Influence of geometrical and electrical parameters of masking layers on the electrochemical etching of silicon for single trench formation

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Abstract. Deep single trenches can be produced at the edge of apertures of protective films masking the surface of silicon samples. This macropore formation, from polarized HF based solutions, is electrically activated depending on the mask geometrical and physical parameters whatever the silicon type or the electrolyte composition. The mask thickness increase is known to induce deeper trenches. In this paper, we show that we can predict and localize this phenomenon by simulating two dimensional hole current distributions below the mask. We demonstrate also the influence of the material permittivity on trench depth. These 2D simulation results are correlated with experimental results.

1. Introduction
Porous silicon (PS) was grown the first time in 1956 during the electro-polishing of silicon in an HF based electrolyte [1]. The interest in this material increased drastically in 1990 [2], when L. Canham observed efficient visible photoluminescence from this material at room temperature. The first foreseen application was in silicon-based optoelectronics [3], but other important applications emerged later, using different morphologies of porous silicon. Very regular arrays of macropores with extremely high aspect ratio were fabricated by Lehmann and co-workers [4] and they were used to develop new capacitor technologies [5] and to produce photonic crystals [6]. On the other hand, the dielectric properties of porous silicon were used in bipolar ICs [7] and in RF applications [8]. Moreover, the high chemical reactivity of microporous silicon to KOH or TMAH solutions makes this material very attractive for use as sacrificial layer for MEMS applications [9].

Macropore arrays fabrication is now a well established process [10]. The pores are in general initiated by an array of regular pits and the pore size and their inter-distance is defined. A parasitic effect observed in both macroporous and nanoporous silicon formation is an increased etch rate at the edges of apertures, formed to define the etched area [13, 14]. The hole accumulation in this area is mainly due to the convergence of the hole current lines [15] and it has been phenomenologically described by Steiner [15] for different masking materials. In this paper, we present a simple model to describe this effect, and we use it to fabricate deep single trenches at the borders of protective layers used as masks for electrochemistry. By monitoring the masking material thickness and permittivity we show that we can fabricate deep single trenches around a non-edged area. Recently, Christophersen et al. [14] have experimentally demonstrated that the trench depth increases in p-type silicon with
increasing the mask thicknesses. The electrolyte used by them consisted of HF diluted in an organic
dimethylformamide (DMF) solution. This behavior was attributed to an increase of the stress at the
carbon-mask interface with increasing the mask thickness. In this paper, we show analog experimental
results in N-type silicon and aqueous HF solutions, for two kinds of protective masks and we
demonstrate that the selective growth of trenches depends mainly on the mask geometry and on the
mask material dielectric properties. To visualize the carriers behavior into the silicon substrate and the
selective growth of the trench, we have proceeded to two dimensional electrical simulations.

2. Experimental setup
In this work, we have used a conventional CZ one-side polished N-type silicon substrate <100>
oriented with a resistivity in the range of 3-10 Ω.cm. Two kinds of protective masks have been tested:
A 300 nm thick APCVD silicon oxide layer covered by a 150 nm thick phosphorous doped
(10^{20} at.cm^{-3}) amorphous silicon layer, and a 100 nm LPCVD nitride film. By means of
photolithography, windows in the masking layers of dimensions 0.5 mm x 0.5 mm were opened
through these layers.

For the anodization, we have used a single-tank anodization cell with a 4.5 wt.% HF water diluted
electrolyte for a bias voltage of 4 V and a global current density of 5.65 mA/cm², during 2 hours. The
samples were illuminated from the back with a 35 W halogen lamp to produce photo-generated holes
into the silicon substrate. Without mask, we have checked in a previous work that these parameters
were suitable to produce porous silicon with randomly distributed macropores [16].

3. Results and discussion

3.1. Experimental results
With the oxide-polysilicon mask, we observed systematically the formation of deep trenches up to 90
µm in depth at the border of the mask, as we can see in figure 1.

![Figure 1. Cross section, SEM micrograph: deep macropore formation at the edge of the oxide/polysilicon mask for an etching current density of 5.65 mA/cm².](image)

The trench growth limits the porous silicon formation in the opened window, where a small porous
silicon nucleation is observed. On the other hand, the anodization process using a nitride mask results
in trenches with smaller depth, below 10 µm. A lateral under-etching is also observed below the masks
in both cases. In order to explain these differences for the same anodization conditions, we have
performed 2D electrical simulations.
3.2 Simulation results

2D electrical simulations were performed using the ISE-TCAD (Integrated System Engineering) tools in order to visualize the hole concentration distribution at the edge of a protective film. To model the electrolyte-N-type silicon electrochemical system we have considered a Schottky contact in an opened insulating film as reported in figure 2. As this is done during the anodization process, the same potential was applied on the Schottky contact, modeling the silicon-electrolyte interface, and the insulating film. The overall structure is then covered with a gold layer (not represented in figure 2). The total dimension of the simulated structure is 300×300 µm². The phosphorous doped silicon (10¹⁵ at.cm⁻³) was illuminated from the back (100 mW/cm², λ = 0.8 µm) to provide hole carriers to the structure. The system is then polarized at 4 V in a reverse state.

![Figure 2](image)

**Figure 2.** Mapping of the hole current density, near the mask edge, simulated in a 2D N-type structure. The arrows show the hole current direction and the shading represents the current density in arbitrary units.

As hole carriers are necessary to produce porous silicon, we have reported the hole current density distribution in the structure (Figure 2). As expected, the hole current density is more important at the edges of the opened window compared with the center of this area. This is due to the convergence of the hole current lines from the substrate toward the mask edge. Once a pit is created in this area, its growth is prolonged as a consequence of an increasing convergence of holes, leading to the formation of a single trench, as we have shown in a previous work [16]. Moreover, the attractive electric field in the space charge region below the oxide film participates in the hole carriers circulation. Indeed, a part of the hole carriers converges from the substrate toward the mask edges and the center of the opened window (black arrows in figure 2), whereas another fraction can reach the silicon-oxide film interface producing a lateral current (white arrows in figure 2). This lateral current could play an important role in the lateral under-etching observed in the micrograph shown in figure 1. To evaluate the impact of the mask thickness, we have calculated the hole current density ratio (Jh_edge/Jh_center) between the edge and the center of the opened area, for different film thicknesses. Hole current densities have been taken at 0.2µm depth from the silicon surface. Considering the SiO₂ mask, we show in figure 3 that the ratio increases from 1.5 to 3 by varying the film thickness from 0.3 to 1.4 µm. Indeed, the increase of the mask thickness reduces its capacitive influence, and then reduces the influence of the electric field below the mask. The capacitive influence of the silicon nitride mask is more pronounced as a consequence of the permittivity increase (ε_{SiN₄} = 7, ε_{SiO₂} = 3.9). So, an increasing hole carrier
accumulation below the silicon nitride film occurs to the detriment of the convergence of the hole carriers from the bulk toward the mask edge. These simulation data are in agreement with our experimental results showing a trench formation of smaller depth when using a silicon nitride mask.

Figure 3. Calculated hole current density ratio between the edge and the center of the window in the mask. The calculated hole. The reverse bias is equal to 4V. Deeper trenches should develop when using a silicon dioxide mask. This is due to its lower permittivity for a given thickness.

4. Conclusion
In this paper, we have used the effect of high hole concentration at a mask edge to produce high aspect ratio single trenches in N-type silicon at the borders of a mask. The carrier distributions have been simulated in a 2D equivalent device. The electrical simulation confirms that the carrier accumulation at the mask edge is the dominating phenomenon leading to the selective trench growth. We have also demonstrated the influence of the thickness and the permittivity of the masking layer on the trench depth. The deepest trenches are obtained by using thicker masking layers from a low permittivity material.

5. References
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