Modelling and Simulation of Porous Silicon Membrane based Fuel Cell

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Introduction: Miniature hydrogen fuel cell based on porous silicon has the potential to power miniature electronics more efficiently as it is easier for it to be integrated on a silicon chip. In such fuel cell, porous silicon acts as proton conducting membrane, Pt layer over porous silicon as anode catalyst and Si substrate over which porous silicon is formed as cathode.

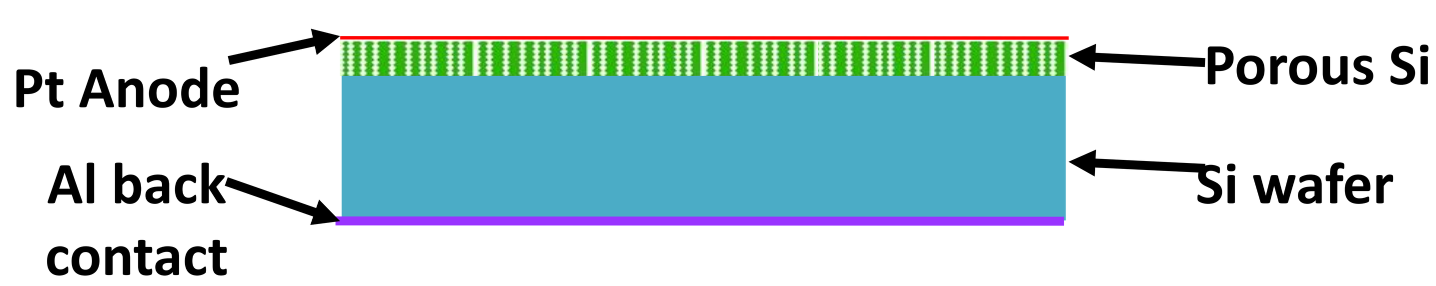


Figure 1. Schematic of fuel cell device

Computational Methods: Pt Anode, Si Cathode catalyst and Porous Si membrane have to be of optimum thickness to obtain good open circuit voltage and current density from such fuel cell. PEM fuel cell model from the COMSOL application library was used and material, physics, and properties of the model were modified to mimic our fuel cell device. Multiple simulations were solved in COMSOL by varying parameters like anode thickness, membrane thickness, cathode thickness, H_2 gas mass flow rate and O_2 gas mass flow rate to find optimum parameters that may lead to the fabrication of good performance fuel cell.

Equations governing reacting flow in porous membrane:

$$\nabla \cdot \mathbf{j}_i + \rho(\mathbf{u} \cdot \nabla)\omega_i = R_i$$

$$\mathbf{N}_i = \mathbf{j}_i + \rho \mathbf{u} \omega_i$$

$$\mathbf{j}_i = -\left(\rho\omega_i \sum_k D_{ik}\mathbf{d}_k + D_i^T \frac{\nabla T}{T}\right)$$

$$\mathbf{d}_k = \nabla x_k + \frac{1}{p_A}[(x_k - \omega_k)\nabla p_A]$$

$$x_k = \frac{\omega_k}{M_k}M_n, \quad M_n = \left(\sum_i \frac{\omega_i}{M_i}\right)^{-1}$$

$$\rho(\mathbf{ua} \cdot \nabla)\mathbf{ua} = \nabla \cdot \left[-pa\mathbf{I} + \mu(\nabla\mathbf{ua} + (\nabla\mathbf{ua})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{ua})\mathbf{I}\right] + \mathbf{F}$$

$$\nabla \cdot (\rho\mathbf{ua}) = 0$$

$$\frac{\rho}{\epsilon_p}\left((\mathbf{ua} \cdot \nabla)\frac{\mathbf{ua}}{\epsilon_p}\right) = \nabla \cdot \left[-pa\mathbf{I} + \frac{\mu}{\epsilon_p}(\nabla\mathbf{ua} + (\nabla\mathbf{ua})^T) - \frac{2\mu}{3\epsilon_p}(\nabla \cdot \mathbf{ua})\mathbf{I}\right] - \left(\mu\kappa^{-1} + \beta_F|\mathbf{ua}| + \frac{Q_{br}}{\epsilon_p^2}\right)\mathbf{ua} + \mathbf{F}$$

$$\nabla \cdot (\rho\mathbf{ua}) = Q_{br}$$

Darcy's Law

$$\nabla \cdot (\rho\mathbf{u}) = Q_m$$

$$\mathbf{u} = -\frac{\kappa}{\mu}\nabla p2$$

Results: In present work through simulation we found that anode catalyst thickness to be kept at 300 nm, porous silicon membrane thickness to be kept below 20 µm, cathode catalyst thickness to be 200 µm and H_2 and O_2 gas flow mass fraction in the ratio of 0.8:0.6. With these parameters such fuel cell generates open circuit voltage upto 1.1 V and current density upto 700 mA/cm^2.

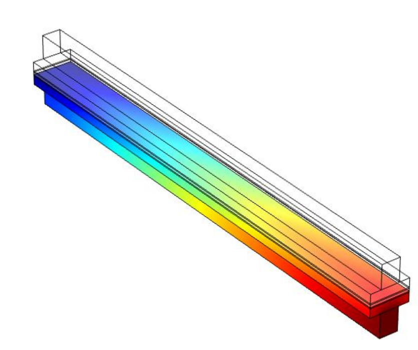
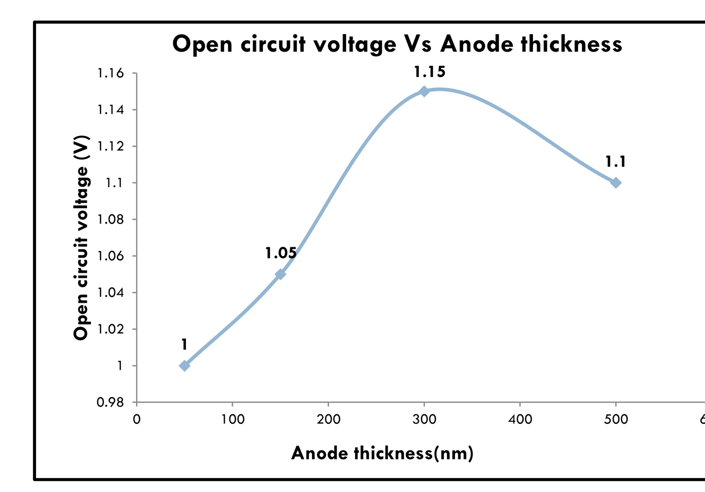
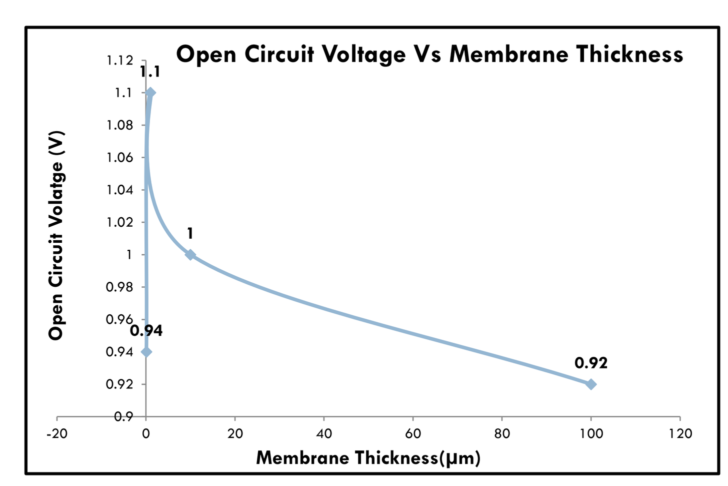
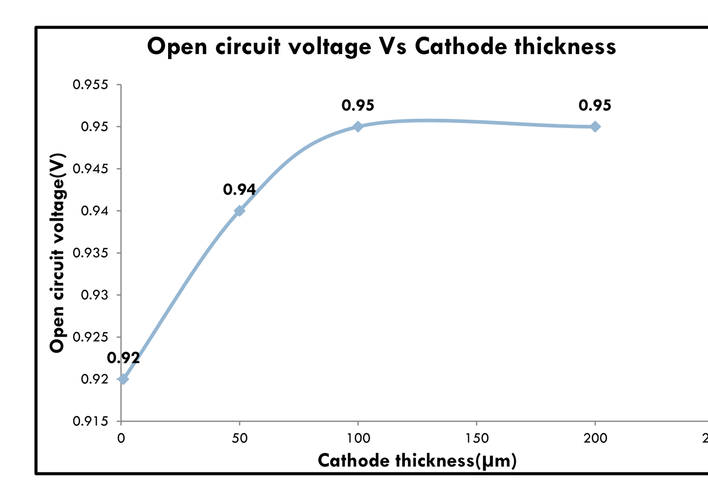
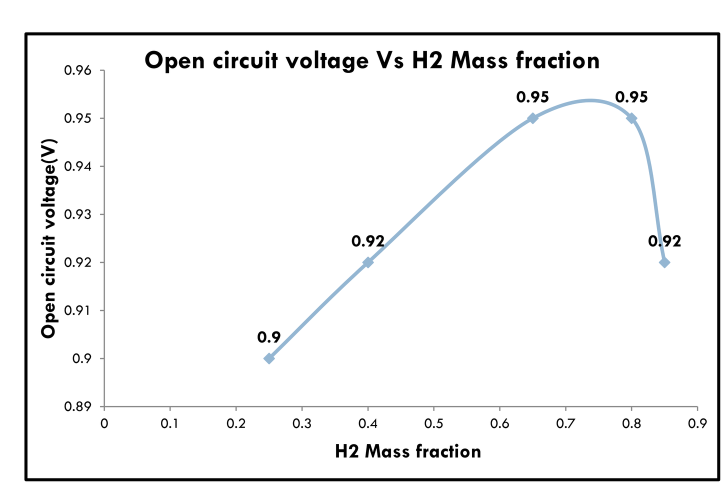


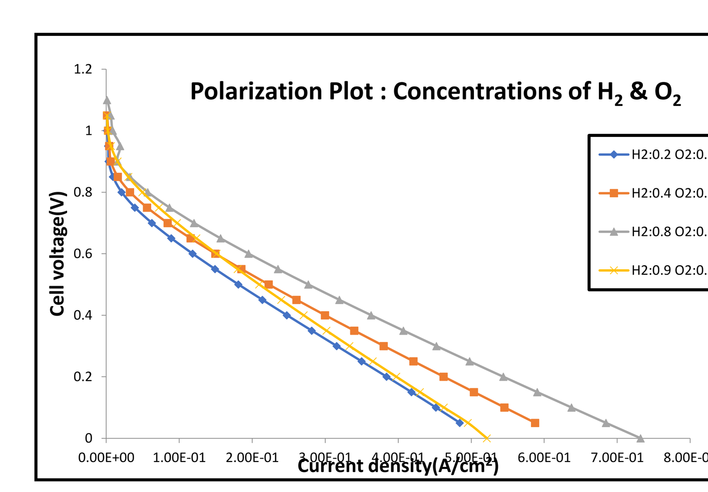
Figure 2. Anode H_2 Concentration in Fuel Cell Model











Conclusions: Open circuit voltage of 1.1 V and current density of 700mA/cm^2 against V_{OC} of 450 mV reported elsewhere from such fuel cell [1-3] is highly encouraging. Using the parameters obtained through COMSOL simulations, our fuel cell device is under fabrication currently. This device may find application in chip scale power for miniature electronics.

References:

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