SEGS: On-line WWW Wet Etch Simulator

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ABSTRACT

This paper presents an interactive on-line wet etch simulator (SEGS) which predicts the etched shape as a function of time for arbitrary isotropic or anisotropic etchants and any initial mask shape. Using any Java-enabled web browser users can draw initial masks, choose the etchant, simulate the etching, and view animation results. SEGS can be accessed at **http://mira.me.tuns.ca/**

Keywords: MEMS, micromachines, silicon, simulations, etching.

INTRODUCTION

Anisotropic wet chemical etching techniques are widely used in silicon micro-electromechanical systems (MEMS) fabrication. The anisotropic rates are due to the crystal structure of silicon, and can drastically change the final etched shape. For common etchants such as EDP, KOH, or TMAH, the (111) planes usually are slowest, (100) and (110) intermediary and higher order planes such as (311) and (522) are fastest. The anisotropisity can be as large as 100 to 1. Because of the differences in rates, some planes grow, while others disappear. Holes enlarge with time while pegs shrink. After long times, holes are dominated by slow planes, while pegs become dominated by fast planes. Within a shape (be it a peg or a hole), there can be two types of corners: convex (peg-like) and concave (hole-like). For example, an ‘L’ shaped hole has five concave corners and one convex corner. While etching convex corners fast planes dominate; for concave corners, slow planes dominate. Due to this complexity, there is an increasing need for computer simulation tools.

There are a number of algorithms and programs available to simulate the anisotropic etching process. The ASEP program [1] uses traveling planes and the intersections between them to define the the shape as a function of time. The Slowness method [2] examines the corners of a shape and predicts the trajectory of those corners. Atomistic [3] and Cellular Automata methods [4] use small cells to model the spatial domain and predict the evolving shape by applying primitive behavior of the cells. Some MEMS FEM systems with etch simulation capability also have been developed, such as MIT’s MEMSCAD [5] and Michigan’s CAEMEMS [6]. Several commercial software packages are also becoming available.

Although there are some programs available to model the etching processes, remote users and researchers who do not have access to the CAD tools cannot take advantage of the simulators. To put these resources to more efficient use and broaden the base of MEMS researchers, this paper presents an interactive on-line etch simulator (SEGS). The simulator accepts arbitrary input mask polygons and arbitrary isotropic or anisotropic etchants. It uses the standard interfaces and formats of the World Wide Web to allow any user on any computer system with a Java-enabled browser users to draw masks, simulate the etching, and view the results. SEGS can be accessed at **http://mira.me.tuns.ca/**

SEGS SIMULATOR

Originally developed at Caltech, SEGS is a fully 3-D simulator [7]. Information on using the SEGS simulator and submitting CIF or GDSII mask layouts for simulation via anonymous FTP can be found at **http://design.caltech.edu/**

The input mask shapes are first converted into polygons, then discretized into lists of small segments (segs) (see Figure 1A). The segments have both a location and an etch rate (velocity) that is dependent on the orientation of the segment. The segments are propagated forward at the appropriate etch rates with new segments inserted into any gaps formed by the displaced segments.

Next excess segments are removed. To determine whether a segment has been etched away, the position vector $\vec{P}_i$ from segment$_{i-1}$ to segment$_i$ is calculated (see Figure 1B). Let the unit tangent in the direction of segment$_{i-1}$ be called $\hat{t}_{i-1}$. Let the component of $\vec{P}_i$ perpendicular to the tangent of segment$_{i-1}$ be called $\vec{P}_{\perp i}$. $\vec{P}_{\perp i}$ can be found using either a cross product or a dot product:

$$\vec{P}_{\perp i} = \vec{P} - \vec{P} \cdot \hat{t}_{i-1} * \hat{t}_{i-1} \quad (1)$$

Since a segment cannot cross over from the unetched half-plane to the etched half-plane, a segment is etched away if the sign of $\vec{P}_{\perp i}$ changes:

$$\vec{P}_{\perp i}(time_j) * \vec{P}_{\perp i}(time_{j+1}) \leq 0 \quad (2)$$

By repeating these calculations for all segments at each time step, all interactions amongst adjacent segments in each polygon list are determined; such interactions are termed local. If the mask polygons are discretized into N segments, then on the order of $2N$ local calculations are required.

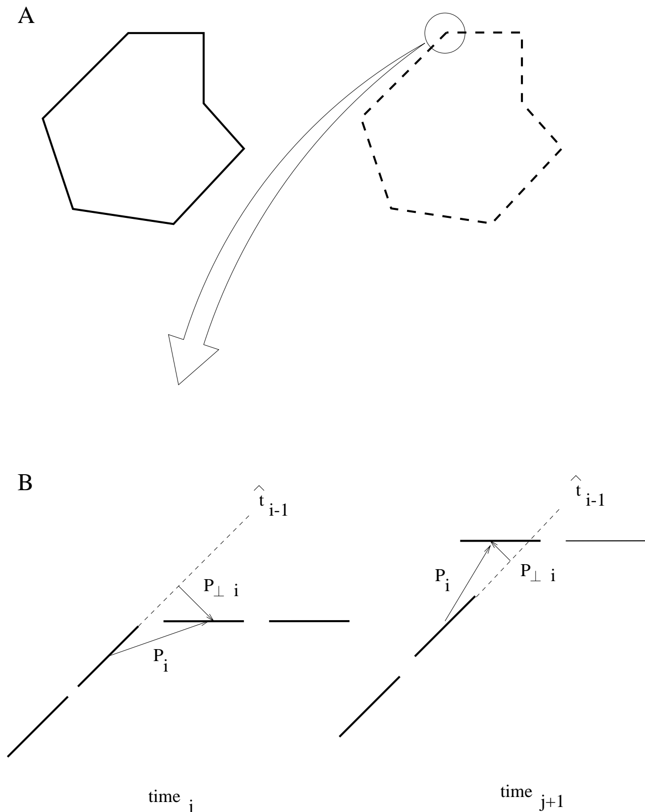

Figure 1: (A) discretization of mask polygons into segment lists. (B) Calculation of segment interactions.

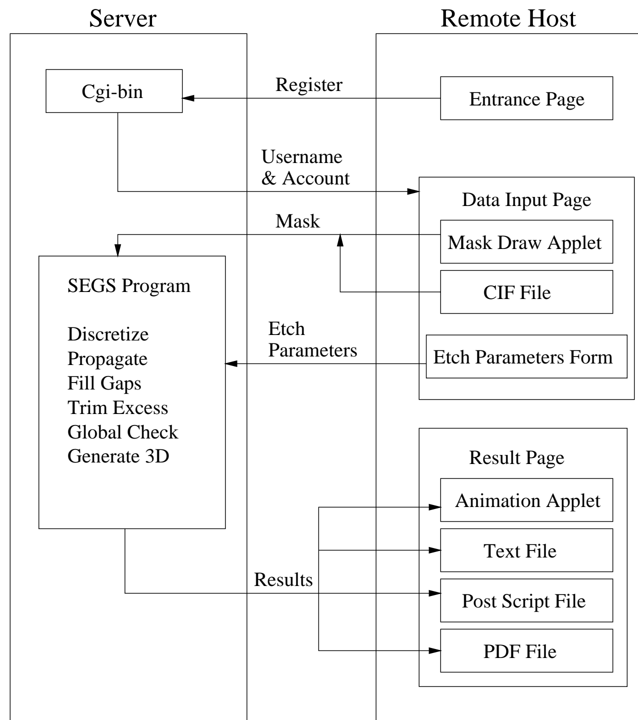

Figure 2: Data Flow

However, complex effects such as compensation and intersecting shapes require the calculation of interactions between segments from different polygons or different parts of a complicated polygon; such interactions are termed global. If the same mechanism as used for local interactions was utilized, then on the order of N^2 calculations would be required. This is so since any of N segments may globally interact within any of the remaining $N-1$ segments. Clearly this will be very inefficient at high resolutions (small segments or large N).

An alternate, less computationally expensive, method is used for calculating global interactions. This is done by overlaying the short segments on a fine grid array. Whenever a segment is moved, the corresponding cell in the grid is filled. The overwriting of a cell by two non-adjacent segments indicates that shapes are intersecting. The two polygons are then joined into one larger polygon; if the intersection is between two parts of one complicated polygon, that polygon is cut in two. Thus, if the mask polygons are discretized into N segments, then on the order of N global calculations are required, resulting in faster simulations especially at higher resolutions. The resolution is effectively limited by memory size since a N x N array must be created.

The division of the interactions into these two classes allows for efficient simulation of a wide variety of etchants and input mask shapes. SEGS has been extensively tested and has been used to model etched shapes such as an optimized concave corner compensated beam root [8].

Three Dimensions

Given the etch rate data, the method outlined above calculates the evolving surface contour of an etched shape. The three dimensional shape can also be calculated. The etch rate data is entered in three dimensional form: a plane vector and an associated rate, *e.g.*, $R(311)$ = 100 μm/hr. First the two dimensional etch rate R_{2D} is calculated: for plane (hkl), $R_{2D} = R(hkl) * \widehat{(hkl)} \cdot \widehat{(hk0)}$. This is the rate information used by SEGS to calculate the two dimensional shape: the change in segment position is $R_{2D} * \Delta time$.

Next the slope of the plane is calculated: for plane (hkl), slope = $|(00l)| \,/\, |(hk0)|$. This can be used to find a contour at some depth within the substrate. After the initial surface shape has been propagated forward, a second contour is propagated backwards by a distance equal to the depth multiplied by the slope. This can be repeated to arbitrary depth. Thus the three dimensional shape is made up of thin slices or contours stacked one atop the other. For the on-line version of SEGS, each shape is represented by two contour lines; one at the surface, and another at some depth. This was done to limit the computation time required.

ON-LINE IMPLEMENTATION

The SEGS software is a command-line based program. It reads three files: rate information, etch times steps, and input

Figure 3: Mask Draw Applet and simulation parameter options.

Figure 4: Animation Output Applet: (initial mask shown in Figure 3) top - isotropic etchant, bottom - anisotropic etchant. Each contour is the two dimensional shape at a different time.

mask. A combination of Java programs and cgi-bin scripts convert the user's browser inputs to the format SEGS expects (see Figure 2).

The rate information and etch defaults are text-based and entered using a standard cgi-bin form. However, the initial mask and the output shape animation are image-based and are communicated via Java applets. When a remote user first logs on, a Java "Mask Draw" applet allows the user to interactively draw and save initial masks (see Figure 3). A Java program running on the SEGS server accepts the remote mask data. Alternatively, a user's CIF file may be transferred from within the web browser using anonymous FTP.

The user may set etching parameters such as etchant and etch times. Standard etchants such as KOH, EDP, TMAH, and Isotropic are available. Users may specify additional etchants by modifying the etch rates of the standard etchants.

Next the simulation is executed by a cgi-bin script which converts the etch parameters, etch rates and mask images into three separate files. It then calls the SEGS program with those files as input parameters. The simulations are done on the local SEGS server and then transmitted to the remote user machine.

The results can be down-loaded directly as ASCII, PostScript or PDF files using the browser. Animations of the etching can be viewed by a second Java "Animation" applet (see Figure 4) which reads the stored results and displays them interactively on the remote machine. The animation time-steps can be stepped through one by one (backward or forward) or can be runs as a movie (backward or forward). An on-line implementation offers several advantages over traditional software distribution:

1. Widespread use of web browsers,

2. Pre-existing GUI (Graphical User interface) via WWW and Java,

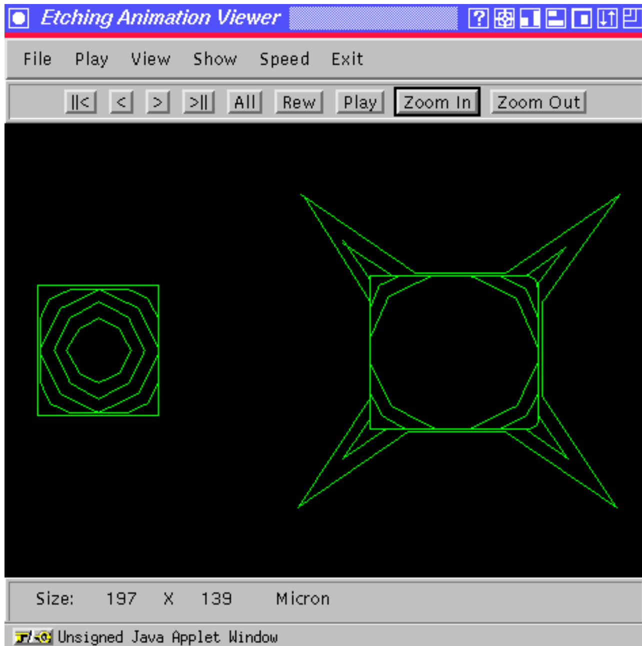

Figure 5: Left: uncompensated square peg, Right: triangular fin compensated rectangular peg. Each contour is the two dimensional shape at a different time. Five time steps are shown.

3. Platform independence - no specific computer system is required,
4. Server control over user access and accounting,
5. Instant software updates - only one server's software need be modified,
6. No hardware technical support,
7. Simplified troubleshooting - only one software version, one hardware configuration, system administrator can check users problems locally.

RESULTS AND DISCUSSION

Simulation time

The simulation time of SEGS is determined by i) the computing power of the server and ii) the data intensity, which is affected by the number and complexity of mask shapes as well as the time resolution required by users. The number of small segments calculated in the program is a linear function of the total perimeter of the shapes and the time resolution. For the SEGS on-line simulator the speed of network data transfer also limits the simulation speed, in many tests the data transfer formed the majority of the total time, especially when the remote user defines small time steps. The current SEGS server is a 166 MHz PC, and simulation times are usually less than one minute.

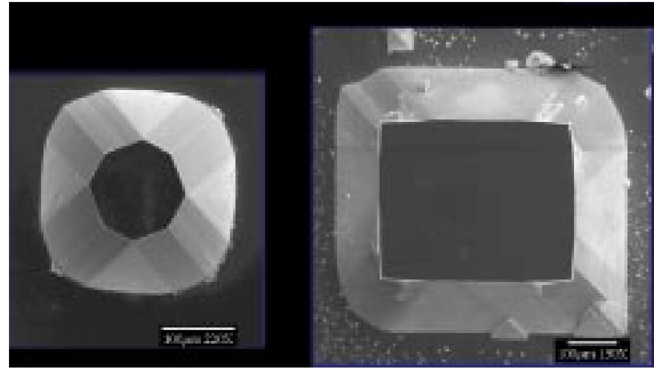

Figure 6: SEM photos of pegs etched in EDP at Caltech Micromachines Lab. Left: uncompensated square peg, Right: triangular fin compensated rectangular peg. Compare with time step three in Figure 5.

Compensation example

In MEMS design a designer may want to compensate or pre-distort an initial mask shape in order to obtain a desired output shape after a certain time of etching. Compensation design is a trial an error procedure, it requires designer's experience and knowledge to obtain the desired the mask shape. Nevertheless, the SEGS on-line etch simulator greatly simplifies and accelerates this procedure. An example of compensation simulation and comparison to experimental results is presented in Figures 5 and 6: triangular fin compensated mask will result in a rectangular peg in time step three.

Complex Intersections

The SEGS on-line simulator can simulate fabrication of multiple interacting shapes. During the etching, the propagating corners of the shapes can meet with each other and merge into a bigger single shape. Due to the difference of the etch rates with different orientations the resultant shape can be very different to the initial mask and difficult to predict without simulation (see Figure 7).

Three dimensions

As outlined above, two dimensional simulations can be extended into three dimensions by stacking successive depth contours. Figures 8 and 9 show the simulation of a cross shaped input mask and the experimental results. Note that the simulation depth is not shown to scale.

Limitations

The SEGS on-line simulator provides an effective tool to predict etch process, but also has some limitations. Because of the polygonization, some input shapes are approximated (see the circle in Figure 3). Additionally, because of the discretization, some output shapes are shifted by on segment length (see the slight shift of the topmost line in the six-sided

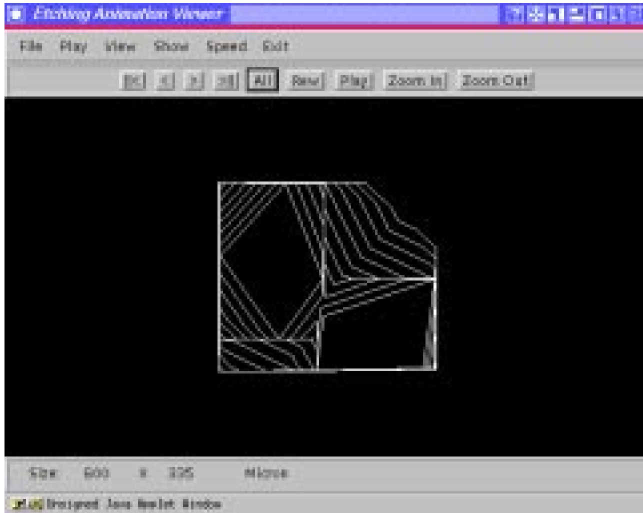

Figure 7: Simulation of complex interactions between shapes etched in KOH. Two initially quadrilateral holes merge to form one larger hole. Each contour is the two dimensional shape at a different time.

polygon of Figure 4). When simulating very complex shapes invalid results may be generated for some shapes. This can occur during grazing intersections of two separate polygons when the calculation results are small and subject to roundoff error. This may also occur when two closely space parallel lines are simulated, since the calculated dot products are also very small and susceptible to round-off error.

CONCLUSIONS

An accurate predictor of etched shapes is needed to reduce the design cycle of MEMS devices. The SEGS on-line simulator has been tested by several dozen groups and has simulated many complex shapes with a variety of etchants. The results can be quickly and easily accessed from any remote machine running a Java-enabled browser.

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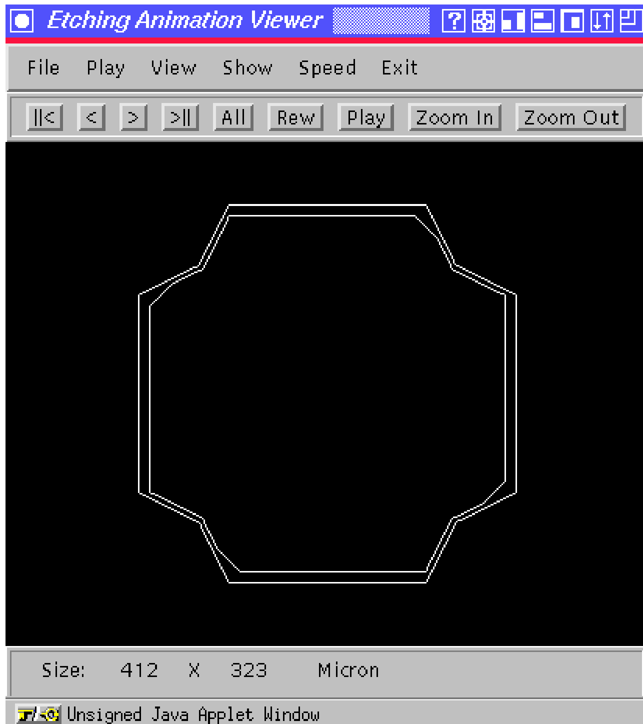

Figure 8: Simulation of three dimensional shape etched in EDP at one time step, the initial mask was a cross shaped hole. The outer contour is the top surface, the inner contour is the etch shape at some arbitrary depth in the substrate (the depth is not to scale).

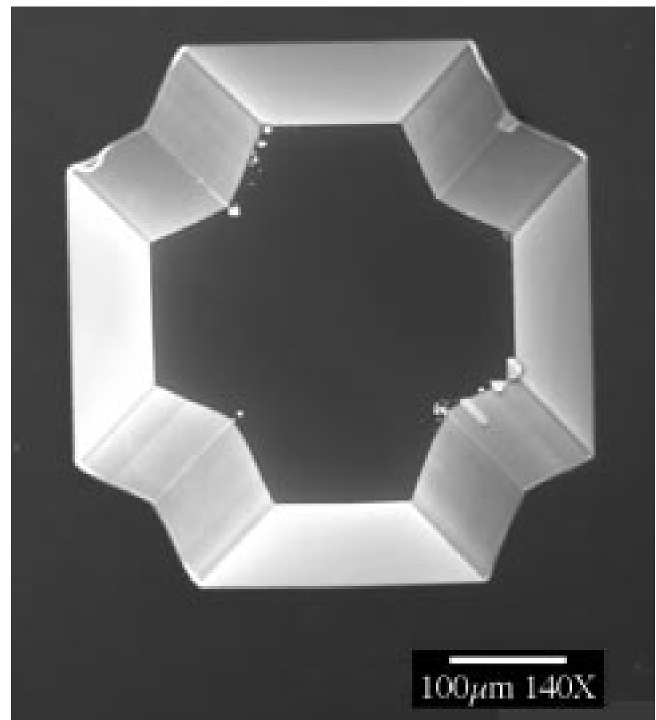

Figure 9: SEM photo of cross shaped mask etched in EDP at Caltech Micromachines Lab. Compare with Figure 8.