Dynamic Simulation of Electrochemical Etching of Silicon

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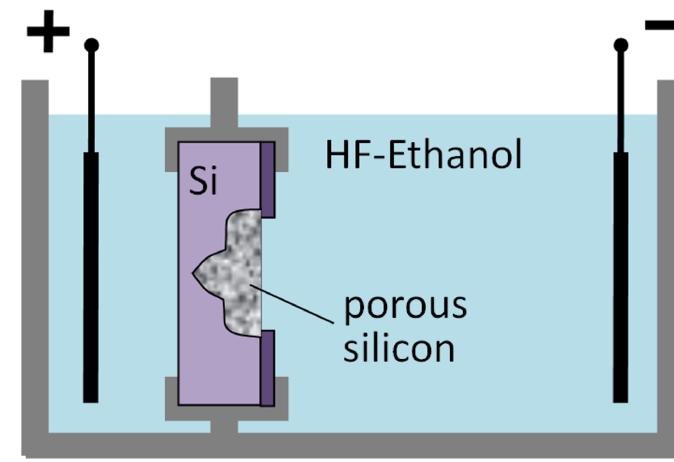
Introduction:

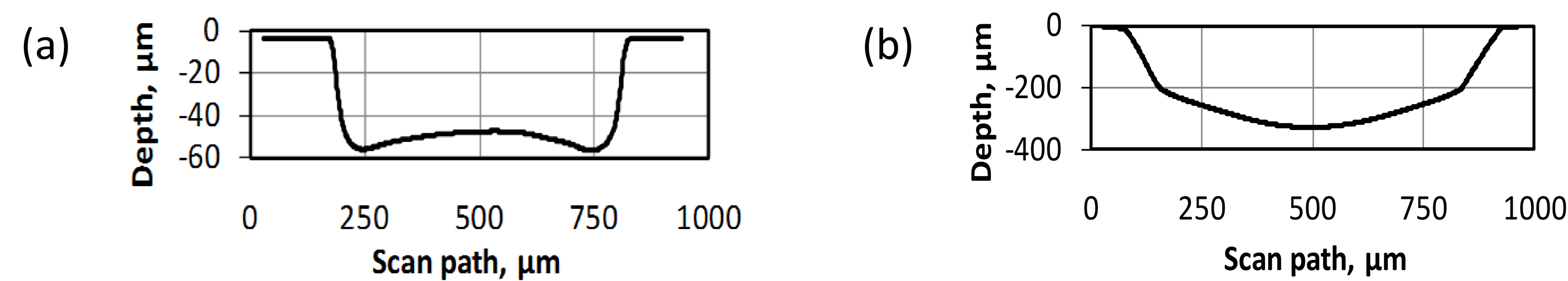
Electrochemical etching of silicon (anodization) in hydrofluoric acid (HF) can be applied for etching of well controlled 3D structures in silicon.



Anodization cell with silicon wafer in cross-section

Typical etch form development observed in silicon anodization process with insulating frontside masking layer at high current:

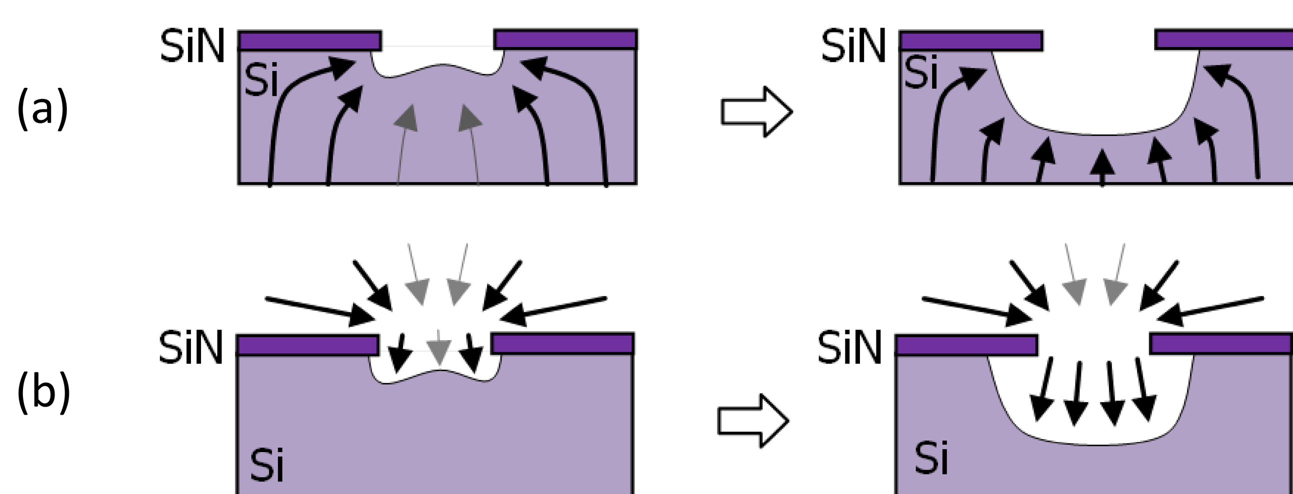
- convex shape in the beginning:
- transformation to concave shape later during the process:



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 for (a) t_{etch} = 1 min and (b) t_{etch} = 10 min

Two mechanisms for this shape transformation are simulated:

- Electrical current distribution in silicon substrate
- Diffusion in electrolyte



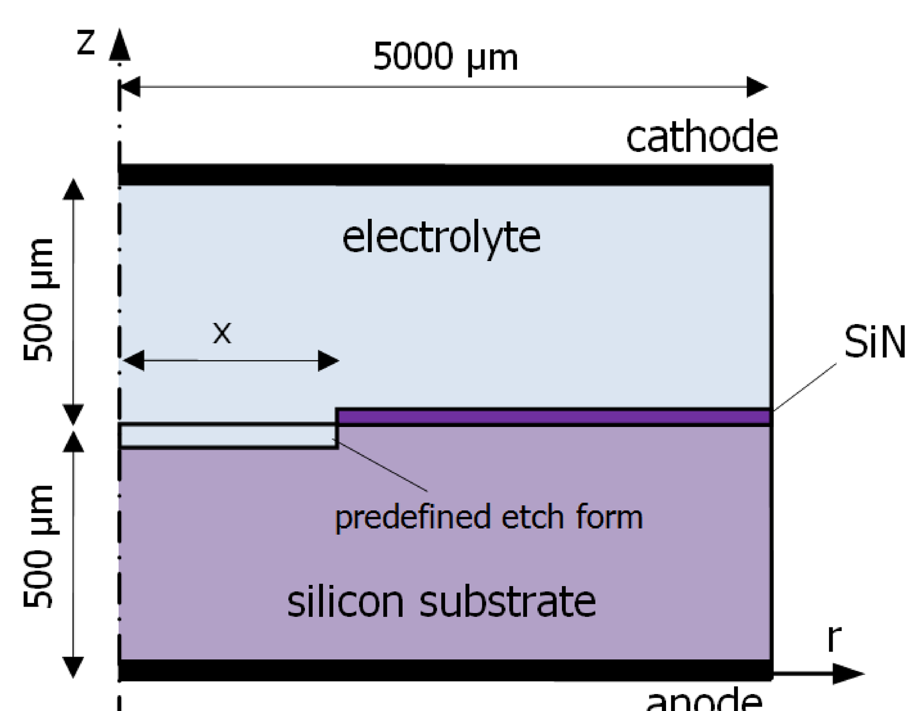
Considered mechanisms for shape transformation: (a) effect of current distribution (arrows represent current flow); (b) effect of diffusion-controlled etching process (arrows represent the flow of F-ions to the reaction site); darker arrows indicate stronger flow

Model geometry and mesh:

Both, the electrical and the diffusion models have been simulated in 2D with axial symmetry. The movement of the etch front was implemented with the moving mesh interface (ale) .

The geometry of the models consists of the following domains:

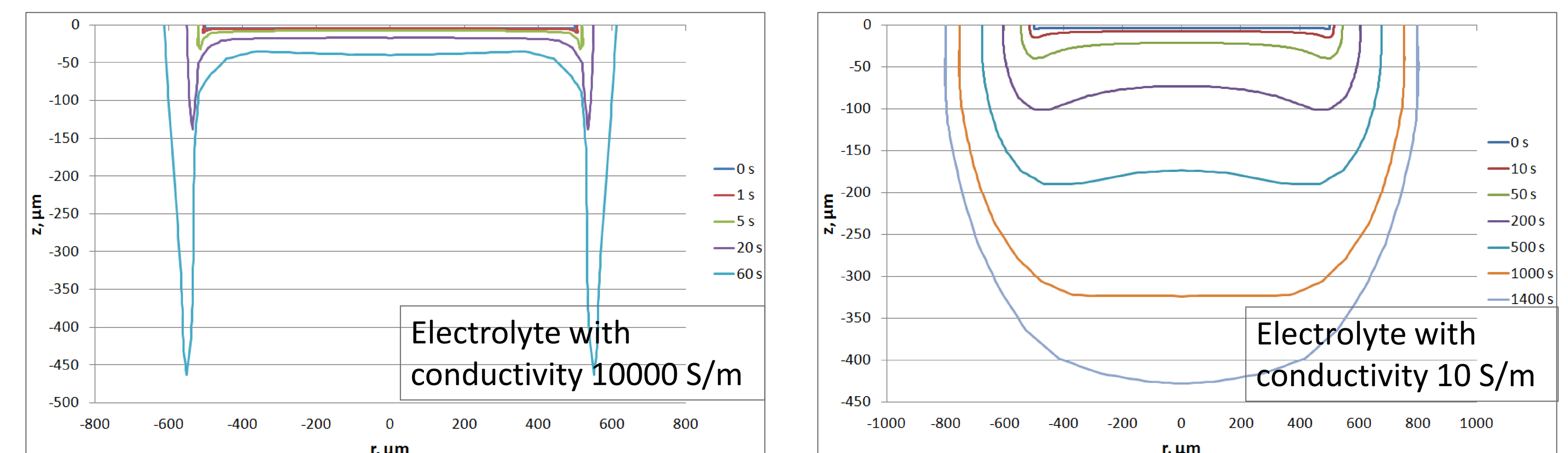
- electrolyte,
- silicon substrate;
- insulating SiN layer (1 µm thick) with an opening of varied radius x in the range 20 µm – 500 µm,
- predefined etch form of thickness 1 µm for enhanced mesh movement.



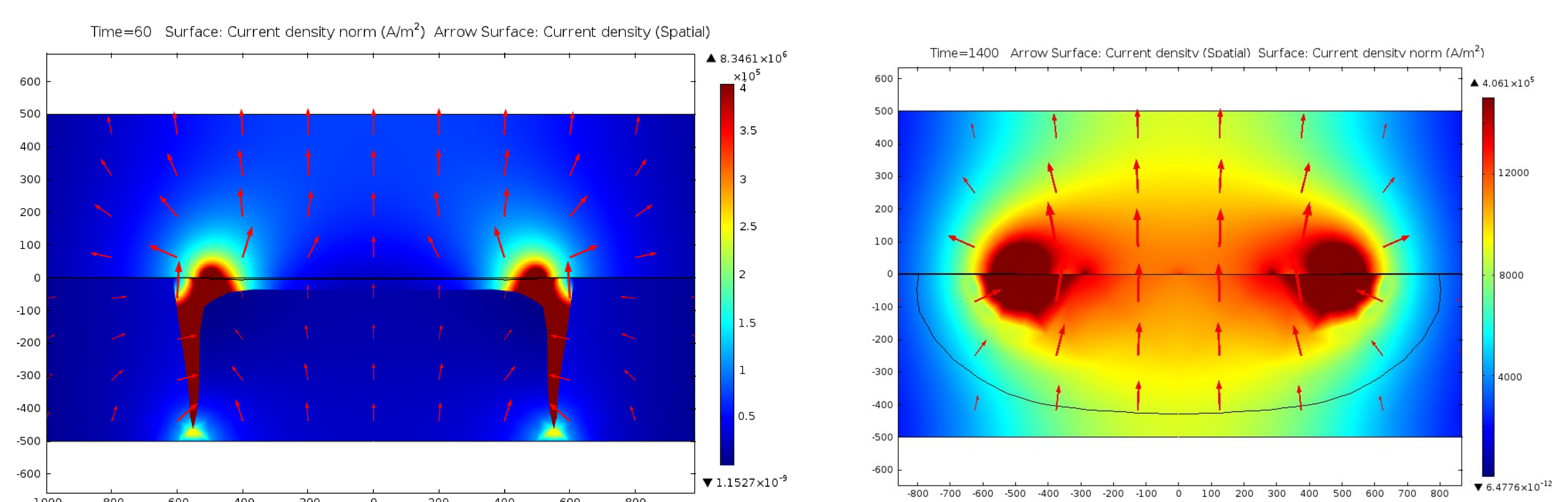
Electrical model (ec):

Etch front movement: $v_r = -K_E \cdot j_r$ $\quad v_z = -K_E \cdot j_z$ $\quad K_E = \frac{1}{z \cdot e} \cdot \frac{M_{Si}}{\rho_{Si} \cdot N_A}$

where *j* – current density and *z* – reaction valence.



Resulting etch forms for diameter of the opening 1000 µm for electrolytes with conductivity (left) 10000 S/m and (right) 10 S/m



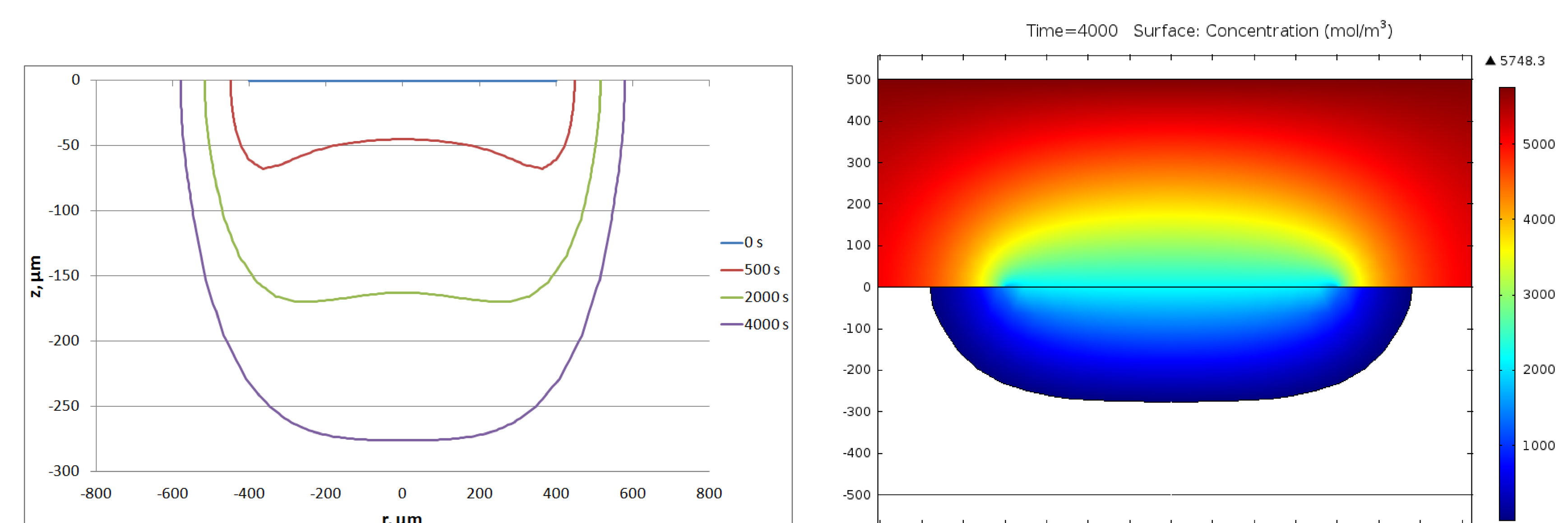
Corresponding current density distributions at the end of the process (for electrolytes with conductivity (left) 10000 S/m and (right) 10 S/m

Diffusion model (chds):

Etch front movement (1st order reaction):

$R = k \cdot c$ $\quad v_r = R \cdot K_D \cdot n_r$ $\quad v_z = R \cdot K_D \cdot n_z$ $\quad K_D = \frac{M_{Si}}{m \cdot \rho_{Si}}$

where *R* – reaction rate at the interface electrolyte-silicon,
k – reaction rate constant, *c* – electrolyte concentration,
m – quantity of F atoms consumed for dissolution of one Si atom.



Resulting etch forms for diameter of the opening 800

Concentration distribution after 4000 s for diameter of the opening 800 µm

Conclusions:

- Two convex-concave shape transformation mechanisms in a silicon anodization process has been considered and demonstrated with electrical and diffusion models.
- In the electrical model transformation of shape to concave was observed only for the electrolyte with low conductivity (equal to the conductivity of Si-substrate). In the case of electrolyte with much higher conductivity, self-amplification of convex shape has occurred.
- In the diffusion model, shape transformation into concave was observed at etch depth 25%-35% of the diameter of the opening.
- Some of the model parameters should be validated with experiments and/or scientific references.

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