COMSOL CONFERENCE EUROPE 2012

HOCHSCHULE FURTWANGEN UNIVERSITY HFU

Dynamic Simulation of Electrochemical Etching of Silicon with COMSOL

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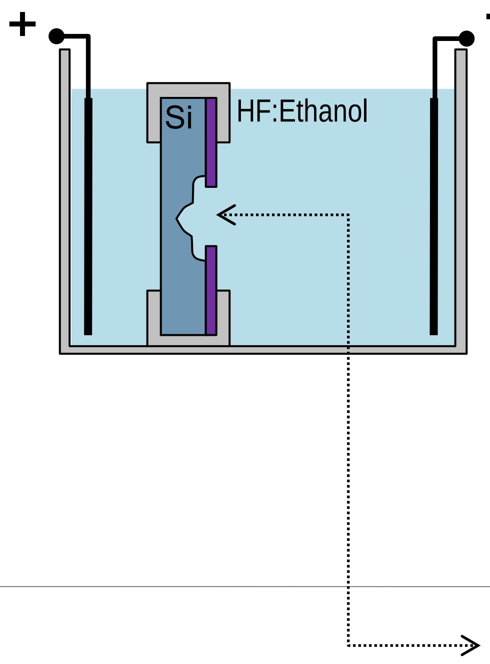
Contents

Electrochemical etching of silicon (anodization)



Chemical reactions:

Low current density: Formation of porous silicon via direct and selective dissolution of silicon atoms:

$$\mathrm{Si} + 4\mathrm{HF}_2^- + h^+ \rightarrow \mathbf{SiF_6^{2-}} + 2\mathrm{HF} + \mathrm{H}_2 + e^-$$

[V. Lehmann]

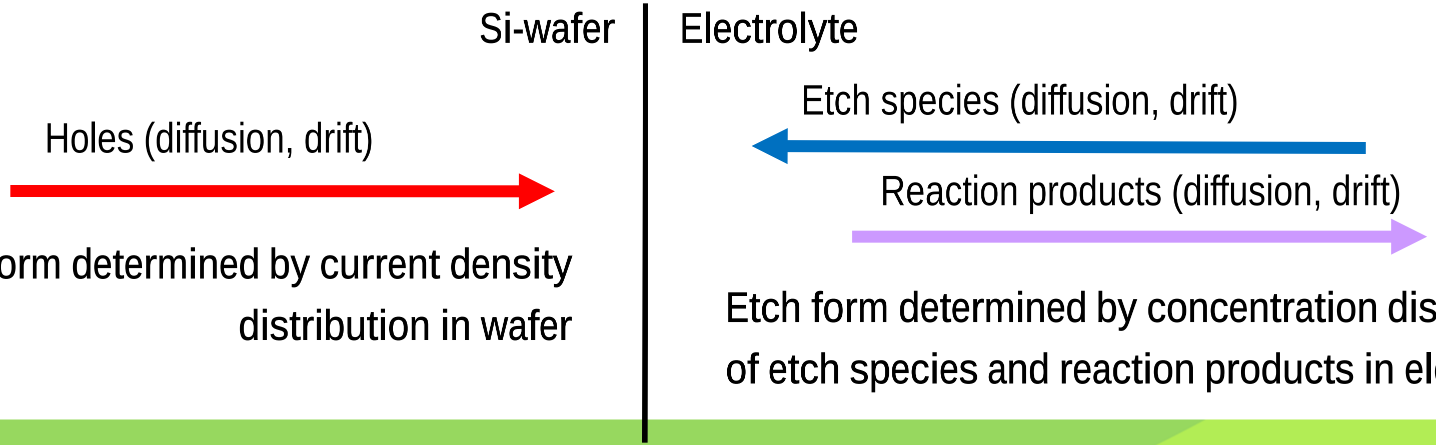
High current density: Electropolishing via silicon anodic oxidation and SiO_2-dissolution:

$$\mathrm{Si} + 2\mathrm{H_2O} + 4h^+ \rightarrow \mathbf{SiO_2} + 4\mathrm{H}^+$$

$$\mathrm{SiO_2} + 2\mathrm{HF}_2^- + \mathbf{2HF} \rightarrow \mathbf{SiF_6^{2-}} + 2\mathrm{H_2O}$$

[V. Lehmann]

At the boundary silicon-electrolyte:



Si-wafer

Holes (diffusion, drift)

Etch form determined by current density distribution in wafer

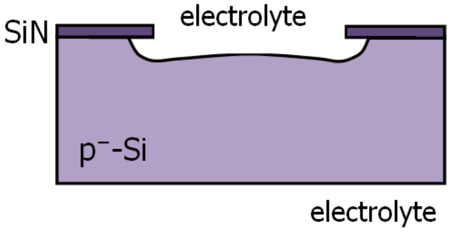
Electrolyte

Etch species (diffusion, drift)

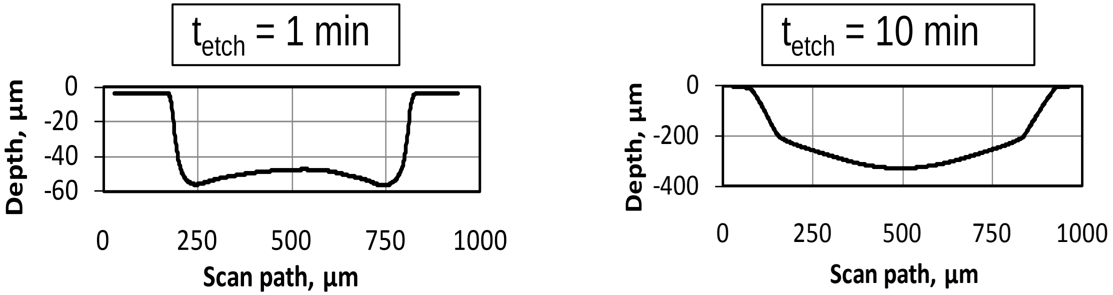
Reaction products (diffusion, drift)

Etch form determined by concentration distribution of etch species and reaction products in electrolyte

Etch form development in the anodization process

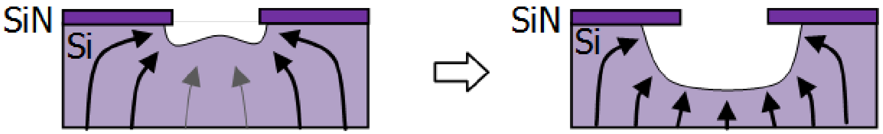


profile of a structure anodized through a 600 µm circular opening in a SiN masking layer in 30 wt.% HF at 2.5 A/cm²

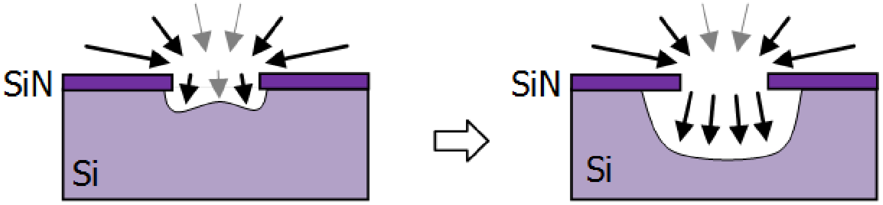


Effect of current distribution

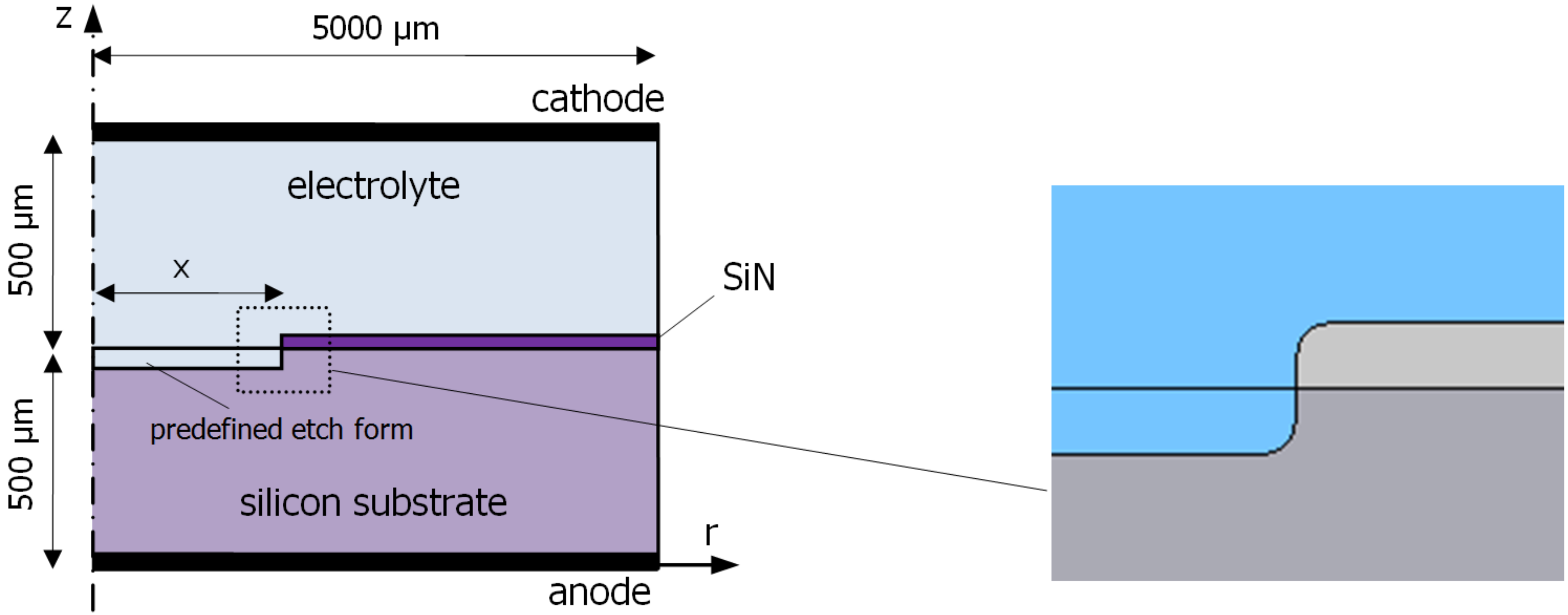
(arrows represent current flow)



Effect of diffusion-controlled etching process (arrows represent the flow of F-ions to the reaction site)



Model mesh and geometry



- The electrical and the diffusion models simulated in 2D with axial symmetry
- The movement of the etch front implemented with the moving mesh interface (ale)
- SiN layer thickness 1 µm, radius of the opening varied in the range 20 µm – 500 µm
- Predefined etch form of thickness 1 µm for enhanced mesh movement

Electrical model: parameters

Etch front movement (ale): $\upsilon_r = -K_E \cdot j_r$ $\upsilon_z = -K_E \cdot j_z$ $K_E = \frac{1}{z \cdot e} \cdot \frac{M_{Si}}{\rho_{Si} \cdot N_A}$

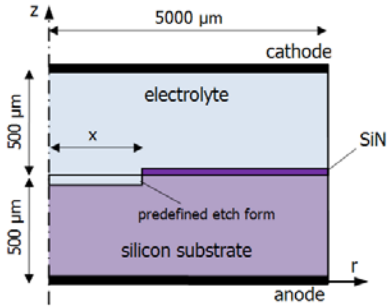
where *j* – current density, *z* - reaction valence, *e* - elementary charge,

M_{si} - silicon molar mass, ρ_{Si} - silicon density and N_A - Avogadro constant.

For the reaction valence of 4 (silicon dioxide formation): $K_E = 3{,}1234 \cdot 10^{-11} \, \frac{\mathrm{m}^3}{\mathrm{A \cdot s}}$

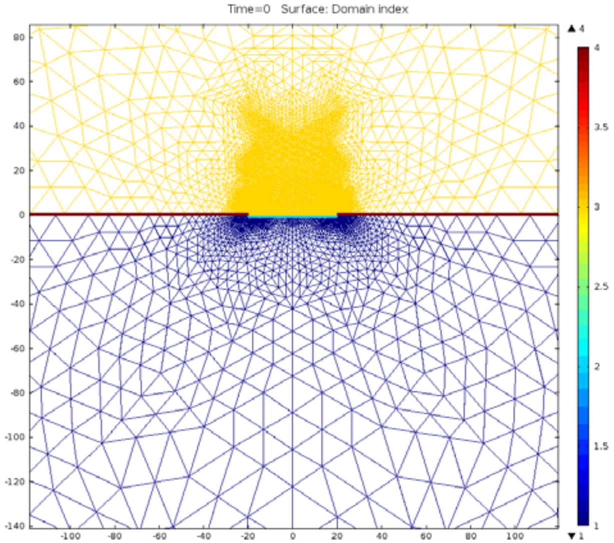
Material properties:

Domain	Electrical conductivity [S/m]	Relative permittivity
Electrolyte	$\sigma_{el.1} = 10^4$ $\sigma_{el.2} = 10$	80.1
Silicon	$\sigma_{Si} = 10$	11.1
Silicon nitride	0	7.5

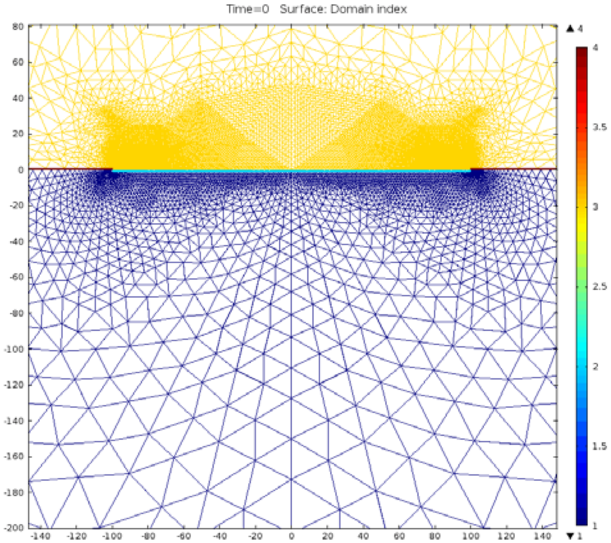


Electrical model: electrolyte with high conductivity σ_1

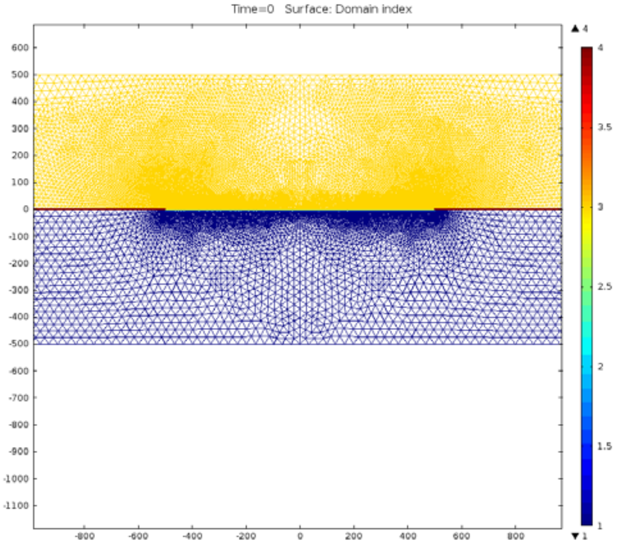
Opening diameter 40 µm



Opening diameter 200 µm



Opening diameter 1000 µm

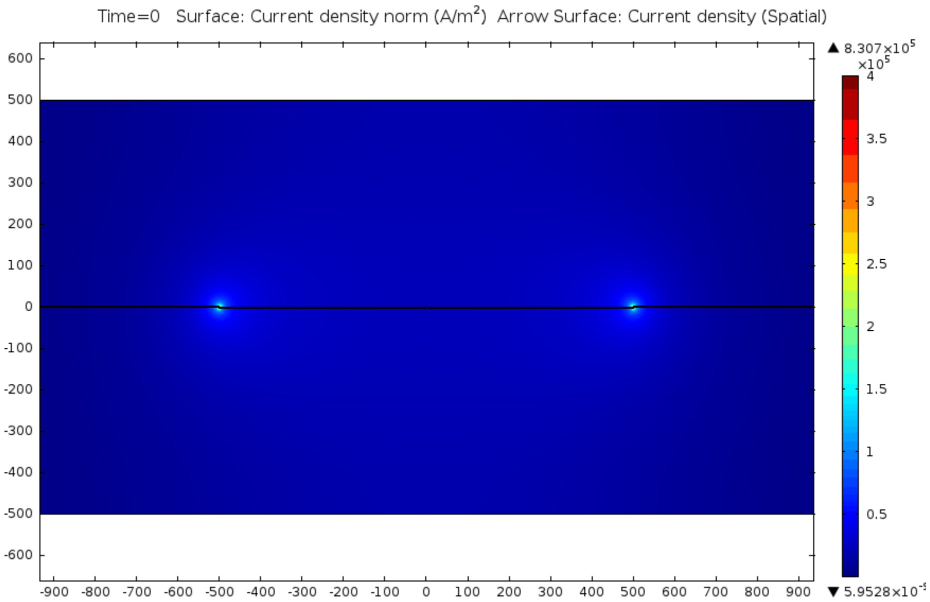


- No convex-concave form transformation
- Higher etching at the edges runs with self-amplification

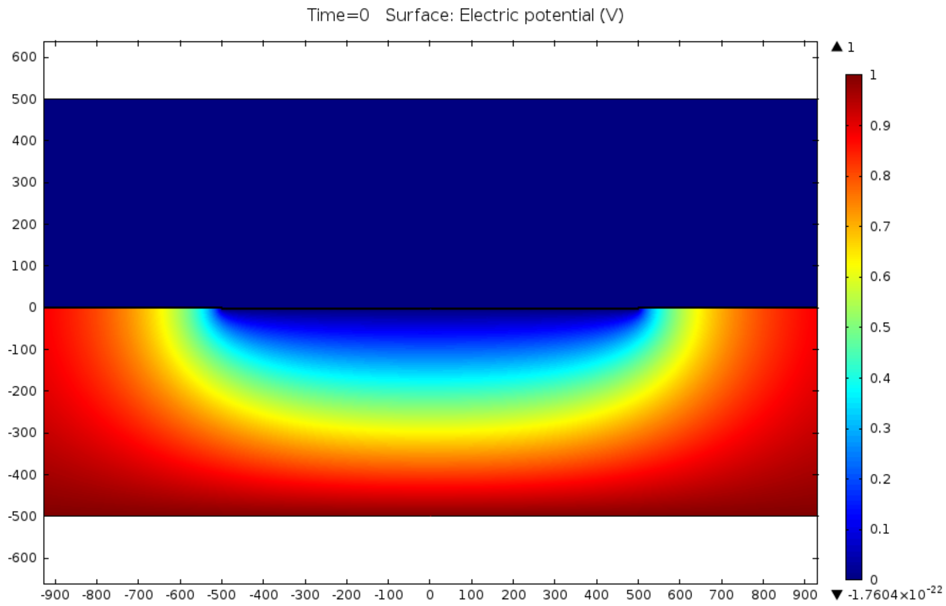
Electrical model: electrolyte with high conductivity σ_1

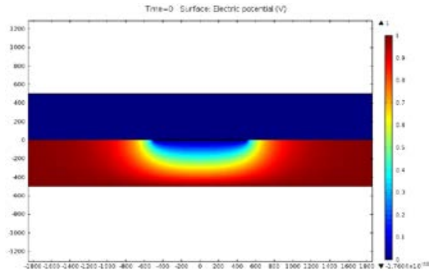
Opening diameter 1000 µm

Current density distribution



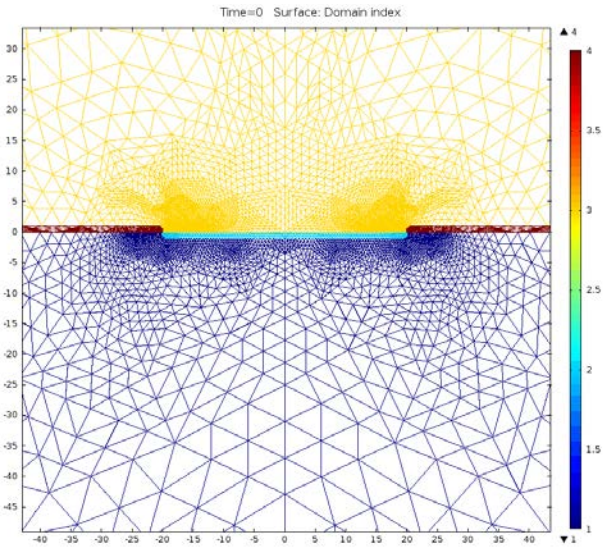
Electric potential distribution



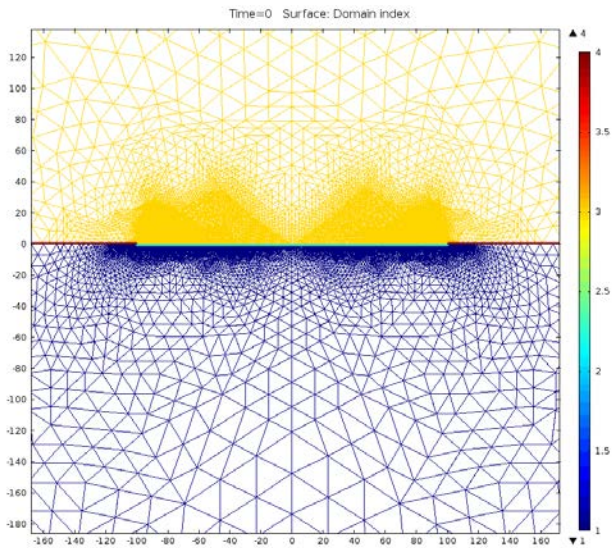


Electrical model: electrolyte with low conductivity σ_2

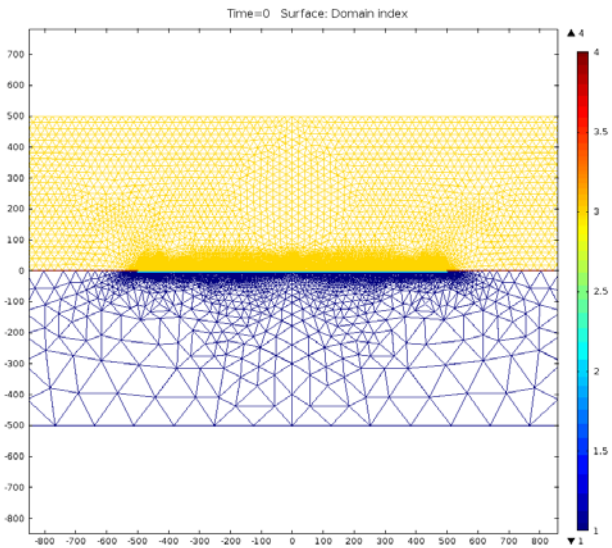
Opening diameter 40 µm



Opening diameter 200 µm



Opening diameter 1000 µm

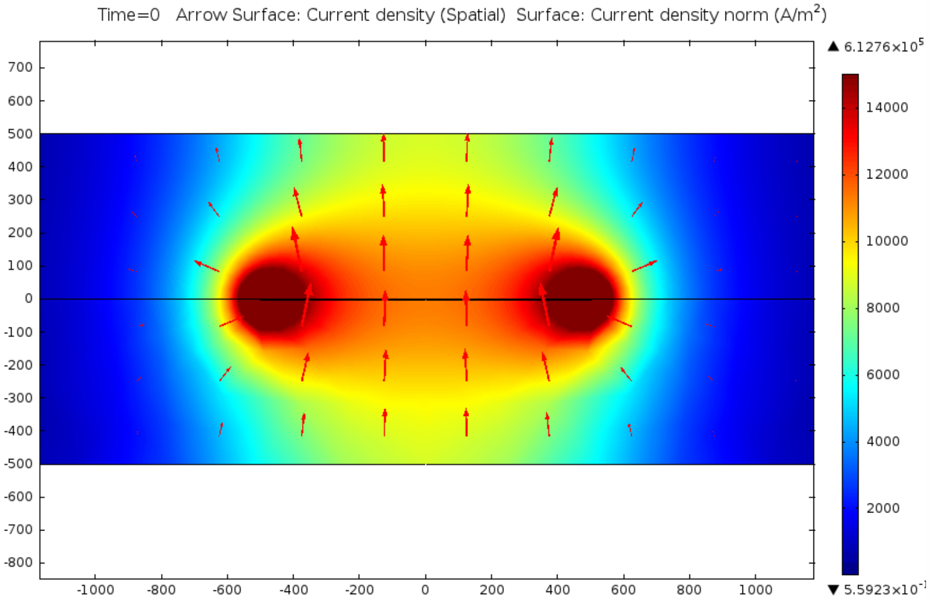


- Etch form transformation convex - concave

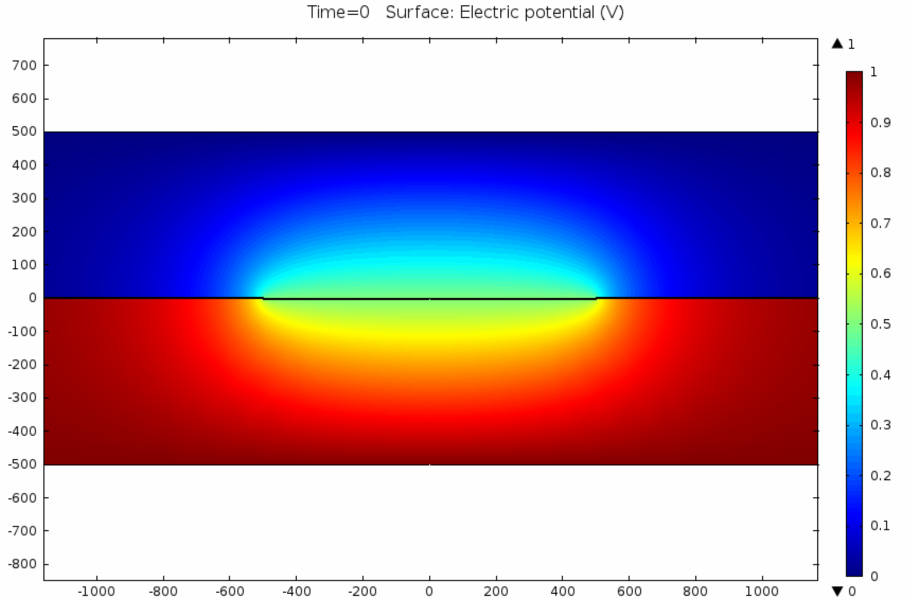
Electrical model: electrolyte with low conductivity σ_2

Opening diameter 1000 µm

Current density distribution



Electric potential distribution



Diffusion model: parameters

Etch front movement (ale), 1st order reaction: $R = k \cdot c$

$$v_r = R \cdot K_D \cdot n_r$$

$$v_z = R \cdot K_D \cdot n_z$$

$$K_D = \frac{M_{Si}}{m \cdot \rho_{Si}}$$

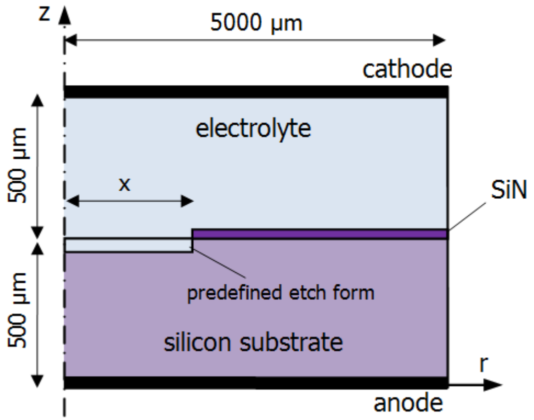
where R is the reaction rate at the boundary silicon-electrolyte, m is a number of Fluor atoms needed for dissolution of one atom of silicon.

For m = 6 (in the electropolishing mode in the reaction of silicon dioxide dissolution):

$$K_D = 2{,}01 \cdot 10^{-6}\ \frac{\mathrm{m}^3}{\mathrm{mol}}$$

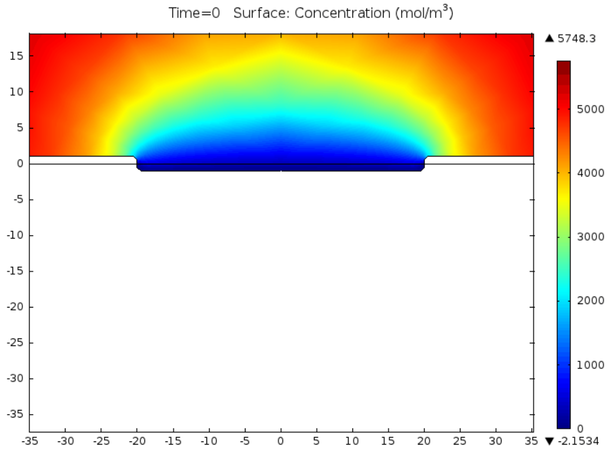
Other model parameters:

- initial electrolyte concentration $c_0 = 5.7483\ \mathrm{M}$
- assumed reaction rate constant *k* = *1* m/s to provide diffusion-controlled process

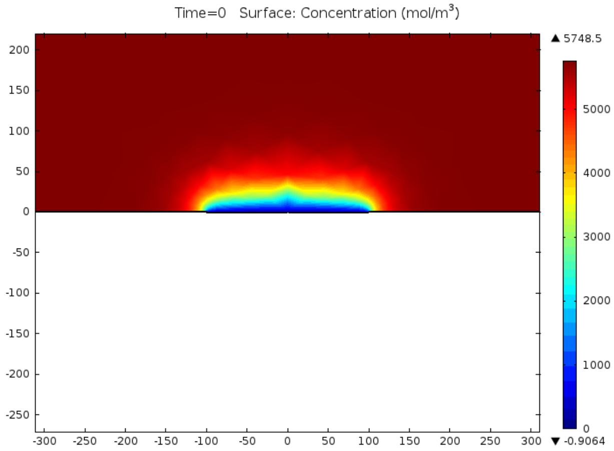


Diffusion model: etch form development

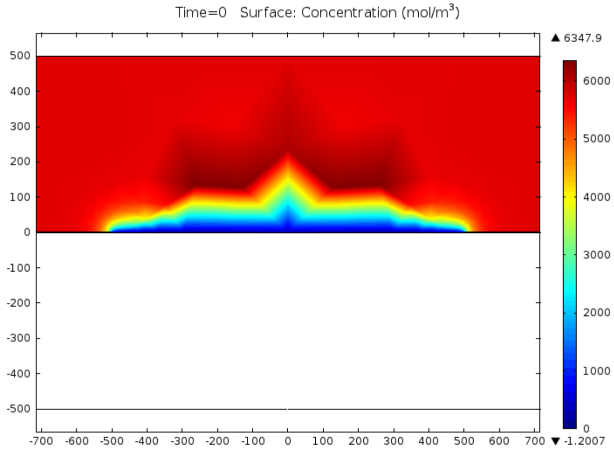
Opening diameter 40 µm



Opening diameter 200 µm



Opening diameter 1000 µm



- Etch form transformation convex – concave

- Concave isotropic form is achieved when the distance from the opening in the masking layer to the etch front is 25%-35% of the diameter of the opening (in the simulated range of openings 40 µm – 1000 µm)

Conclusions

- Models for the dynamic simulation of etch front in silicon anodization process presented

- Convex-concave shape transformation was demonstrated with electrical and diffusion mechanisms

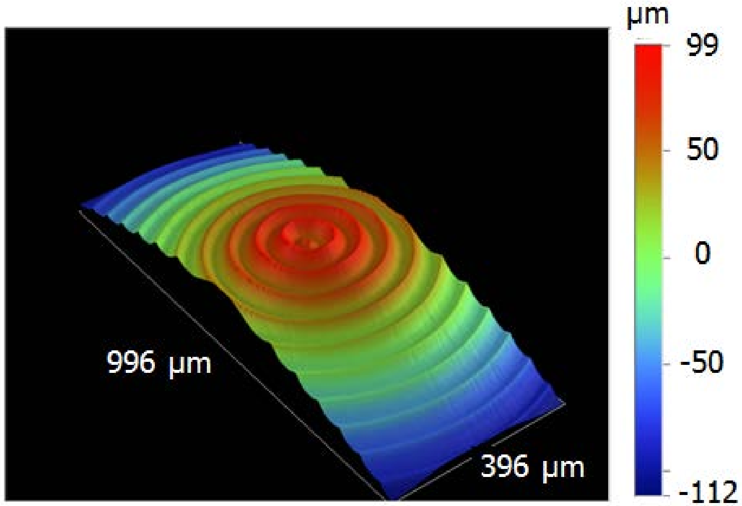
- The shape transformation in the electrical model observed only for the electrolyte with low conductivity

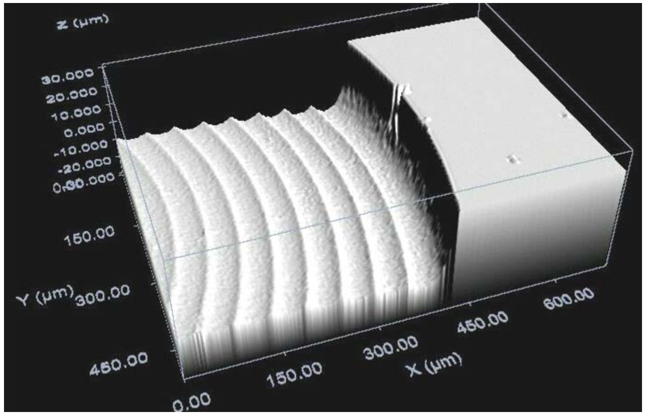
- The shape transformation in the diffusion model occurs at the etch depth 25%-35% of the diameter of the opening

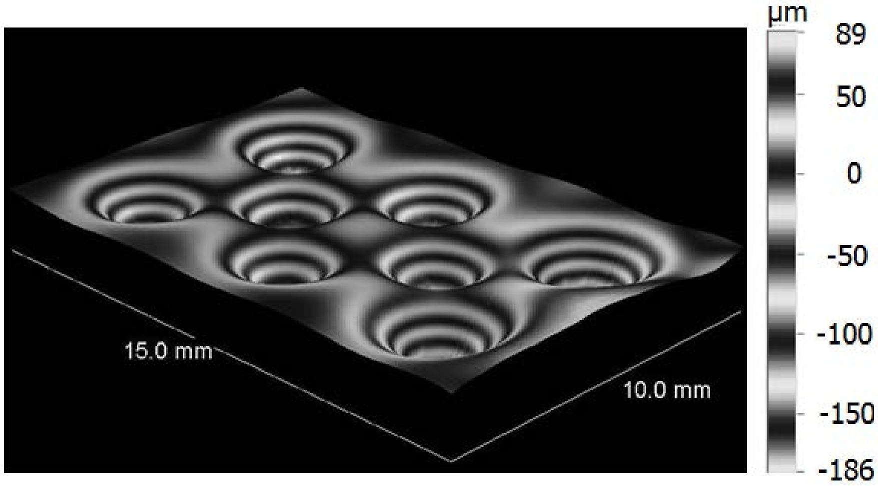
Further work:

- Some assumptions require further investigations (e.g. order of the reaction in the diffusion model)

- Development of the general model with both electrical and chemical properties







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Thank you for your attention!