Experimental Validation of Model of Electro-Chemical-Mechanical Planarization (ECMP) of Copper

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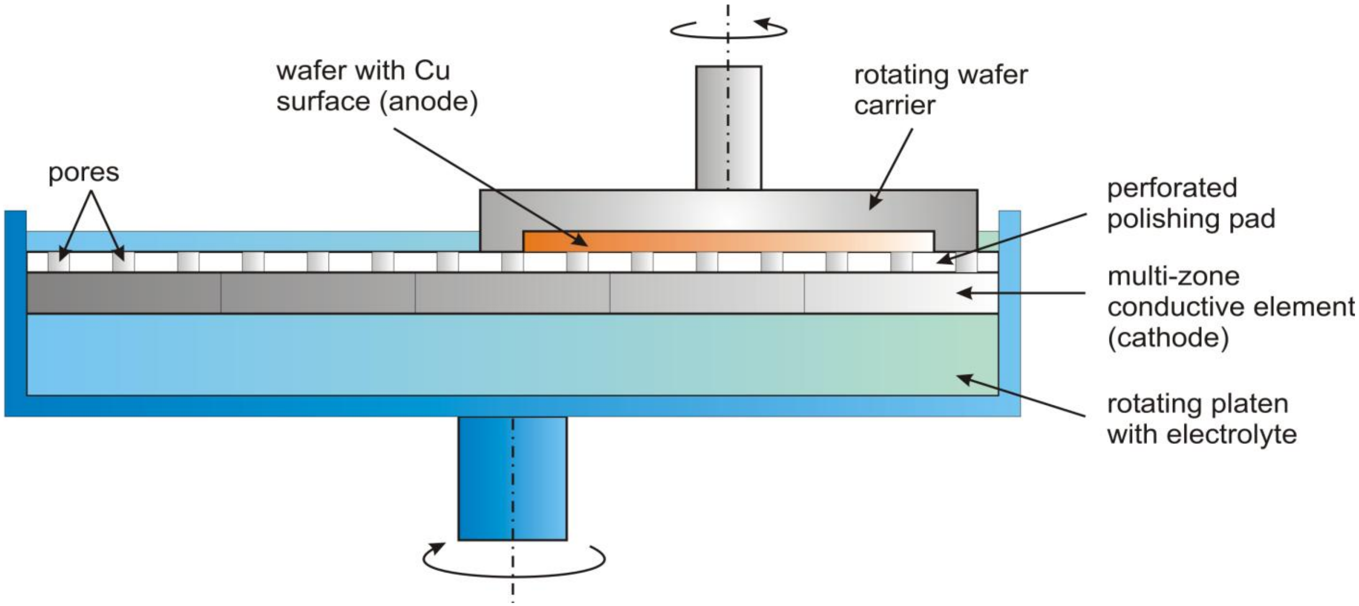
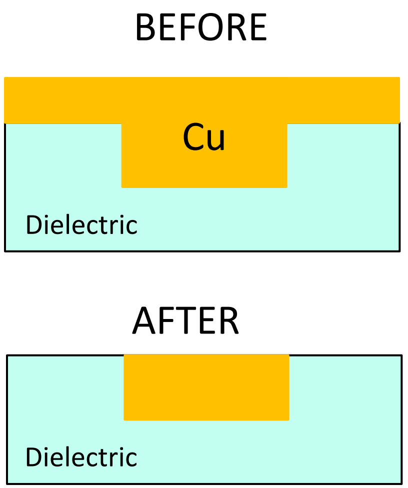
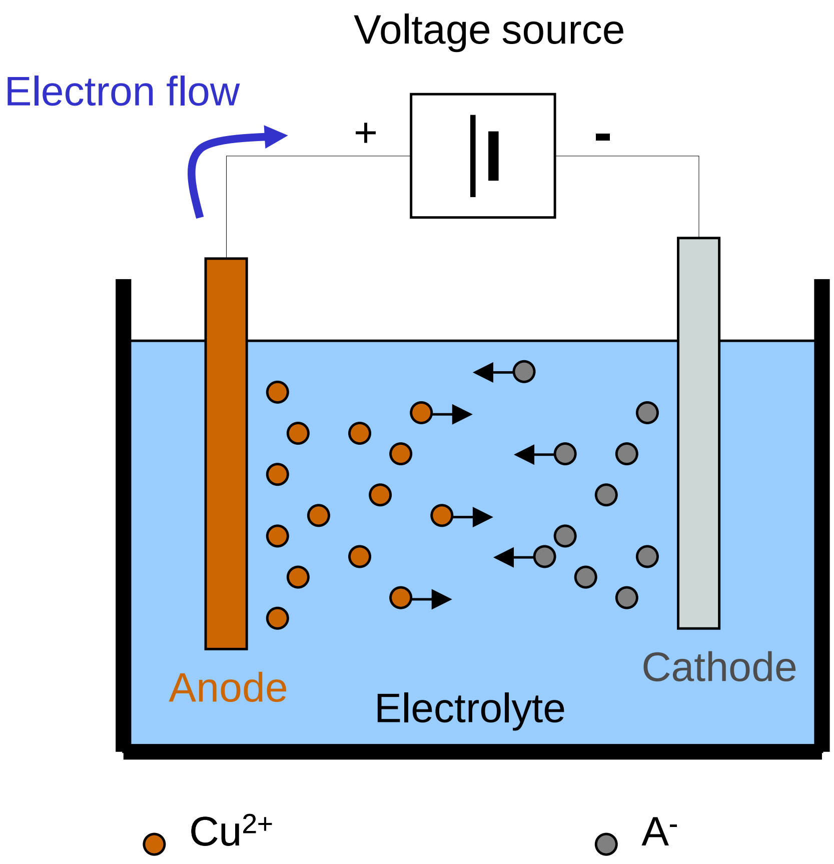
Overview of ECMP Process and Equipment





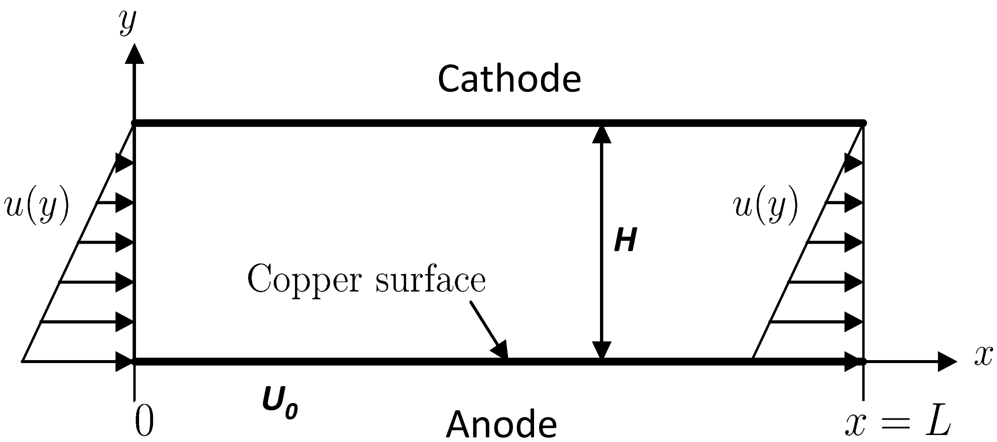
- **Electro-Chemical Mechanical Planarization (ECMP) is used for polishing semiconductor wafers as part of the IC fabrication process.**
- **ECMP uses a combination of mechanical pressure, chemical reaction, and electrochemistry to remove the metallic (copper) layers between steps such as thin film deposition and etch.**
- **Unlike conventional Chemical Mechanical Planarization (CMP), ECMP is more gentle on fragile low-k dielectric layers.**
- **The copper layer acts as anode and the conductive layer on polishing pad acts as cathode with a thin layer of electrolyte flowing between the rotating pad and wafer.**

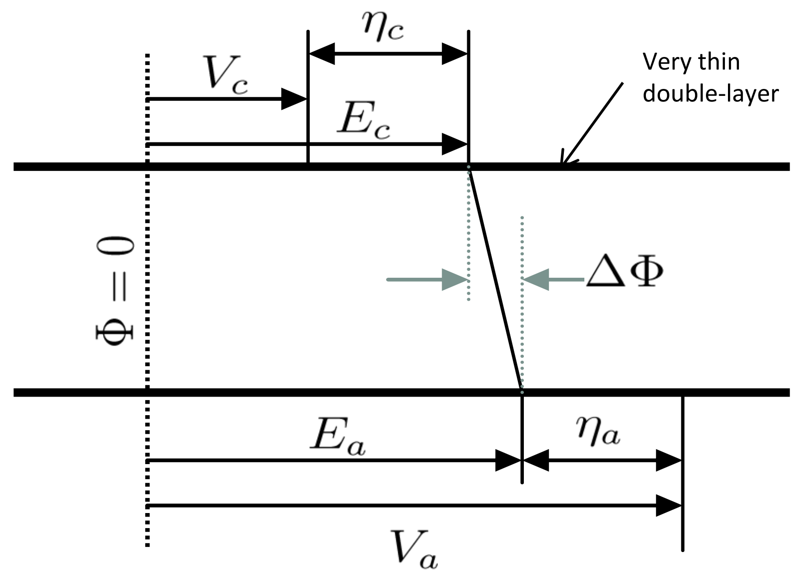
ECMP Electrochemistry



- Anode is copper film on wafer.
- Cathode is on the pad.
- As voltage rises, copper ions (Cu^{2+}) are generated at anode.
- Cu^{2+} at anode surface combines with water to form a copper complex according to the *acceptor model* (Vidal and West, 1995 and Suni and Du, 2005):
  $Cu + 6H_2O \leftrightarrow [Cu(H_2O)_6^{+}]^{2+} + 2e^-$
- Dissociation reaction of phosphoric acid (electrolyte):
  $H_3PO_4 + H_2O \leftrightarrow H_2PO_4^- + H_3O^+$
  The hydronium ion, H_3O^+, migrates to cathode and is reduced to hydrogen.

2D Geometry for ECMP Model





2D geometry for ECMP model in COMSOL:

- 2D geometry is sufficient to test our ability to model ECMP process with sufficient accuracy for control purposes.
- Flow conditions shown in the figure on left. Electrolyte flow enters from the left.
- Polishing occurs at the copper anode (bottom “wall”) which is moving at velocity U_0 with respect to the pad (top “wall”).
- Electrical boundary conditions shown in figure on right.

ECMP Equations

Species

$$c_1 = [H_2O], \quad z_1 = 0$$
$$c_2 = [Cu(H_2O)_6^{2+}], \quad z_2 = 2$$
$$c_3 = [H^+], \quad z_3 = 1$$
$$c_4 = [H_2PO_4^-], \quad z_4 = -1$$

Species Conservation

$$\nabla \cdot \mathbf{N}_i = 0, \quad i = 1, 2$$
$$\mathbf{N}_i = -\kappa_i \nabla \Phi - D_i \nabla c_i + c_i \mathbf{v}$$
$$\kappa_i = z_i D_i F c_i / RT$$

Electrolyte Potential

$$\nabla \cdot \left[-\kappa \nabla \Phi - F \sum_i z_i D_i \nabla c_i \right] = 0$$
$$\kappa = (F^2/RT) \sum_i z_i^2 D_i c_i$$

Dissociation/Charge Neutrality

$$c_3 = -c_2 + \sqrt{c_2^2 + k}$$
$$c_4 = k/c_3$$
$$k = K_a[H_3PO_4]$$

Anode and Cathode Reaction

$$Cu(s) + 6H_2O \leftrightarrow [Cu(H_2O)_6]^{2+} + 2e^-$$

Anode B.C.'s (input V_a)

$$\mathbf{N}_2 \cdot \hat{y} = \frac{i_0}{zF} \left[\exp\left(\frac{\alpha_a F}{RT}\eta_s\right) - \exp\left(-\frac{\alpha_c F}{RT}\eta_s\right) \right]$$
$$\mathbf{N}_1 \cdot \hat{y} = -6\mathbf{N}_2 \cdot \hat{y}$$

Butler-Volmer Equation

$$\Phi = E$$

where

$$E = E^o - \frac{RT}{nF} log\left(\frac{c_2}{c_1^6}\right)$$

Nernst Equation

$$\eta_s = V_a - E$$

Cathode B.C.'s (input V_c)

$$\mathbf{N}_2 \cdot \hat{y} = \frac{i_0}{zF} \left[\exp\left(\frac{\alpha_a F}{RT}\eta_s\right) - \exp\left(-\frac{\alpha_c F}{RT}\eta_s\right) \right]$$
$$\mathbf{N}_1 \cdot \hat{y} = -6\mathbf{N}_2 \cdot \hat{y}$$
$$\Phi = E$$

where

$$E = E^o + \frac{RT}{nF} log\left(\frac{c_2}{c_1^6}\right)$$
$$\eta_s = V_c - E$$

Inlet Flow Boundary

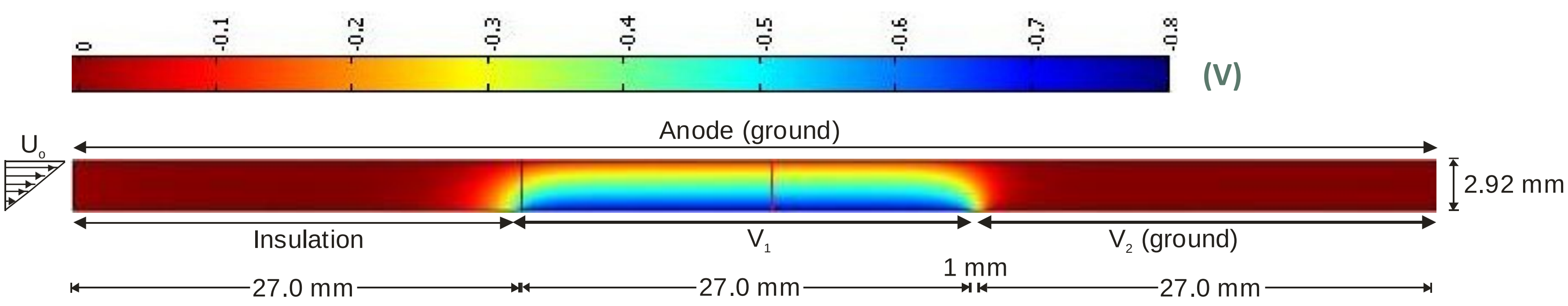
$$c_1 = c_{1,0}$$
$$c_2 = c_{2,0}$$
$$\partial \Phi / \partial x = 0$$

Outlet Flow Boundary

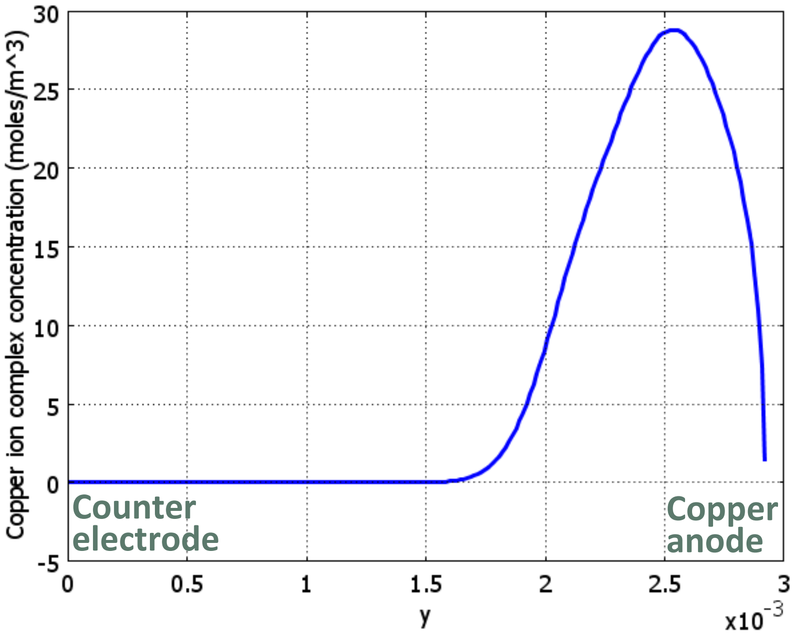
$$\mathbf{N}_1 \cdot \hat{x} = u c_1$$
$$\mathbf{N}_2 \cdot \hat{x} = u c_2$$
$$\partial \Phi / \partial x = 0$$

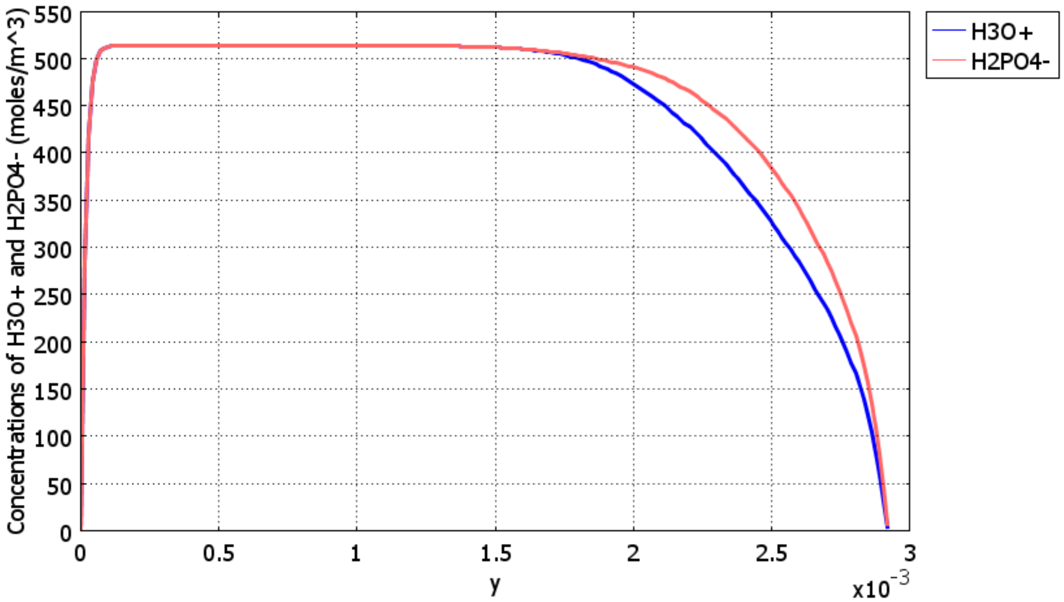
2D COMSOL Model for ECMP

- **COMSOL's PDE Interface was used to specify the equations and boundary conditions for electrochemistry, while the Physics Interface was used to specify the species transport problem.**
- **A simple 2D geometry for ECMP model allowed focus on electrochemistry.**
  - **Electrolyte flow enters from the left with linear velocity profile.**
  - **Polishing occurs at the copper anode (top "wall") which is moving at velocity U_0 with respect to the cathode on the pad (bottom "wall").**
  - **1 mm gap of insulation between the segmented counter-electrodes on the pad with voltages V_1 and V_2.**



COMSOL Model Results

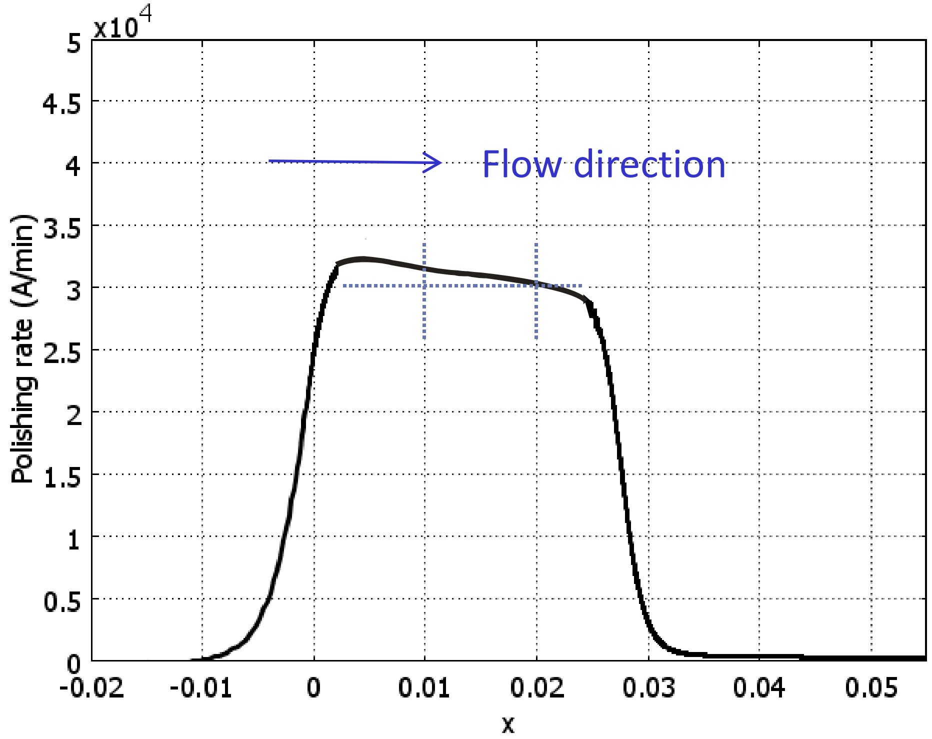




- Molar concentration of $Cu(H_2O)_6^{2+}$ in the vertical (*y*) direction at *x* = 15 mm.
- Copper complex concentration maximum just below the anode where $Cu(H_2O)_6^{2+}$ diffuses to add to that generated upstream.

- Molar concentrations of $H_2PO_4^-$ and H_3O^+ in *y* direction.
- Both species concentrations near the anode where water is depleted to form the copper complex.

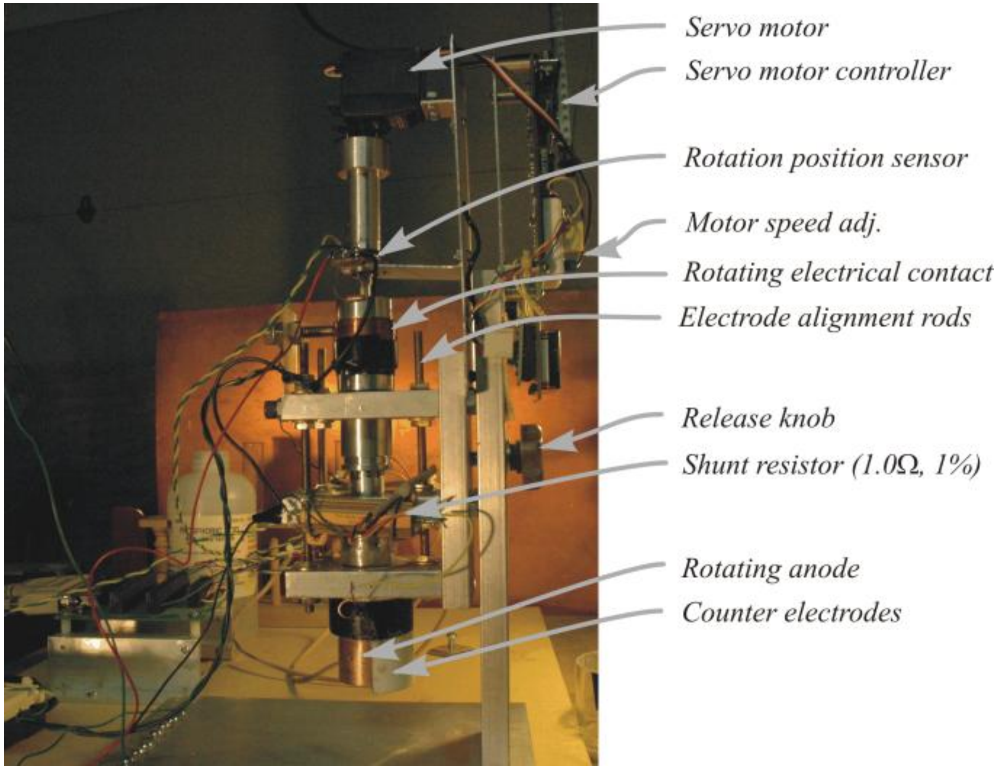
COMSOL Model Results (Continued)

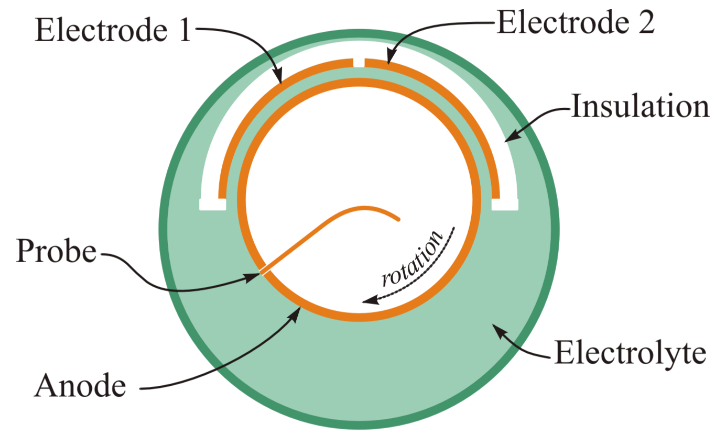


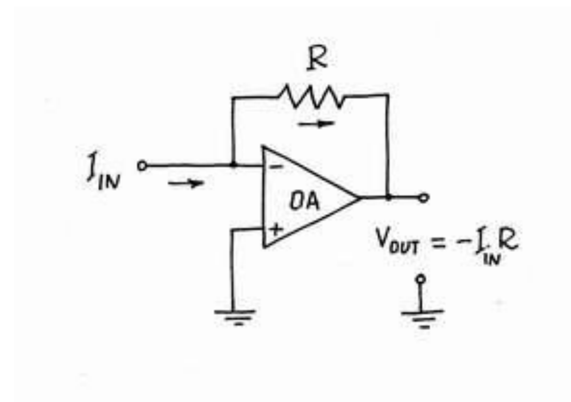
- **Copper polish rates in Å/minute computed from the gradient of the copper complex flux at anode.**

- **Rate decreases in flow direction as available water decrease.**

Experimental Validation of COMSOL Model



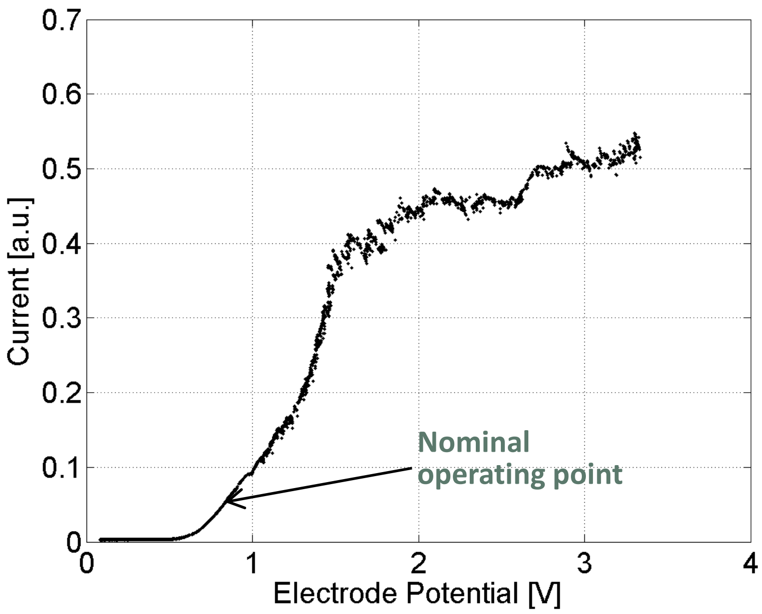




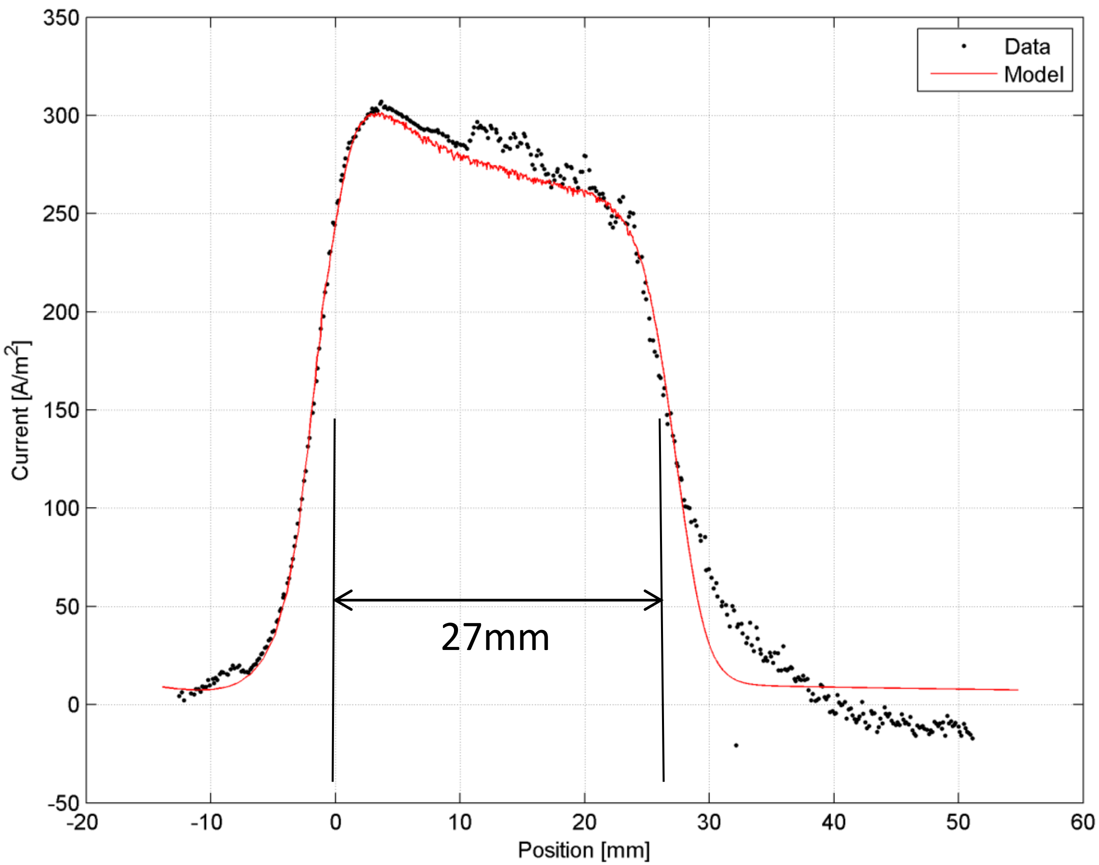
Experimental apparatus:

- Cylindrical copper electrode (anode) and two adjacent partial cylindrical electrodes (Electrode 1 and 2).
- Rotating anode is a copper cylinder of approx. 32 mm diameter.
- Wire probe in cylinder wall measures current distribution.

Experimental Validation of COMSOL Model (Continued)



- **Electrode 1 current *vs.* voltage from anode to counter-electrode.**
- **Linear region between 0.6 V and 1.3 V.**
- **Noise increases with voltage due to increased evolution of hydrogen at counter-electrode.**



Anode current along electrode. Counter-electrode at 0.8 V. Very good agreement between experimental data and COMSOL model prediction.

Summary and Conclusions

- **We have developed a COMSOL model of the ECMP process that incorporates copper dissolution and species transport in the electrolyte, ion transport including convection, diffusion, and migration, and electrodic reactions represented by the Butler-Volmer equation.**

- **Model predicts removal rate and uniformity as a function of electrolyte concentration and applied voltage.**

- **A successful experiment was conducted to validate this model. Good agreement seen between COMSOL model predictions and measured anode current.**

- **Reduced-order version of this validated physical model may now be used for developing multivariable feedback control of ECMP.**