# A Novel Simulation Methodology for Isotropic Gas Phase Etching

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## ABSTRACT

In this paper, we will present our achievements on simulating a gas phase isotropic etching process. The simulation is based on random movements of individual etchant molecules, and subsequently, removal of substrate atoms based on the etch parameters. This is contrary to the layer-by-layer removal of substrate material in most other etch simulators. The main simulation parameters are the mean free path of the etchant gas at the etching pressure, the probability of the reaction between the etchant and substrate molecules, and a scaling factor. Having performed the simulations, it was concluded that the ratio of the mask opening diameter to the mean free path of the etchant molecules is the most important factor in determining the etch profile. Simulation results were compared to experimental data taken from silicon samples etched in a xenon difluoride etching system and were in good agreement. The small number of simulation parameters will enable this method to be easily expandable to other gas phase isotropic etching processes.

***Keywords:*** etch simulation; Monte Carlo method; mean free path; xenon difluoride.

## 1 INTRODUCTION

Gas phase etching of a substrate is a common process in microelectronic and micromachining industries. Anisotropic etching is generally preferred to isotropic etching for various reasons. However, gas phase anisotropic etching of a material requires an external energy source, such as an electromagnetic field, and is generally done in a plasma environment. However, starting and maintaining a plasma is difficult and expensive. Etching silicon (or polysilicon) is of particular importance, due to its wide spread application in microfabrication. There are a number of materials which can be used to etch silicon in their gaseous form, such as xenon difluoride ($XeF_2$) [1] and bromine trifluoride ($BrF_3$) [2]. These gases generally etch silicon isotropically and are very selective to silicon compared to other materials which are commonly used in microfabrication.

One problem with using isotropic gas phase etchants is poor control over the final shape of the etch profiles. Since the etchant gas molecules are not subject to any external force, their movements in the etching chamber is uncontrolled. This can lead to variable etch rate across a wafer due to loading effect at adjacent etched regions. In addition, local etch rates along the profile depend on the geometry of the mask opening and the current undercut profile under the mask (trenching effect). Most of today's etch simulators try to extract the etch rates along different crystallographic orientations inside a substrate, and in some cases, the mass transport issues are also taken into account based on the geometry of the mask opening. Using this data, they usually remove layers from the surface of the substrate to reach the desired etch depth [3, 4, 5]. These methods, however, will not take into account the effect of adjacent holes on each other (loading effect) or the dependence of the local etch rate along the profile (trenching effect).

The random movement of molecules suggests that the Monte Carlo method can be an appropriate choice for modeling the etching of a substrate. In this study, this hypothesis is verified by comparison of simulation results and experimental data taken from silicon samples etched in a xenon difluoride ($XeF_2$) etching system. $XeF_2$ is a crystalline white solid with a sublimation pressure of about 4Torr. It directly etches silicon in its gaseous form, usually at a pressure of about 1Torr [6]. Since it is an isotropic etchant of silicon without requiring a plasma environment, it was selected as a reference etchant for our simulations.

## 2 ETCH MODEL

In the proposed etch model, it is assumed that the etchant gas molecules move in the etching chamber freely and randomly until they hit either the substrate or the mask. Gas molecules will travel on average one mean free path (MFP) until they collide with another gas molecule. The MFP for a gas molecule can be found from the following equation:

$$\lambda = \frac{RT}{\sqrt{2}\,\pi\, d^2\, P\, N_A} \qquad (1)$$

where $R$ is the universal gas constant (8.3145 J/mole K), $T$ is temperature, $d$ is the molecule diameter, $N_A$ is Avogadro's constant, and $P$ is pressure. For $XeF_2$ the MFP is ~20μm at the etching pressure of ~1Torr.

Since the gas molecules are not subject to any external force, their direction of movements after colliding with other molecules is random. If a gas molecule hits the mask, it should bounce back and continue its movements in free space. But if it impinges on the substrate, it may react with substrate material or bounce back, depending on the reaction probability of the etchant and substrate.

It is assumed that the reaction probability represents all

the chemistry behind the reactions, including the existence of the boundary layer [7]. If present, this boundary layer is ignored, since it is very thin at the etching pressures of our interest (less than one MFP).

## 2.1 Simulation Setup

Before the simulation begins, the user enters the mask data and values for the different etch parameters. The user also enters the value of the MFP of the etchant molecules at the etching pressure, and the probability of the reaction between the etchant and substrate material. Since each pixel on the screen is assumed to be equivalent to 1μm, a *scaling factor* is defined to compensate for the difference between the actual size of substrate atoms and what is shown on the screen. A scaling factor of greater than one will result in more accurate results at the expense of computation time.

Two arrays of random numbers are generated at the beginning to reduce the amount of calculations during the actual simulation. The first array is composed of uniform random numbers between 0° and 360°, which is later used to calculate the direction of movements of gas molecules. A Wichmann/Hill linear congruential generator is used to create this array with a period of about $6.95\times10^{12}$ [8]. This ensures the quality of generated random numbers during the simulation. The initial seed for the generator is taken from the system clock. The second array is a separately generated Gaussian random variable whose average is equal to the MFP of the etchant gas molecule. This array is used to determine the radius of movements after each collision between the simulated gas molecule and other virtual gas molecules.

## 2.2 Simulation Algorithm

The simulation algorithm is based on the etching model described above. First, a gas molecule is generated at a random location above the substrate. This molecule is then randomly moved in the free space until it impinges on either the mask or the substrate. The radius of movements is taken from the array of Gaussian random variables. The direction of movements, in accordance to the isotropic nature of the etch, is taken from the array of random variable, ranging from 0° to 360°.

If the gas molecule hits the mask, it rebounds (assuming an elastic collision) and continues its movements in free space until it impinges on the substrate. Based on the assigned reaction probability (RP), the etchant may either react with a substrate atom or it may rebound with a random direction.

If the user sets the scaling factor to a value larger than one, each substrate particle must be hit that many times before it is removed. This in effect is the same as reducing the relative dimensions of etchant and substrate particles to approach the real case scenario.

The whole simulation data is saved at regular intervals in a bitmap format and can be viewed outside of the simulation program.

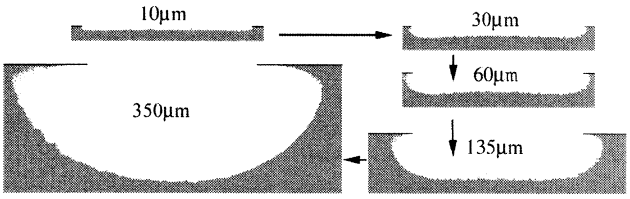

Figure 1: Variations of profile as the etch depth increases.

# 3 SIMULATION RESULTS

Three different general shapes are possible for etched profiles: spherical, flat bottom, and trenched. It should be noted, however, that after long etching periods the overall shape of the etch profile will approach a hemisphere. This can be observed in Figure 1, where the changes in the etch profile of a given mask opening are shown as the etching proceeds.

## 3.1 Trenching and Effect of MFP

Based on the proposed etch model, the mask opening diameter to MFP ratio ($\alpha$) is found to be the most important factor in determining the overall shape of a profile, and hence, can be used as the figure of merit.

A small $\alpha$ (<5) will result in spherical bottom profile and the etching process is mainly limited by the mass transport of etchant gas molecules. The spherical profile gradually approaches a flat bottom profile as $\alpha$ increases. For a large $\alpha$ (>20), the bottom profile shows trenches at edges of the etched region. There are two phenomena which contribute to the formation of tranches at the edges of large profiles. Firstly, a spot in the middle of a profile is subject to loading from all of the neighboring locations. For a spot at the edge of the profile, the loading effect is smaller. The other phenomenon is the higher reaction probability at the edges of profiles. Suppose that an etchant gas molecule hits the bottom profile of a large mask opening and does not react with the substrate. If this location is far from the edges of the profile, the gas molecule has a lot of room to rebound away from the surface. However, if the gas molecule hits the substrate near the sides of the profile, the molecule is partially surrounded by the etched substrate sidewall and the mask overhang due to etch undercut. Thus, the molecule may continue to rebound in this region. As a result, the probability of the reaction is enhanced near the sides of the etch profile. Hence, the etch rate, and so the depth, is larger near the sides of a hole compared to its center. Figure 2 illustrates the simulation results for different values of MFP. Variation of etch profile with MFP is shown in the simulation results of Figure 2.

## 3.2 Loading Effect

Loading effect of adjacent holes on each other is also related to the MFP. If the distance between two holes is on the order of a few MFP's or less, strong loading of etched profiles occurs. Unlike most other etch simulators, this simulator is capable of illustrating this effect (Figure 3).

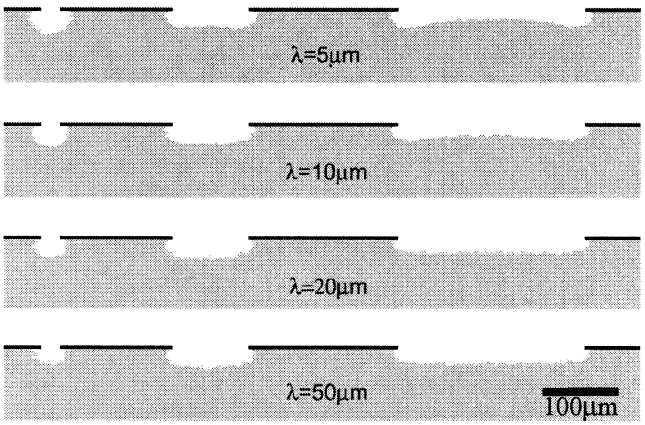


Figure 2: Illustration of dependence of profile on diameter of mask opening with RP=0.1. The hole diameters, from left to right, are 25μm, 100μm , and 250μm, respectively.

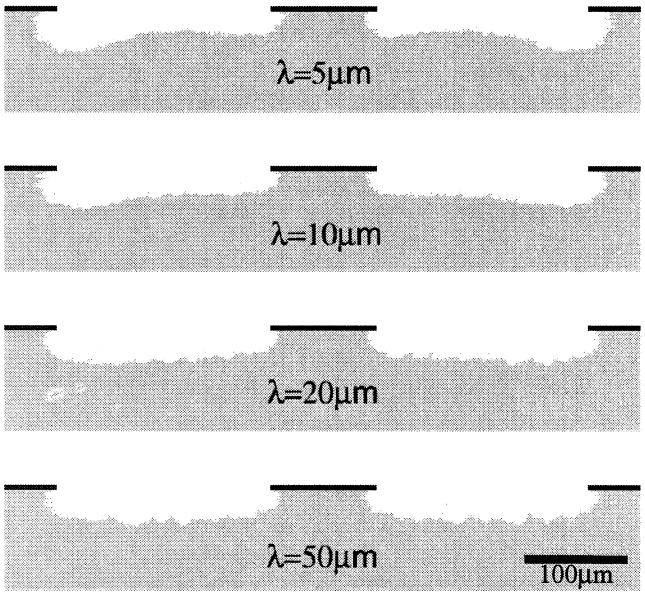


Figure 3: Dependence of loading effect on the MFP. The mask openings are 200μm wide and the distance between them is 100μm.

## 3.2 Reaction Probability

The most pronounced effect of changing the reaction probability (RP) on the simulated profiles is the variation in surface roughness. In Figure 4, the RP is changed by 3 orders of magnitude. However, the overall etch profile is not too sensitive to RP and small changes in RP do not contribute to observable variations of the etched profile. However, choosing small values for RP significantly increases the computation time.

# 4 VERIFICATION OF SIMULATIONS

Simulation results were compared against experimental data to verify their accuracy. Holes were etched by $XeF_2$ on

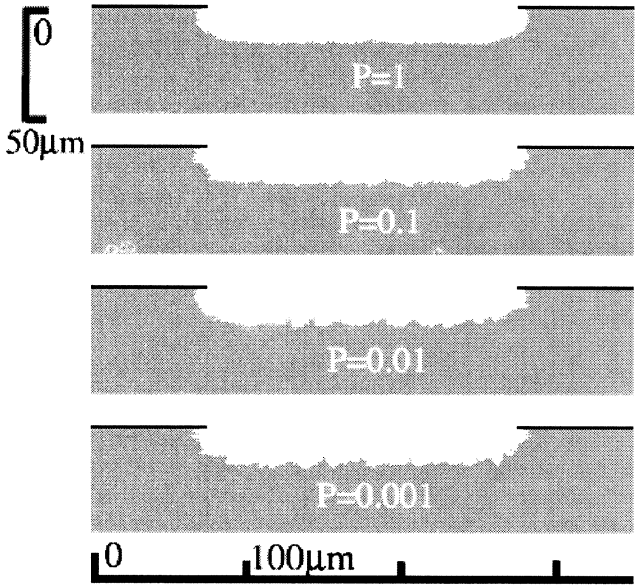


Figure 4: Effect of changing the RP on etch profile. For the simulations MFP was set to 20μm.

a silicon substrate with an $SiO_2$ mask. Profiles were measured by a Tencor Alpha-Step 500 surface profiler [6]. Simulations were performed with the same mask specifications to reach the target etch depth. Since the effect of changing RP was examined and shown to have small effect on the final profile, the reaction probability between silicon and $XeF_2$ was set to 0.05 to speed up the simulations. This is greater than the actual RP of 0.013, as reported in literature [9, 10].

As can be seen in Figures. 5, 6, and 7, the simulation results for the overall shape of the bottom profile of different holes approximately match the experimental data in all cases. However, the simulation slightly overestimated the depth of the trenches in the large hole of Figure 7 (6 μm deep vs. 5μm deep for the experimentally etched sample). The sidewall profiles of the measured holes appear linear in Figures 5, 6, and 7. It should be noted that the linear shape of the sidewall profiles is due to the slope of the Alpha-Step 500 probe tip. The actual etch sidewalls possess a curved slope, as is expected in isotropic etching of silicon.

# 5 CONCLUSIONS

A simulation program was written to study the isotropic gas phase etching of a substrate. The simulation results were compared against the experimental data from silicon samples etched by $XeF_2$. Etching parameters, according to the proposed etch model, can be set, and the effect of varying these parameters on the simulation results was tested and discussed. The simulation algorithm does not involve the chemistry behind the reactions, and hence, is easily expandable to etching of other materials, once the simulation parameters are known.

Current research concentrates on extending the proposed

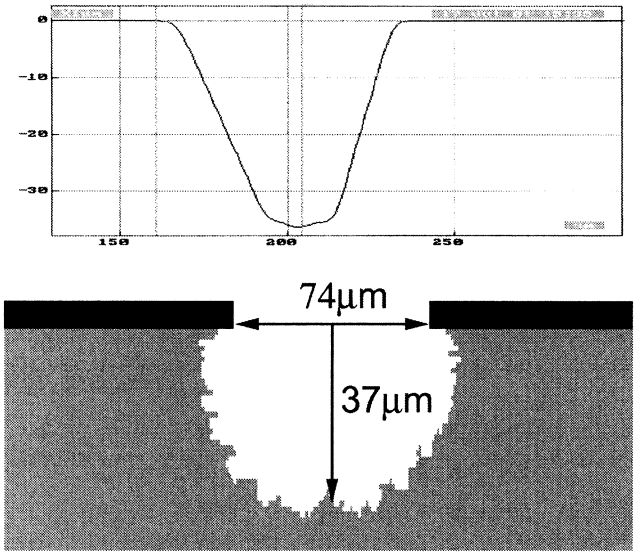


Figure 5: Comparison of simulation and experimental results for a 74μm mask opening.

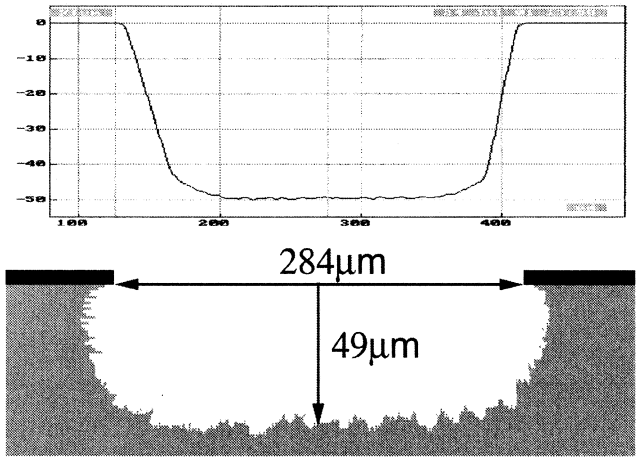


Figure 6: Comparison of simulation and experimental results for a 284μm mask opening.

algorithm to cover other dry etching mechanisms, such as high pressure reactive plasma etching, reactive ion etching (RIE), and ion milling.

## 6 ACKNOWLEDGMENTS

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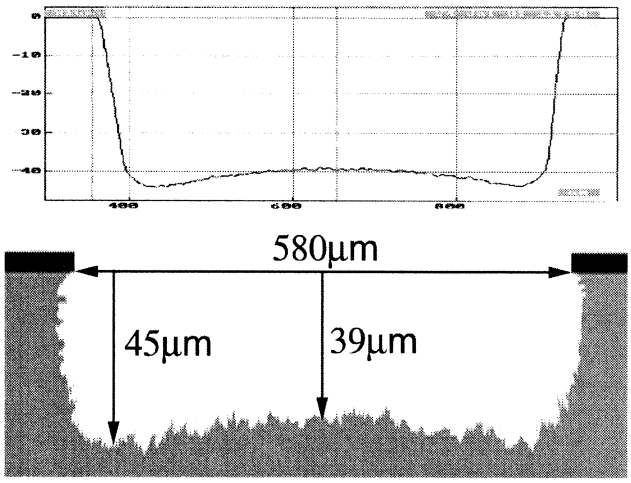


Figure 7: Comparison of simulation and experimental results for a 580μm mask opening.

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