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

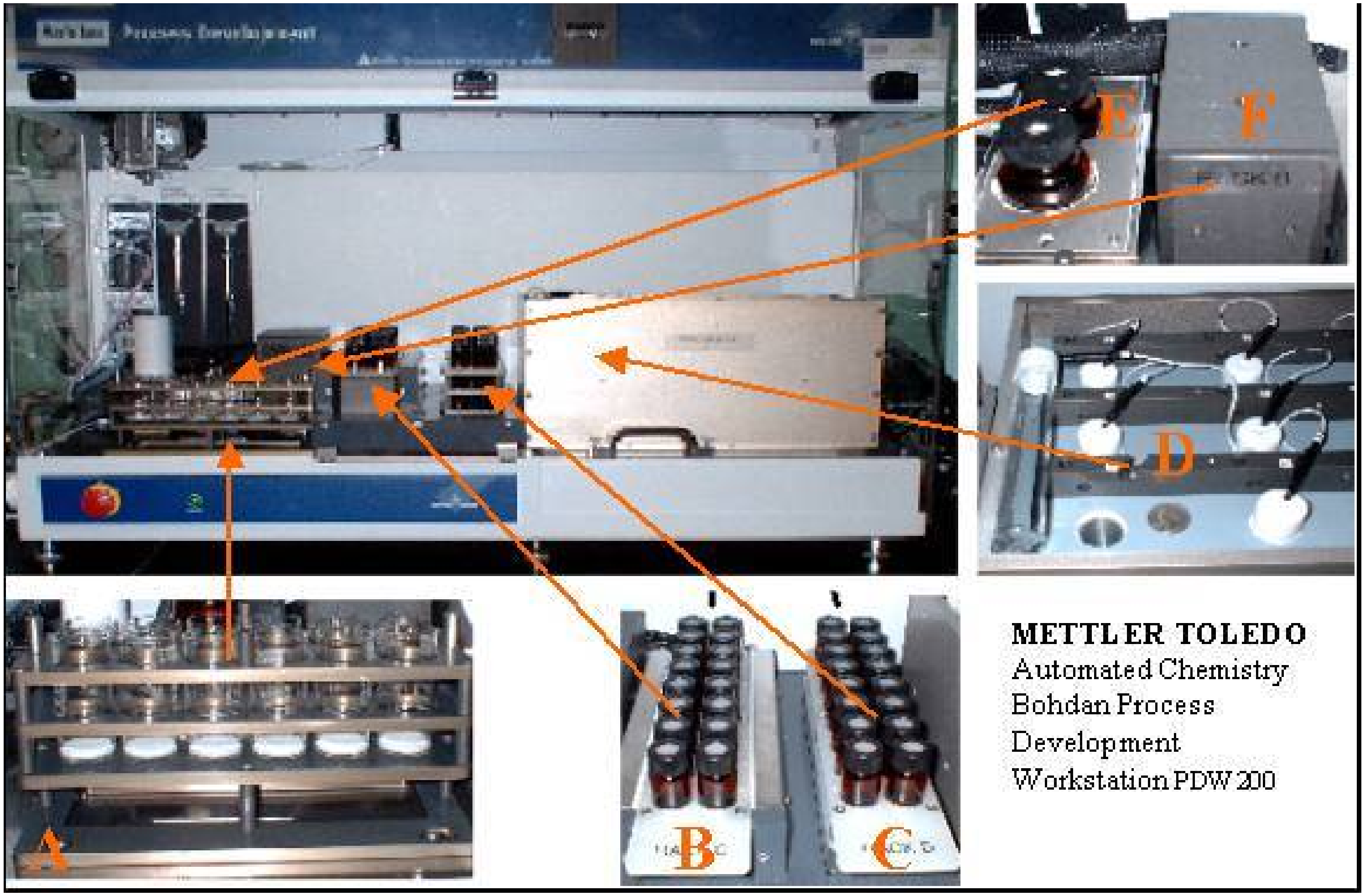
Assist DOE in the discovery of a PEMFC cathode catalyst with an order-of magnitude improvement over state-of-art catalysts to decrease the cathode cost and improve cathode performance.

- **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

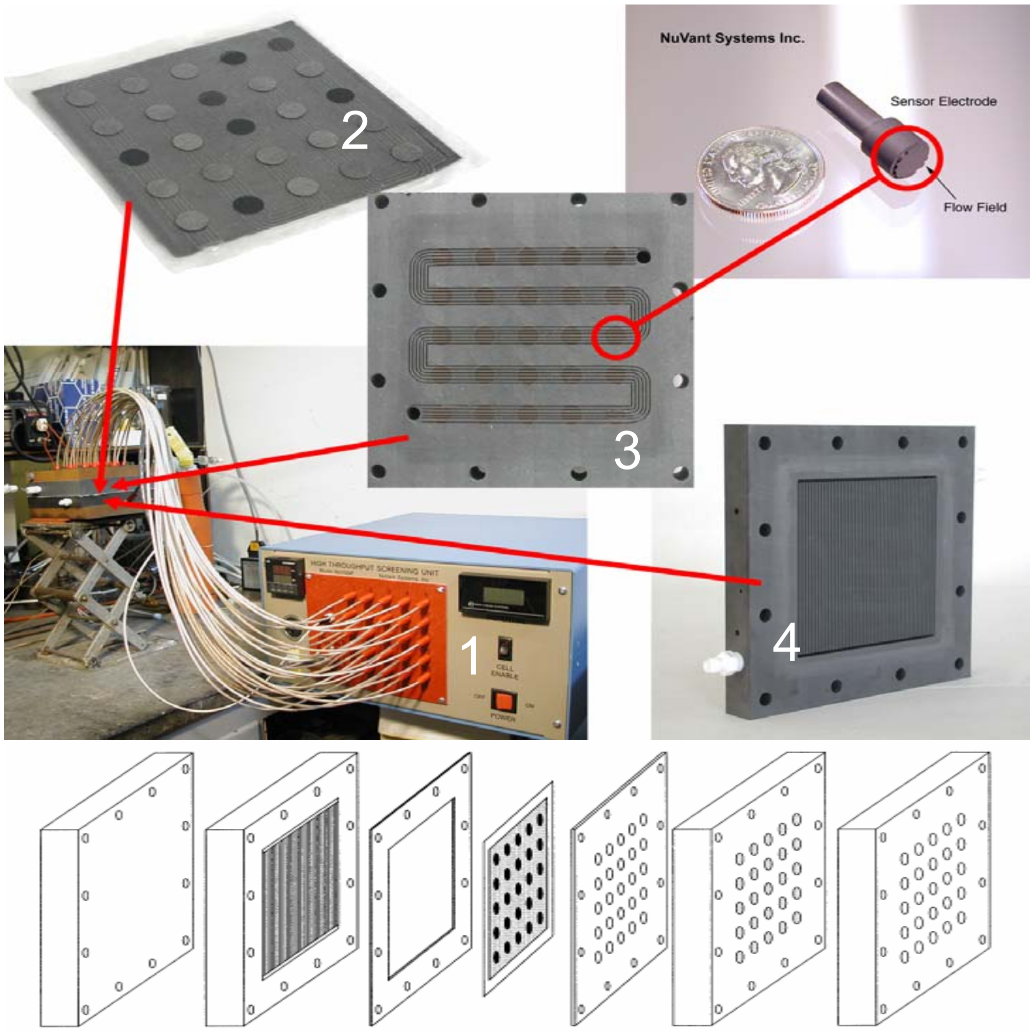
- Development of revolutionary cathode catalysts for the PEMFC through an integrated discovery program
  - Efficient factorial search strategies
  - High throughput synthesis using customized process control robotics
  - High throughput focus screening
  - Development of synthetic routes
- Demonstration 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.

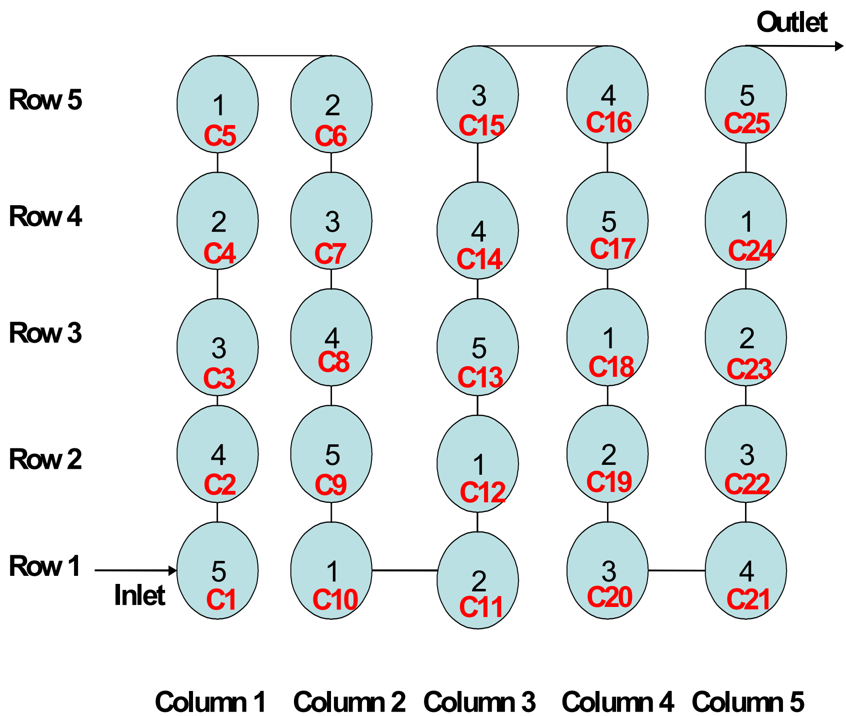
Conditions for control experiments

Loadings:
Sample 1: 2.02 mg cm^{-2}, JM 20 wt%Pt/C
Sample 2: 2.01 mg cm^{-2}, JM 20 wt%Pt/C
Sample 3: 2.05 mg cm^{-2}, JM 20 wt%Pt/C
Sample 4: 2.02 mg cm^{-2}, JM 20 wt%Pt/C
Sample 5: 2.03 mg cm^{-2}, JM 20 wt%Pt/C
Counter electrode: 2 mg cm^{-2} JM 20 wt%Pt/C

Operating conditions:
Cell temperature: 60 ^{o}C
Oxygen/air side: 1000 SCCM O_2/air with sparger 60 ^{o}C and tube 60 ^{o}C
Hydrogen side: 200 SCCM with sparger 65 ^{o}C and tube 65 ^{o}C

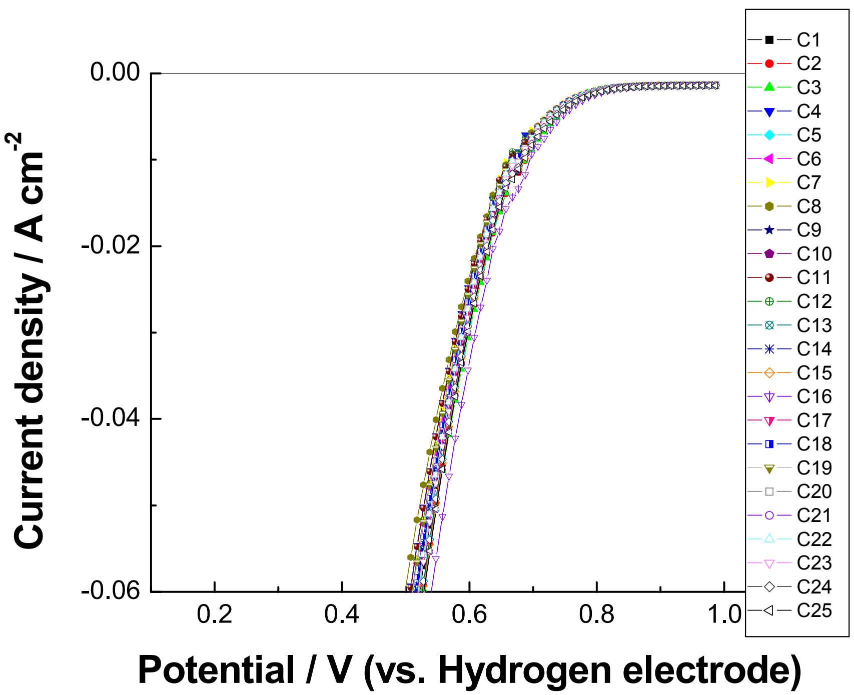
Measurement
Scanning potential from 1.0 to 0.60 V at 10 mV s^{-1}

Sample maps (Latin square sample design)

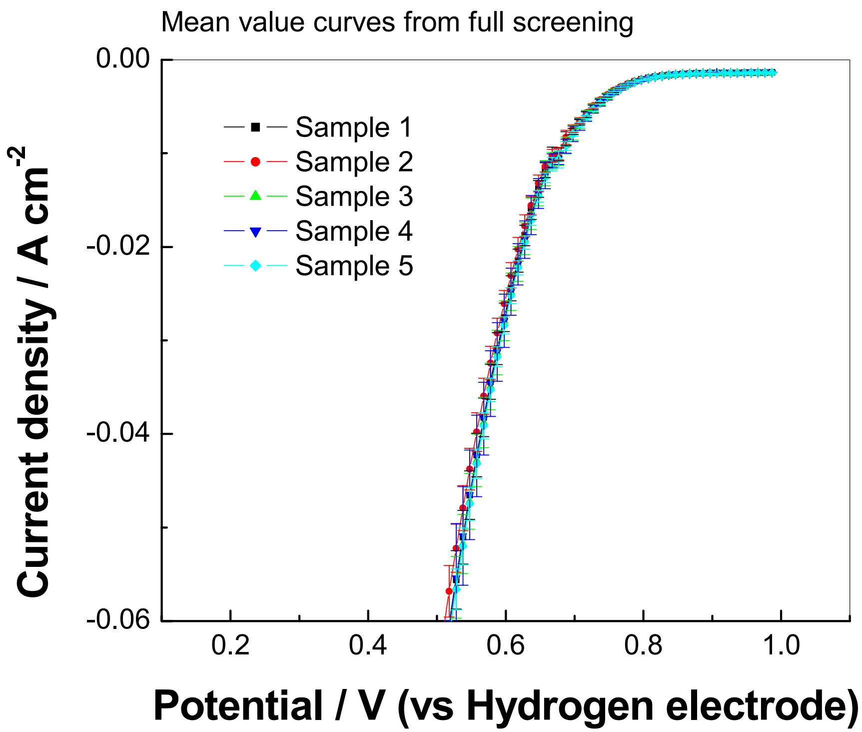


Data for H_2-Air control experiment

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



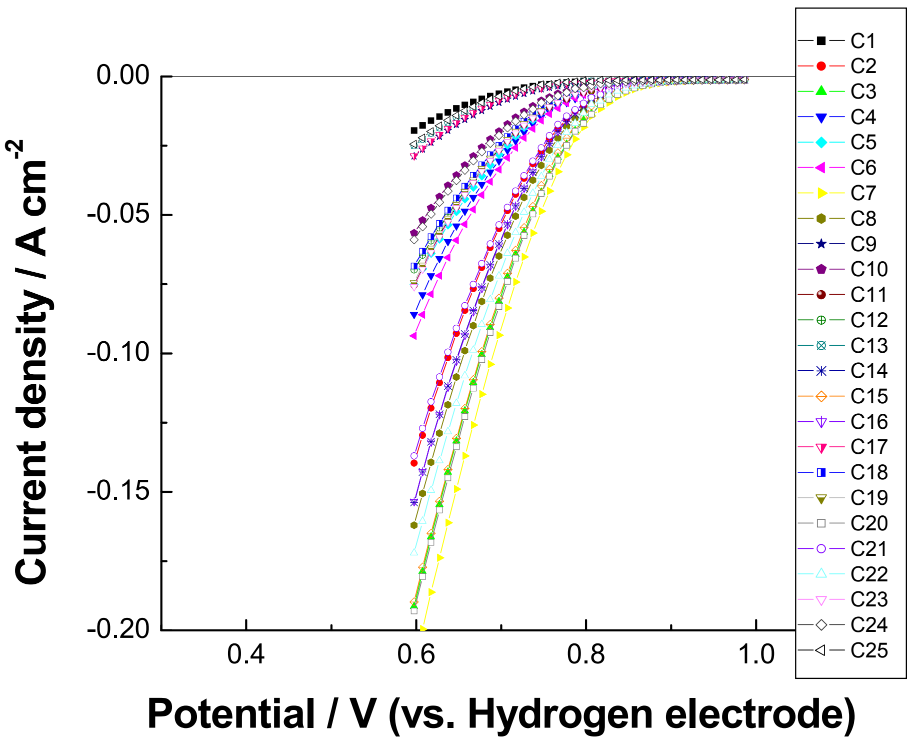
(b) Mean value curves for sample 1-5



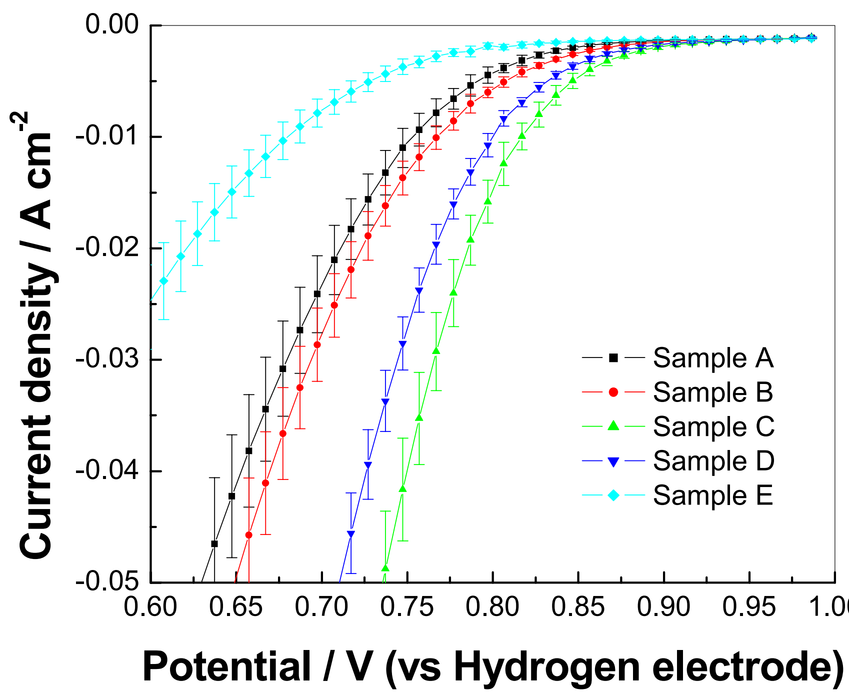
- **Good uniformity is obtained at 25 spots in the control experiments.**
- **The mean value curves for five samples are very close.**
- **Difference of 10 % in the activity can be distinguished at 0.80 V where the reaction is in kinetic control.**

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

(a) Full polarization curves at 25 spots

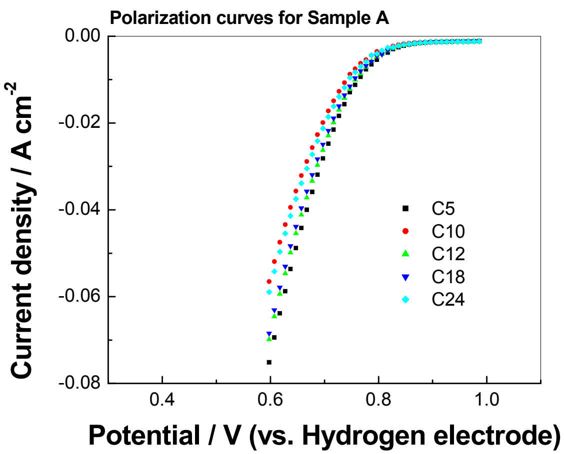


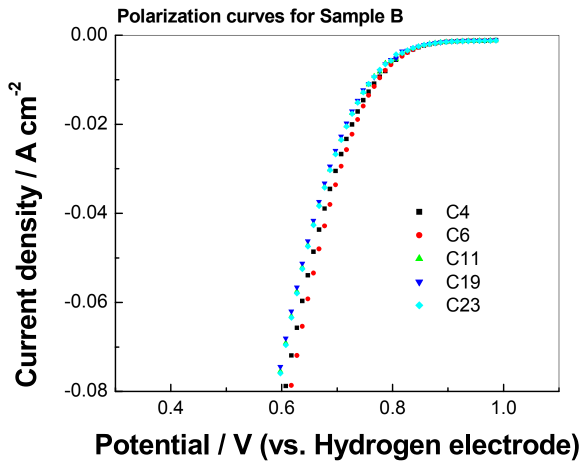
(b) Mean value curves for sample A-E

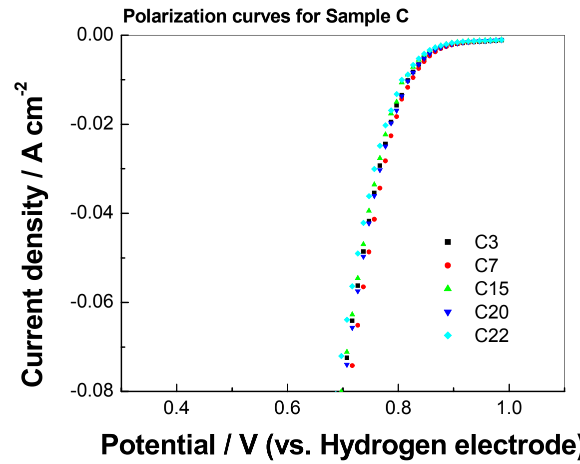


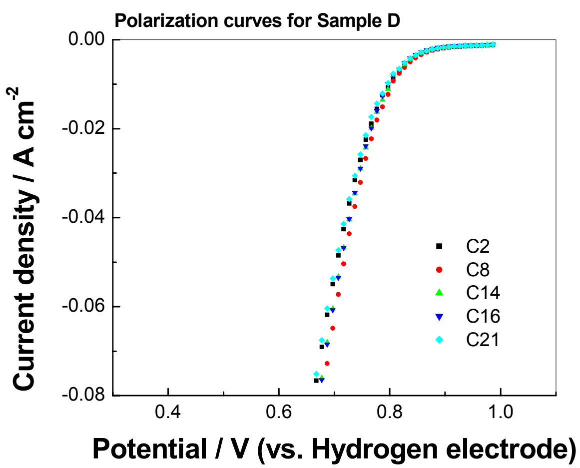
- Five samples are arranged in a 5x5 Latin square
- Good uniformity is obtained for each sample
- The ranking at 0.80 V for five samples is: C>D>B>A>E

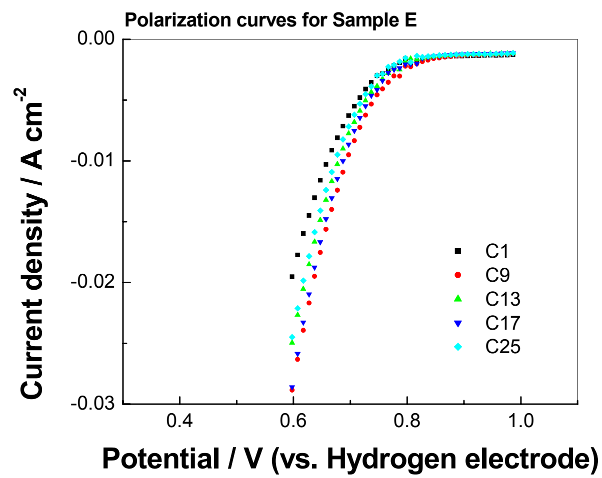
One example of polarization curves for individual sample at 60 °C and with air







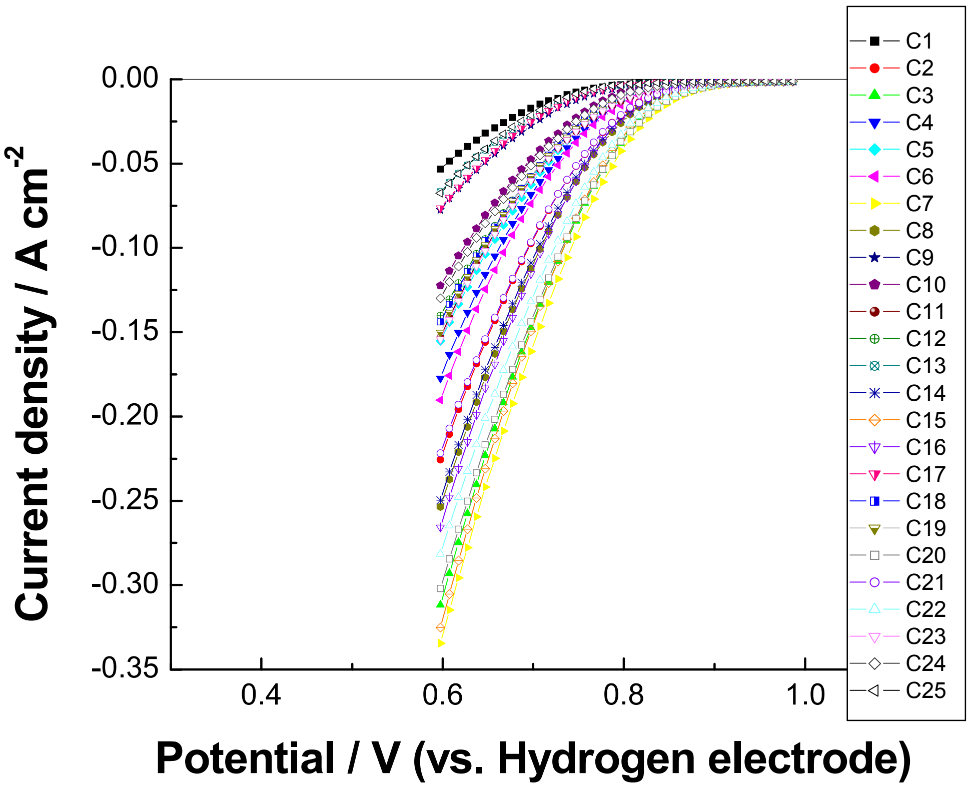




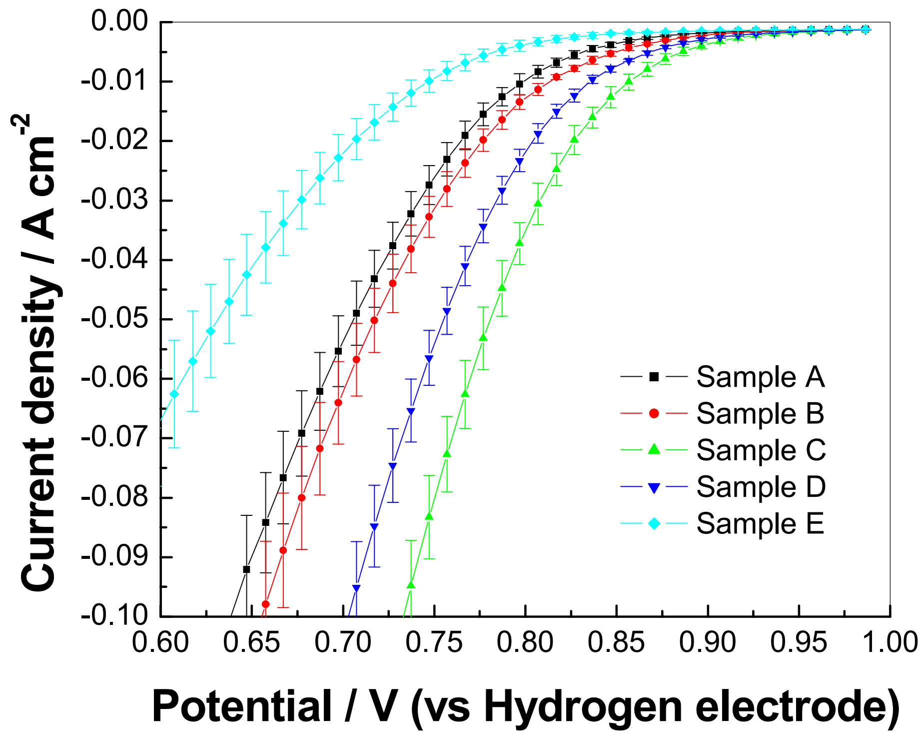
- **For the same sample, the polarization curves at different spots are very close.**

Screening of 5 catalysts (A-E) at 60˚C with O_2

(a) Full polarization curves at 25 spots



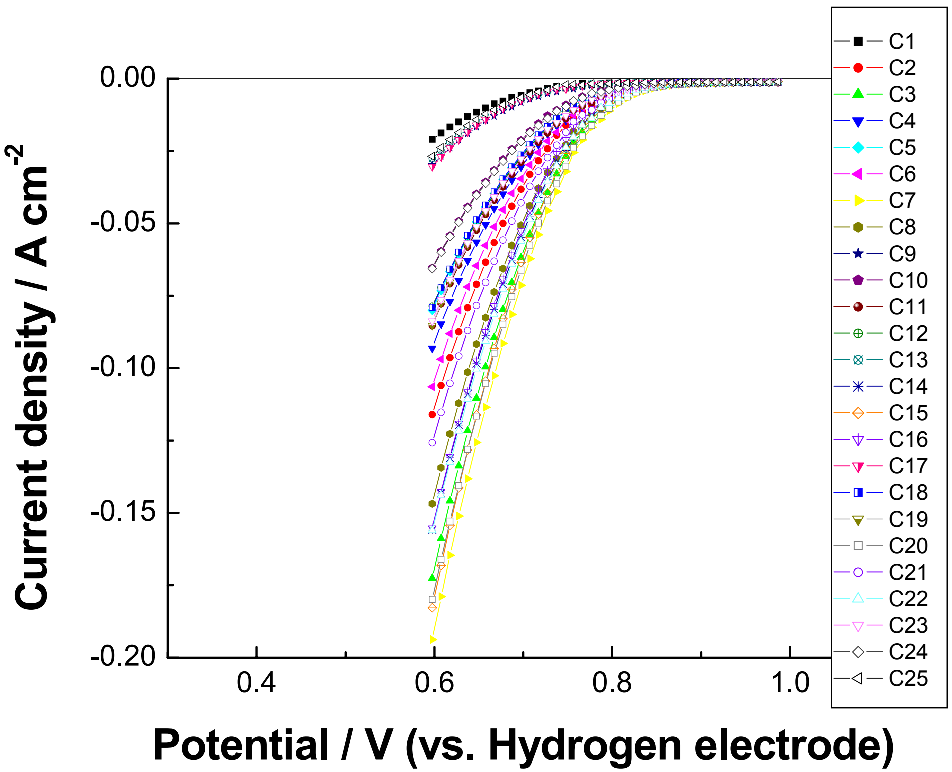
(b) Mean value curves for sample A-E



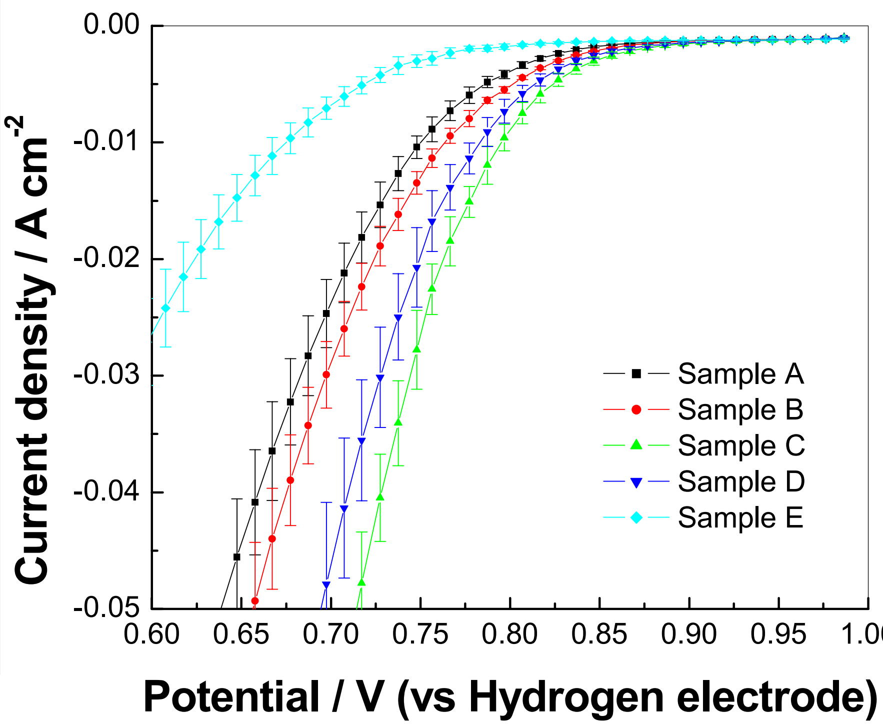
- **Ranking at 0.80 V: C>D>B>A>E**

Screening 5 catalysts (A-E) at 80 ^{o}C with air

(a) Full polarization curves at 25 spots



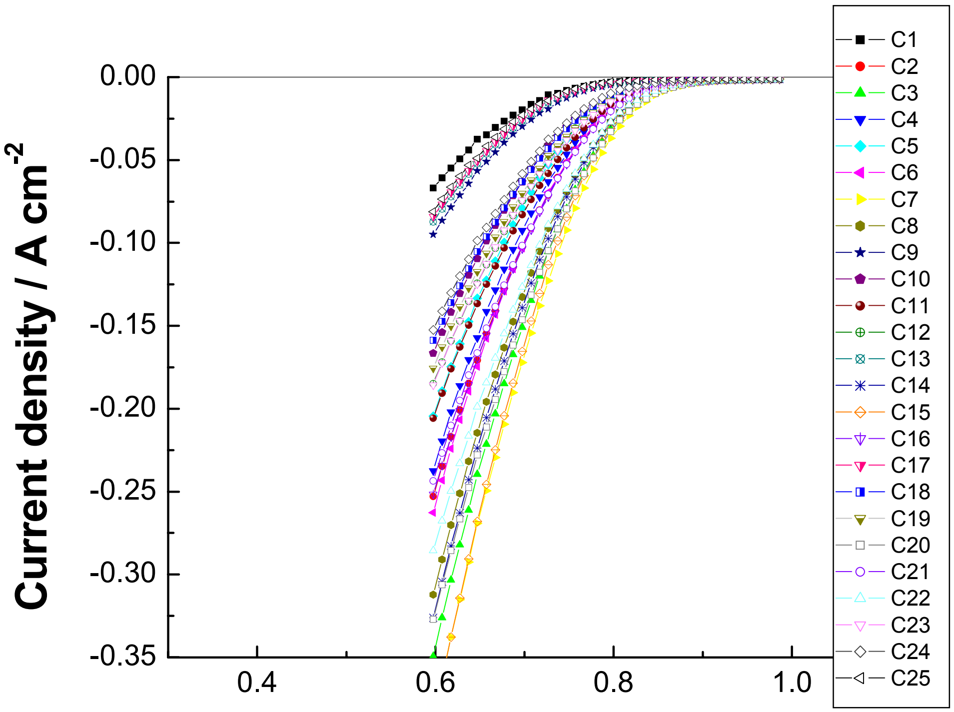
(b) Mean value curves for sample A-E



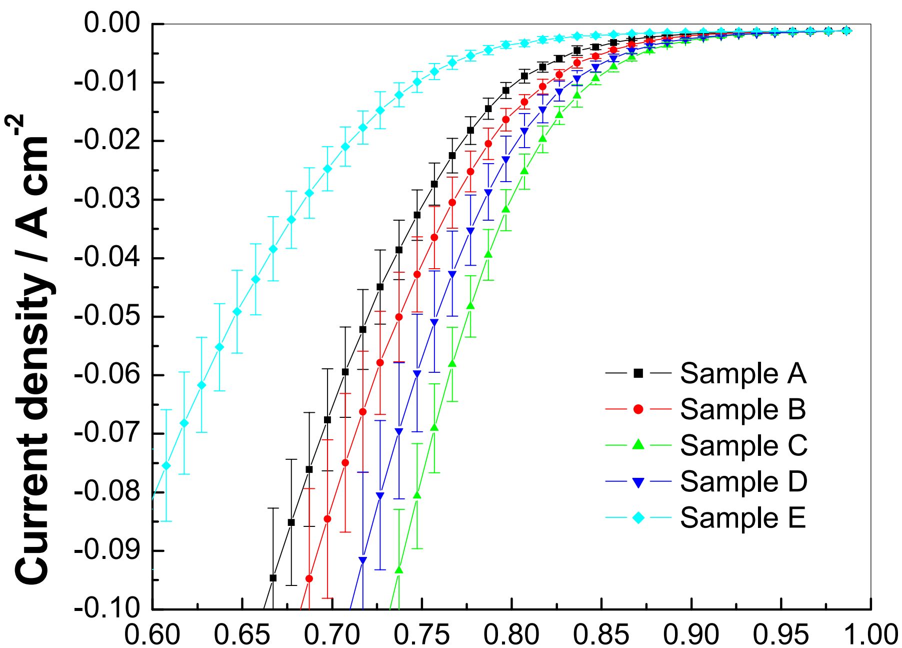
- **Ranking at 0.80 V: C>D>B>A>E**

Screening % catalysts (A-E) at 80 °C with O_2

(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^{o}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^{o}C and 80^{o}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.