

# Characterization and Modeling of Silicon Migration by Hydrogen Annealing

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## Abstract:

In this work, we studied silicon migration rates as a function of ambient temperature and pressure. We etched periodic trenches in crystalline silicon with a width of 400 nm and a separation of 500 nm, and then examined the effect of annealing them in various hydrogen ambient conditions. Anneals were performed at pressures between 20 and 80 Torr and temperature values of 1050°C and 1100°C. We then measured the change in the surface topology by imaging cross sections under an scanning electron microscope (SEM). The resulting change was then compared to a dimensionless transient simulation of the phenomenon to characterize the magnitude coefficient. Experimental values for the magnitude coefficient can be calculated with the model and the dependence of this coefficient upon pressure and temperature can then be determined. This work will bring the micro and nanotechnology community closer to building an accurate quantitative model for silicon migration induced shape transformations as well as a better understanding of the effectiveness of direct applications of the process.

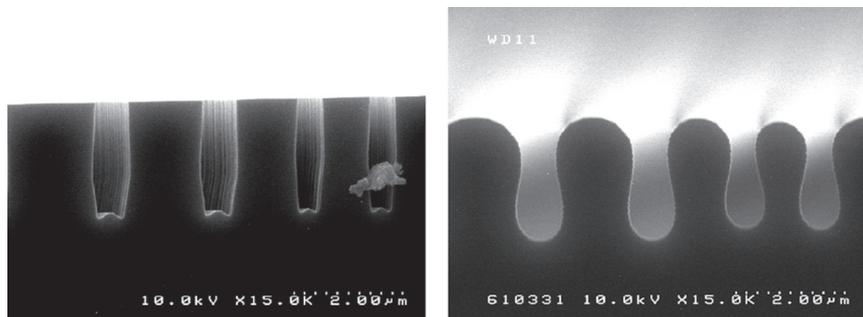


Figure 1: Four plasma etched trenches before (left) and after (right) silicon migration.

## Introduction:

A key challenge in creating devices with structure in the nanometer regime is creation of smooth, symmetric, defect-free surfaces with high reproducibility. Silicon migration is a diffusive process that increases symmetry and smoothness of silicon surfaces as atoms flow into lower energy configurations. This process is distinctly different from the usual methods of shaping silicon, as it is a fluidic transformation as opposed to a sharp cut or etch (Figure 1).

Applications for this process are currently being developed, such as enhancement of photonic crystal optical properties via symmetry improvement. A more complete characterization of the process as a function of temperature and pressure would greatly improve the ease and potential effectiveness of process applications.

## Experimental Procedure:

Wafers were put through a standard process of oxide hard mask growth, patterning via optical lithography, and oxide removal. The completed wafers were then annealed in hydrogen ambient in a hot wall epitaxial chemical vapor deposition system. The main anneal steps in the recipe were a basic run up period to allow the machine to reach main anneal temperature and pressure, a 300 second anneal period at those values and then a cool down period. A wafer was run through the warm up and cool down steps of the recipe without the

main anneal step and analyzed to verify these steps were not observably effecting results. The pressure quickly attained the desired value in both steps, the temperature lagged a bit but ultimately reached the desired level linearly in the span of approximately one minute. Upon removal from the reactor, wafers were then immediately spin coated with a 7  $\mu\text{m}$  layer of photoresist to prevent particle contamination during the cleaving process. The wafers were then cleaved across the surface trench features by hand with a diamond scribe. The photoresist was then removed and the samples were mounted in cross-section under SEM and imaged. Several rounds of procedure modifications were undertaken to reach this final process.

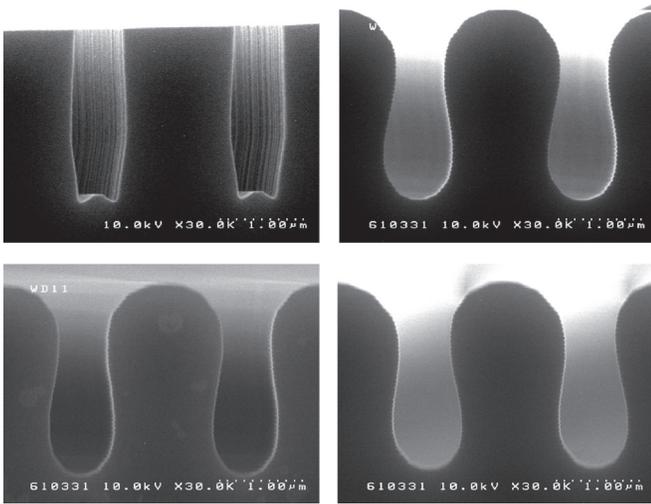


Figure 2: Close-ups of trenches (clockwise from top left) without anneal; with anneal for 300 seconds at 1050°C, 20 torr; 1050°C, 80 torr; 1100°C, 80 torr.

**Results:**

Of the thirty wafers that were initially prepared, twenty three reached the annealing stage (several were lost to etcher malfunction). Of these, seven reached the analysis stage and produced quality images (Figure 2).

To define the process quantitatively, a mathematical model of the Mullins equation (Figure 3) for surface diffusion [1] was implemented using level set modeling techniques. We then implemented the Canny edge detection algorithm [2] for finding the surface edges in an image. Images of the initial surface geometry of a sample, which had gone through the entire process without the anneal, were then scanned into the model using this method and the model was run to time-evolve the surface (Figure 4).

**Future Work:**

Obtaining a more precise image of the initial surface geometry of the samples can lead to a more accurate final prediction

**Mullins Equation:**

$$r_n = \frac{D_s \Omega^2 v}{kT} \frac{\partial^2 K}{\partial s^2} = B \frac{\partial^2 K}{\partial s^2}$$

- $r_n$  → normal velocity
- $D_s$  → diffusion const.
- $\gamma$  → surface tension const.
- $v$  → # atoms per unit area
- $\Omega$  → molecular volume
- $K$  → surface curvature

Figure 3: Mullins equation.

from the modeling software. We hope to eventually use the model to evaluate the final images and then work backwards to bring it into exact agreement with the data. Magnitude coefficient values can be extracted and then plotted versus temperature and pressure of the anneal to generate an equation for it as a function of these variables. With a small amount of improvement it will be ready to be packaged and used as a system capable of inputting any surface geometry and outputting an image of the final surface for a given time and pressure, allowing far greater application in various areas of MEMS and nano-scale engineering.

**Acknowledgements:**

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**References:**

- [1] Mullins, W.W., J. of Applied Physics, 1957. 28(3): p. 333-339.
- [2] Canny, J.F., IEEE Trans. Pattern Analysis and Machine Intelligence, 1986. p. 679-698.

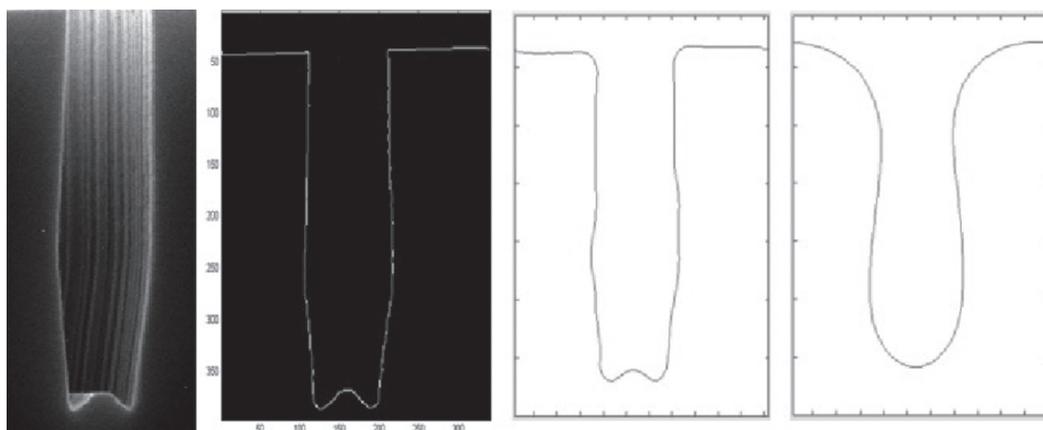


Figure 4: Four steps in the model (from left); Initial surface image, surface edge detection, fitting of an initial condition, image of evolved surface after migration.