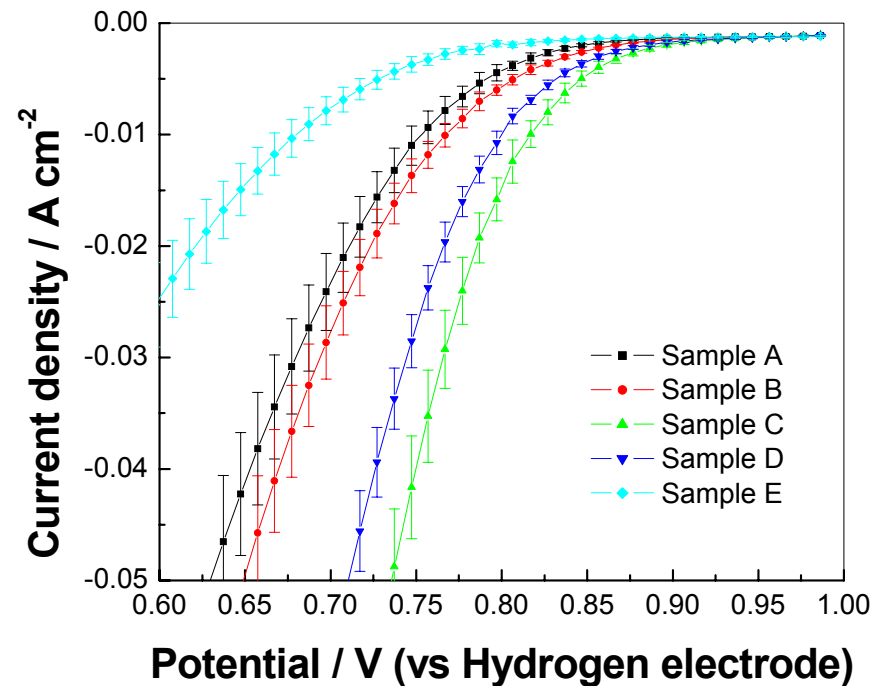


# Screening of five different catalysts (A-E) at 60°C with air

(a) Full polarization curves at 25 spots

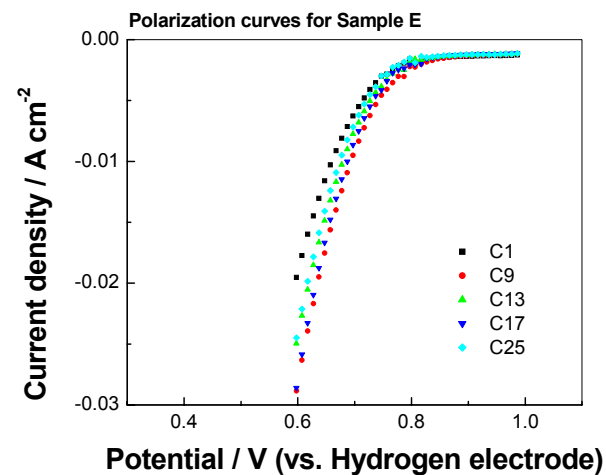
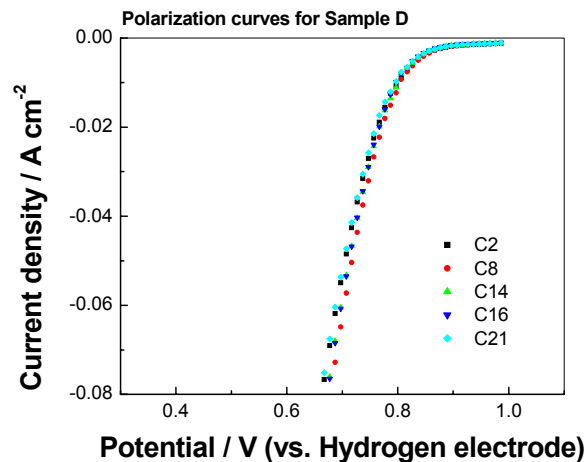
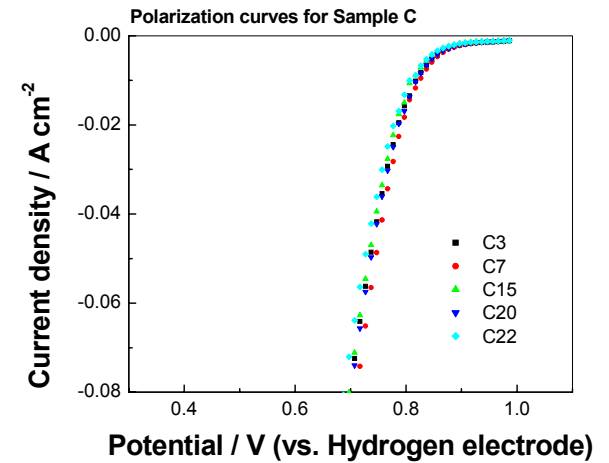
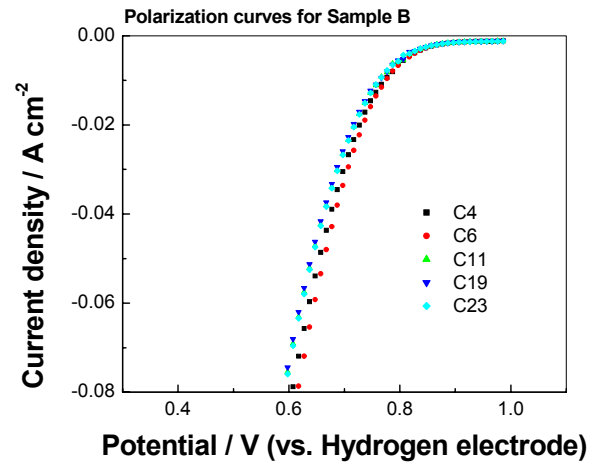
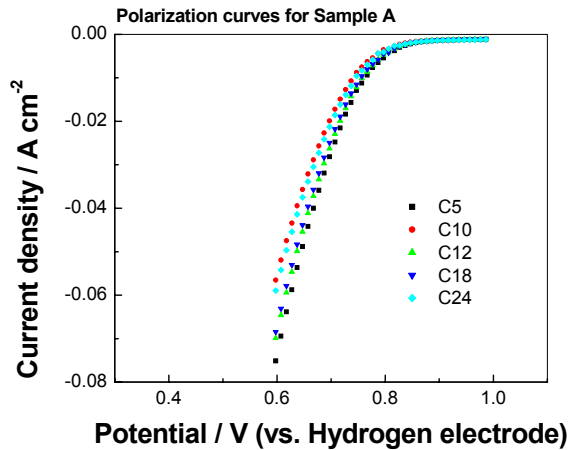


(b) Mean value curves for sample A-E



- Five samples are arranged in a 5x5 Latin square
- Good uniformity is obtained for each sample
- The ranking at 0.80 V for five samples is: C > D > B > A > E

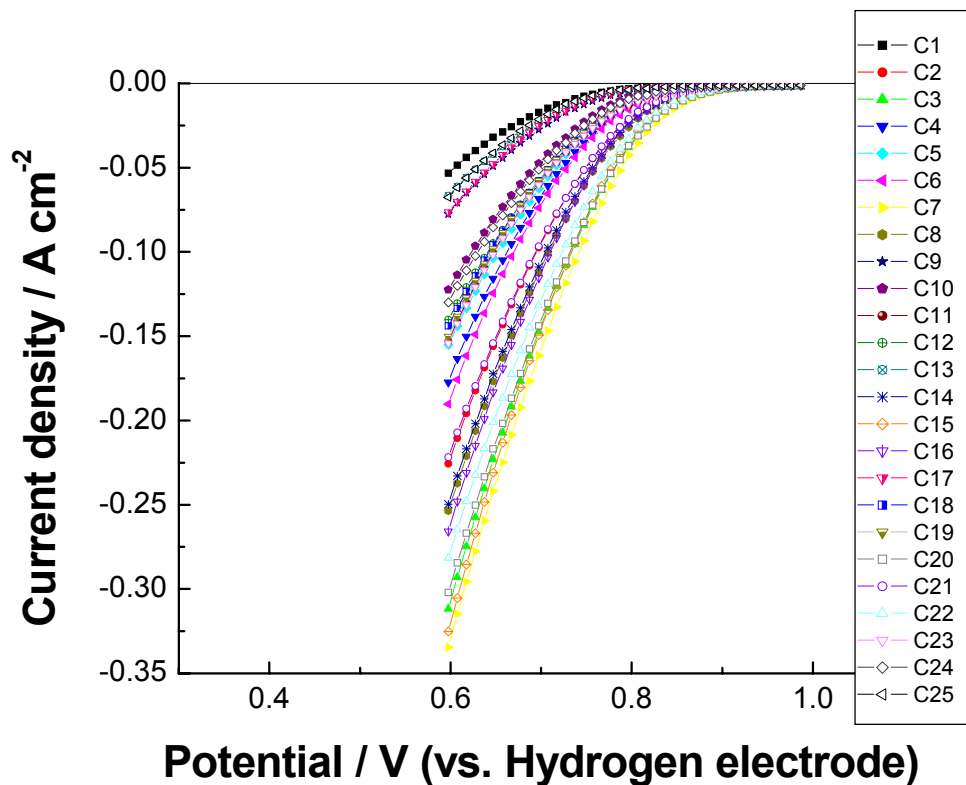
# One example of polarization curves for individual sample at 60 °C and with air



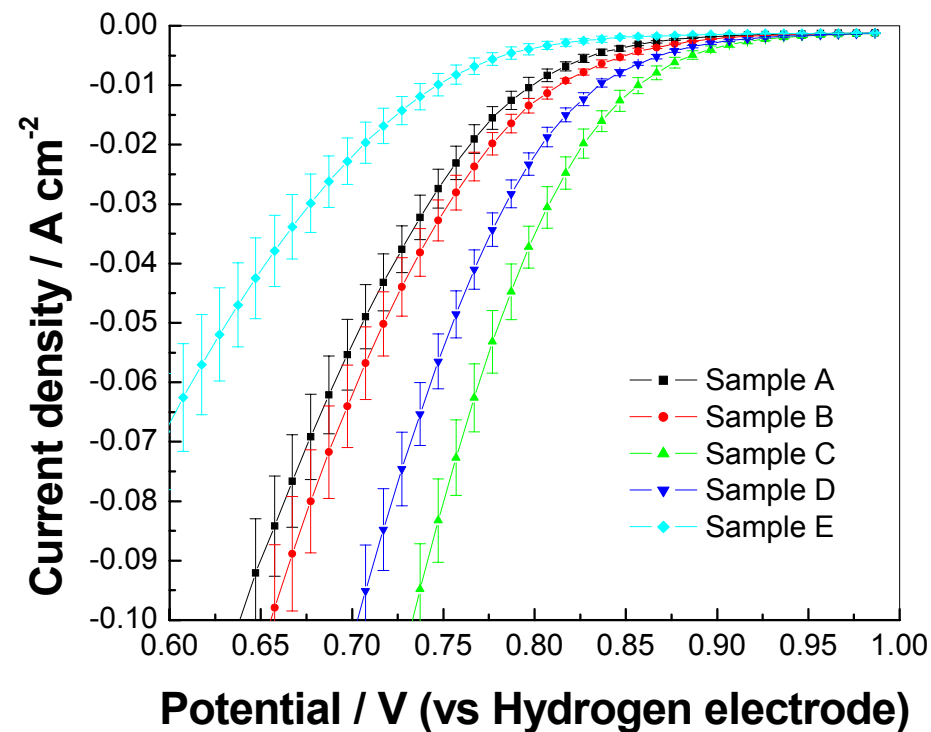
- For the same sample, the polarization curves at different spots are very close.

# Screening of 5 catalysts (A-E) at 60°C with O<sub>2</sub>

(a) Full polarization curves at 25 spots



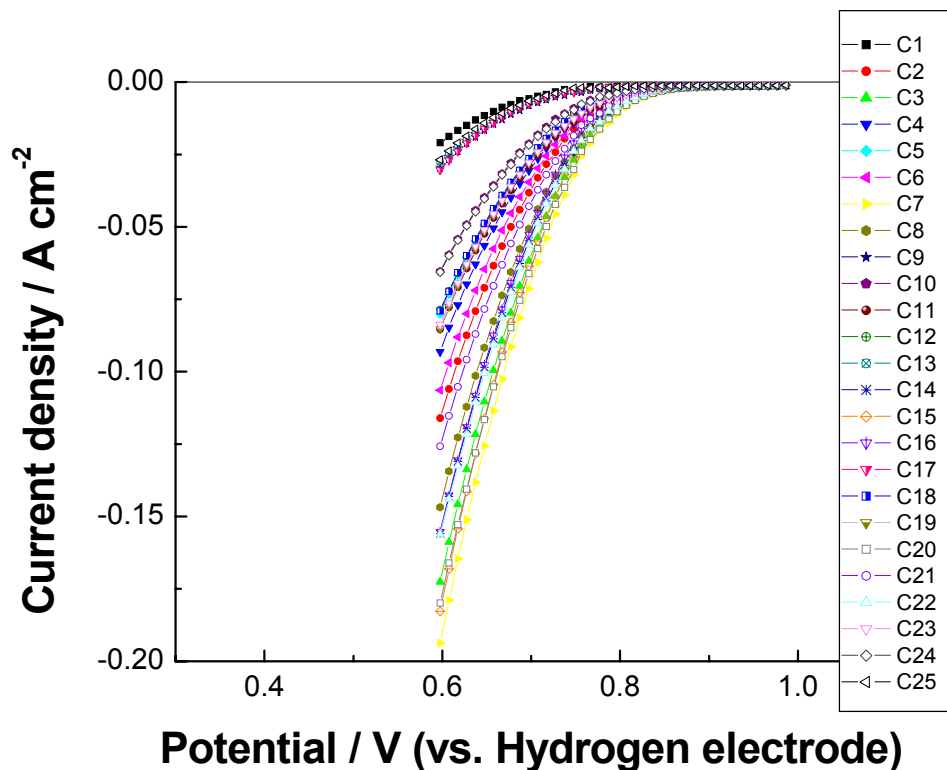
(b) Mean value curves for sample A-E



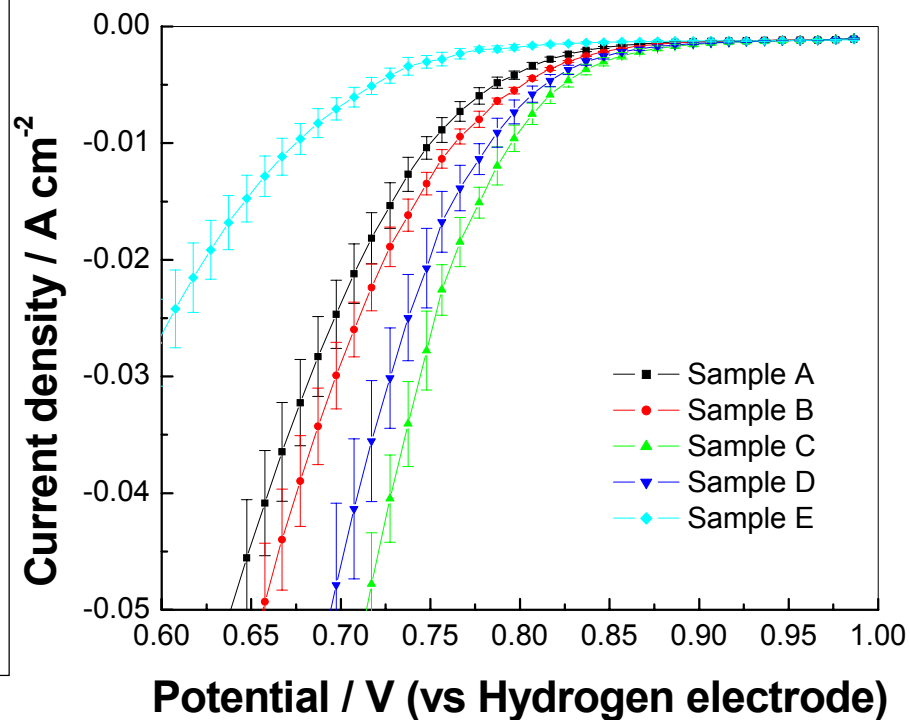
• Ranking at 0.80 V: C>D>B>A>E

# Screening 5 catalysts (A-E) at 80 °C with air

(a) Full polarization curves at 25 spots



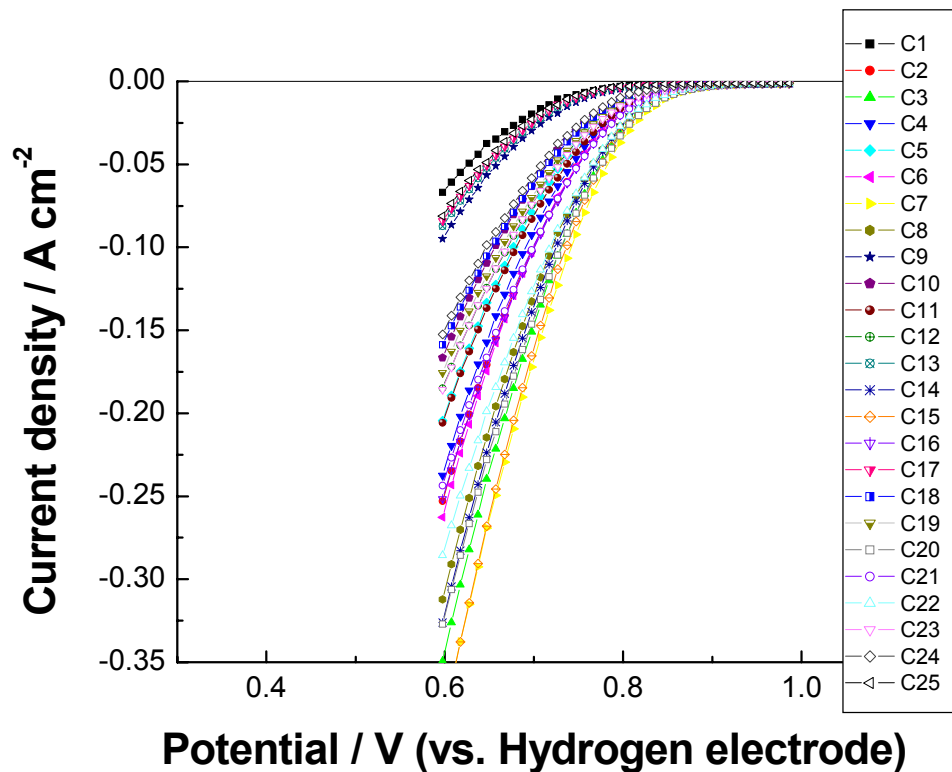
(b) Mean value curves for sample A-E



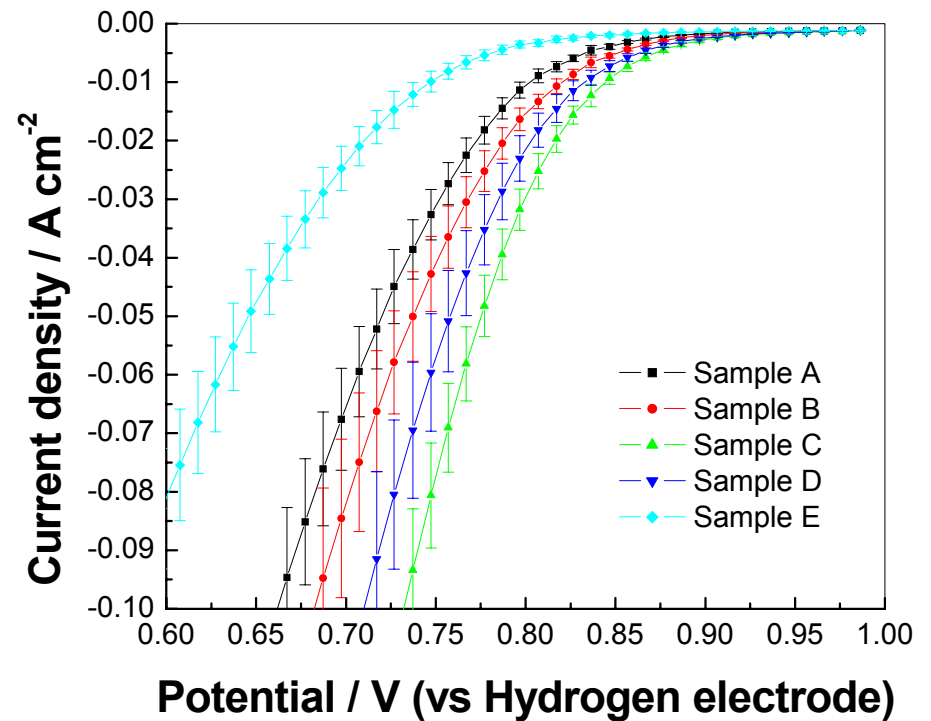
- Ranking at 0.80 V: C>D>B>A>E

# Screening % catalysts (A-E) at 80 °C with O<sub>2</sub>

(a) Full polarization curves at 25 spots



(b) Mean value curves for sample A-E



- Ranking at 0.80 V: C>D>B>A>E

## Conclusions

- The NUV100P system, a 25-channel potentiostat and a serpentine flow field, has been validated for high precision screening of cathode catalysts.
- Catalysts can be screened at temperatures ranging from room temperature to 80°C, in air or oxygen.

## Conclusions (contd..)

- Five different cathode catalysts were ranked using NuVant's NUV100P system composed of a 25-channel potentiostat and a serpentine flow field
- The rankings for the five catalysts at 0.80 V follow  $C > D > B > A > E$ , and remain the same at 60°C and 80°C, independent upon the air or oxygen.
- These rankings show high precision and validate the screening system.

# Future Work

- Remainder of FY 2004
  - High throughput synthesis and activation of the catalysts on the robot-controlled work station
  - High throughput screening of the samples above
  - Optimization of the conditions for the synthesis multi-component catalysts
- FY 2005
  - Continuous combinatorial screening of catalysts
  - Size-controlled synthesis of five promising candidates
  - Demonstration of the five candidates with optimized size in a single cell
  - Develop and utilize heuristic rules for the development of next generation PEMFC cathode catalysts



# Publications and Presentations

E. S. Smotkin, J. Jiang, A. Nayar, S. Chung, R. Liu, High-throughput screening of fuel cell electrocatalysts, Applied Surface Science, submitted 2005.

# Hydrogen Safety

The most significant hydrogen hazard associated with this project is:

Possible fire hazard with fuel side.

# Hydrogen Safety

Our approach to deal with this hazard is:

We place hydrogen cylinder and oxygen cylinders 10 ft apart and have flash arrestors at the inlets of the fuel cell. Outlet gases are vented to a fume hood that vents to the outside of the lab.