Topography Simulation of Trench Etch Using Monte Carlo Plasma Etch Model with Polymer Re-deposition

1. Introduction

The topography simulation module, ***Elite*** has constantly been improved in order to simulate advanced processes, which are becoming more complex with device miniaturization and further integration of VLSI circuits. ***Elite*** is a two dimensional topography simulation module that works within ***ATHENA***, and includes the etching and deposition models neccessary to simulate diverse modern technologies.

One of the more important features of ***Elite*** , is the physics based Monte Carlo Etch Model, which is more accurate than conventional direction-rate based etching models. The Monte Carlo Etch Model involves calculation of the plasma distribution, and takes into account the redeposition of the polymer material generated as a mixture of incoming ions and etched (sputtered) molecules of substrate material.

In this article, we will discuss the relationship between the process conditions of the reaction chamber and the resulting etched profile. The example combines topography simulation together with plasma sheath reaction and surface reaction modelling.

The pioneering efferts of S. Takagi, et al. [1] reported both experimental results and plasma/topography simulation using the ***ATHENA/Elite*** Monte Carlo Etch Model. In this article, we are concentrating on how to specify the many complicated simulation parameters of the Monte Carlo Etch Model, referring to the results and calibration work of S. Takagi, et al. [1].

2. Simulation Model and Parameters

2-1. Incoming ions and neutrals

It is assumed that ion and neutral fluxes leaving the plasma sheath are represented by bimaxwell velocity distribution function [2] along the direction determined by user specified incident angle:

$$f(\upsilon_{\parallel}, \upsilon_{\perp}) \sim I \cdot \exp\left(\frac{\upsilon_{\parallel}}{T_{\parallel}} - \frac{\upsilon_{\perp}}{T_{\perp}}\right) \qquad \text{Eq. 1}$$

where $v_{//}$ is the ion velocity component parallel to the incident direction, $v_{\perp}$ is the ion velocity component perpendicular to the incident direction, I is the ion (or neutral) current density, $T_{//}$ is the dimensionless parallel temperature and $T_{\perp}$ is the dimensionless lateral temperature.

The contribution of parallel and lateral components have a relation to RF power and gas pressure as shown in reference [1], Figure 6.

2-2. Reflection Ratio of Ions

The experimental depth dependent etch rate was compared to ion flux simulations in the trench. By changing the reflection ratio of ions on the oxide wall, the relationship between the trench depth and the ion flux was simulated. S. Takagi, et al. [1] determined that a reflection ratio R of 0.4 showed good agreement to experimental results, so this value was chosen as a base value.

R=0.4 (mc.alb1 for oxide) .

2-3. Etch Rate

The etch rate is calculated with the microscopic etch rate parameter (EtchParam) and ion velocity (see equation 2). The perpendicular etch rate as a function of the RIE reactor conditions was reported in [1]. The details of the surface reaction model and the parameters used (including those mentioned in section 2-2 and 2-3) will be described in the next section.

$$EtchRate\ (mat) = \sum_{ion\ types} EtchParm\ (mat, ion) \cdot Vabs \qquad \text{Eq. 2}$$

So far we have discussed the base line physical parameters extracted from experiments in Takagi's work [1]. The next section will discuss simulation examples using other parameters available to the user.

3. Elementary Process of Oxide Trench Etching

The procedure to specify input parameters can be broken down into the following four steps:

step 1. Set base physical parameters refered to in the previous section.

step 2. Tune smoothing parameters

The main tuning parameter is mc.sm [3] A value of 0.1 is suggested as a starting point. The smoothness should be tuned for the best balance of the surface segment reaction, as shown in Figure 1, combined with the number of particles set by mc.parts1, mc.polympt, and mc.dt.fact. The parameter mc.dt.fact controls etching time discretization.

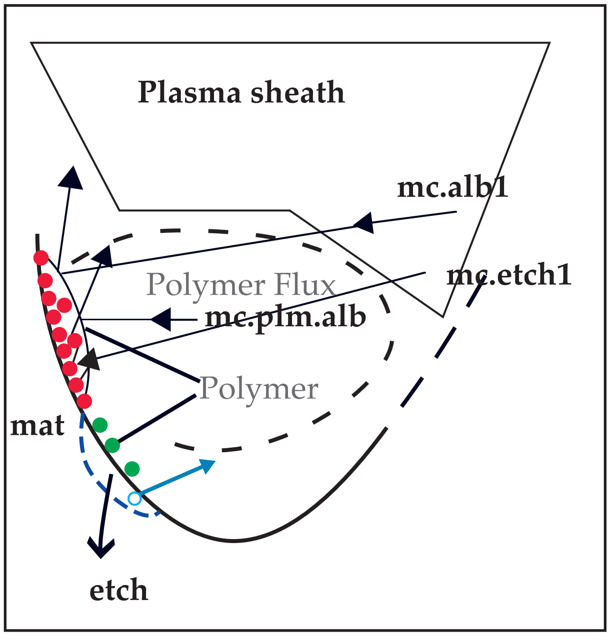

Figure 1. Surface reaction model described by tracing particles from plasma sheath and polymer flux. Parameters depicted in this diagram is for polymer material, which is etch/deposition target of incident particles.

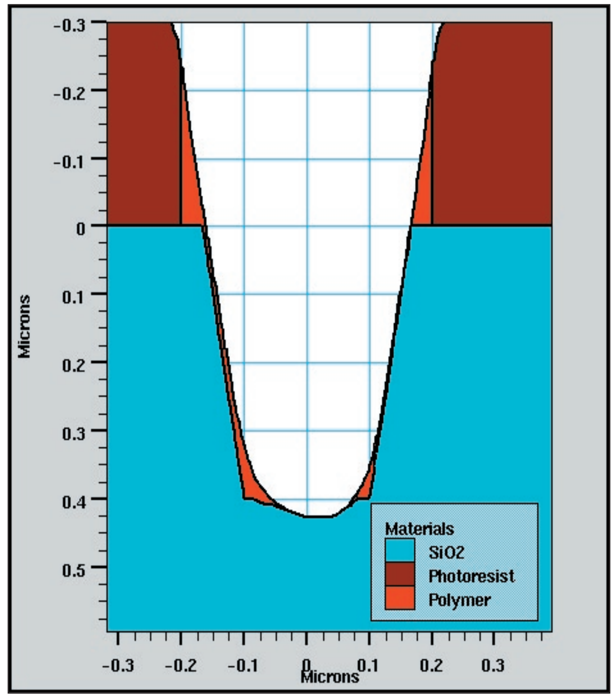

Figure 2. The result of oxide trench etch.

The three physical parameters, mc.etch1, mc.alb1, and mc.plm.alb (seen in Figure 1) control the surface evolution in the surface reaction model [2].

The parameter mc.etch1 concerns the etch rate of the particles from the plasma sheath against the respective materials, described by the right hand side of equation 2.

mc.alb1 represents the reflection ratio parameters of the particles from the plasma sheath against the respective materials described in 2-2.

mc.plm.alb represents the reflection ratio parameters of particles from polymer flux against the respective materials.

If an inappropriate value for the above parameters is not specified, rough surface elements with a "zig-zag" form will result.

step 3. Further tuning of the physical parameters

Here we show an example of trench RIE simulation to illustrate the effect of polymer growth and surface reactions.

We consider oxide trench fabrication, and define three rate.etch statements for oxide, resist and polymer materials respectively. There are more than 15 parameters included in these three rate.etch statements and etch statement, i.e.

3 x 3 (see Figure 1 for three materials) + 2 (Temperature of sheath) + 4 (smoothness parameters discussed in 2)) = 15 .

The effect of polymer re-deposition could be increased either by decreasing the polymer etch rate, or decreasing the polymer etch particle reflection from the polymer layer (mc.plm.alb).

Surface evolution was calculated at the polymer etch rate (mc.etch1=0.01e-5) 1/45 times slower than the etch rate for oxide.

In this example, the basic oxide trench was first created with a geometrical trapezoid etch which was then followed by the second physical monte-carlo etch. To illustrate the physical etching capabilities, the first geometric etch left the left haand side of the trench covered with a 10nm layer of polymer.

Due to the intentional polymer deposition only on the left side of the trench, an asymmetrical etch shape is generated as shown in Figure 3. This is the effect of the polymer re-deposition during the etching of the trench. The extent of the asymmetry of the trench geometry depends on the polymer etch rate (mc.etch1) and the polymer reflection (mc.plm.alb) parameters.

Figure 4 shows the sensitivity of the resulting etch asymetry to the value of these parameters. The figure illustrates a 2x2 experimental matrix of the polymer etch rate, mc.etch 1, reflection parameters, mc.plm.alb.

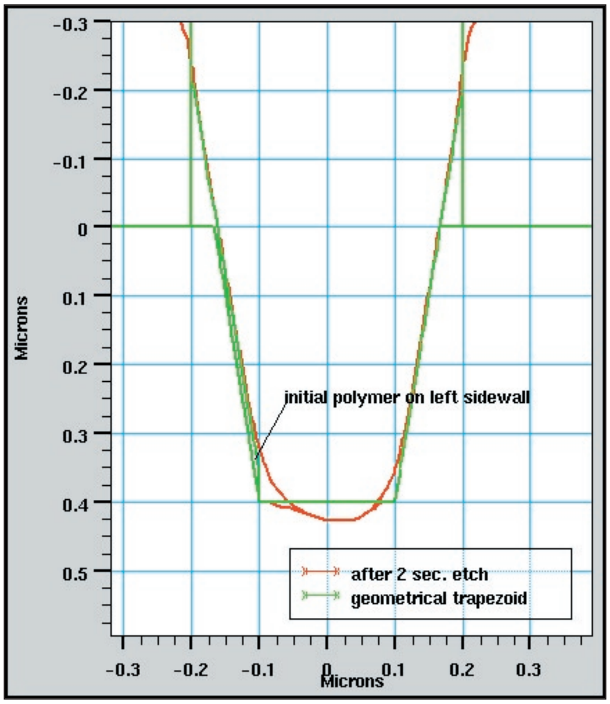

Figure 3. Overlay of geometrical trapezoid shape and subsequent two second etch

Shown in the top left of Figure 4, the symmetry of the bottom right trench is deeper for mc.etch1=0.01e-5 and mc.plm.alb=0.8; the top right shape is almost symmetric for mc.etch1=0.01e-5 and mc.plm.alb=0.05 (decreased from a), but a thin polymer covers the left side of the trench bottom.

Simulation time is less than 10 seconds for this short etch step, with mc.patrs1=mc.polympt=10000 MC particles.

4. Process Condition Dependence

In this section we will summerize the trench etching simulation example using the modeling parameters discussed in the previous sections.

By using the same parameter values (except mc.etch1=0.8e-5 and mc.plm.alb=0.8) the shape of the oxide trench (shown in Figure 5) is formed during a 1 minute etch. The value used for polymer etch rate (mc.etch1=0.8e-5) is two times larger than the etch rate for oxide. The ratio coresponds to the optimized etch rate ratio against polymer and oxide, which is compared experimentaly in [1].

Regarding simulation result dependency on the simulated process conditions, we quote two figures with the permission of Jpn. J. Appl. Phys. These two figures compare the simulation results with experiment. RF power and gas pressure dependency results were taken from Takagi et al. [1].

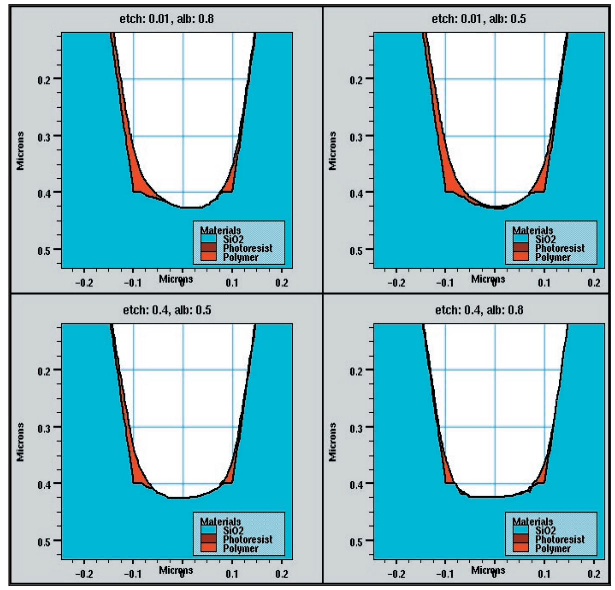

Figure 4. Effect of redeposition comparing four different set of parameters on symmetric/asymmetric trench geometry.

Figure 6 (Figure 13 in reference [1]) shows the etch depth and width, respectively. The simulation reproduces the tendencies of etch depth increasing with Rf power, whereas etch width remains almost constant. The dependence of etch depth and width on gas pressure are shown in Figure 7 (Figure 14 in ref [1]). The simulation reproduces the tendencies of etch depth and width which increase slightly with increased gas pressure.

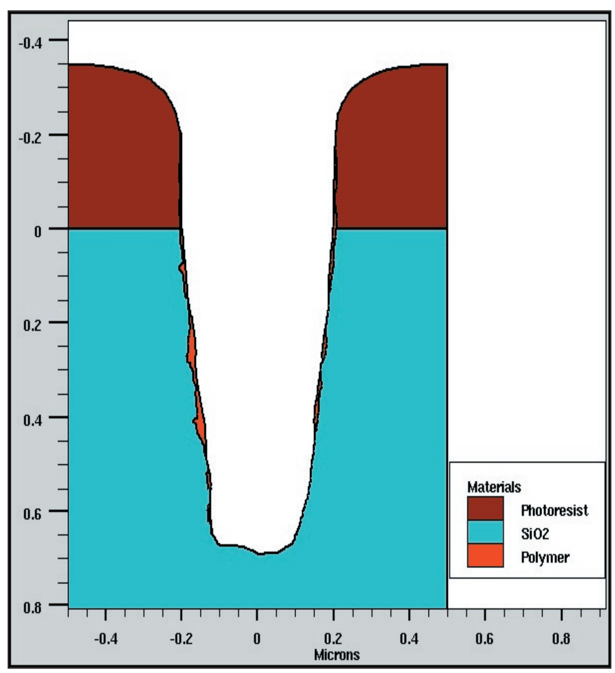

Figure 5. Simulated oxide trench with one minute etch using plasma etch parameters described in secion-3.

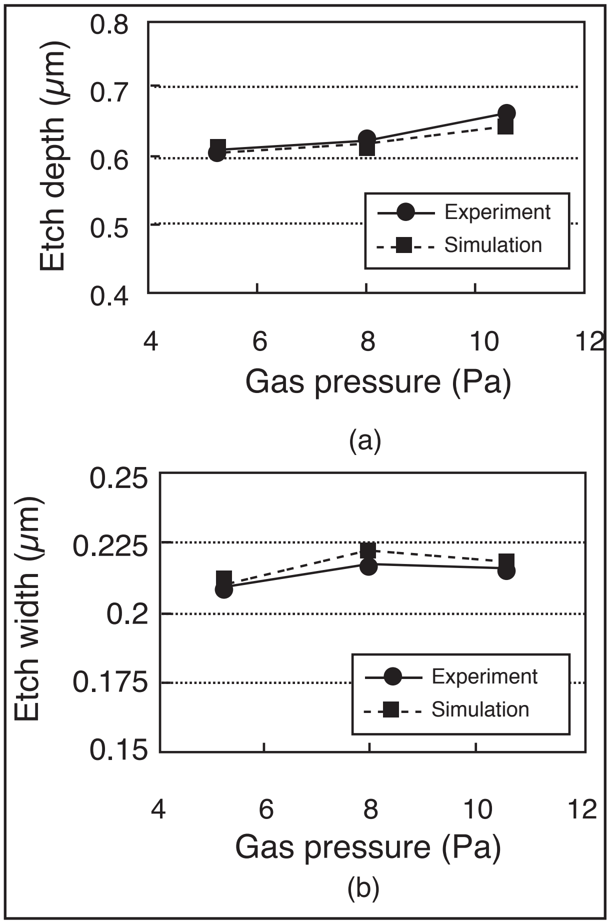

Figure 6. Comparison of experimental results and simulation results (RF power dependence):(a)etch depth, (b)etch width.

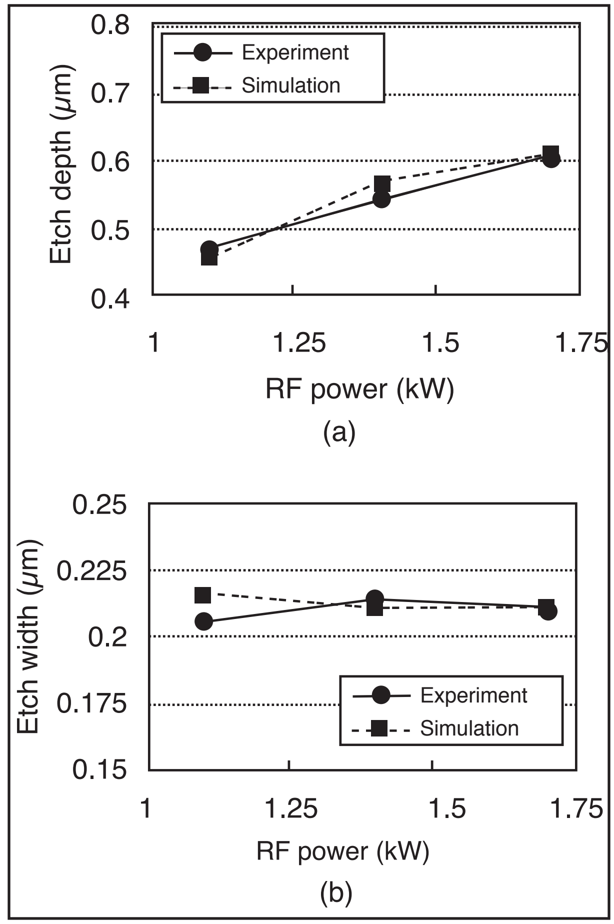

Figure 7. Comparison of experimental results and simulation results (gas pressure dependency):(a)etch depth, (b)etch width.

5. Summary

This article has shows the procedure to specify suitable model parameters to perform Monte Carlo plasma etch simulations. The parameters include polymer etch and polymer particle reflection from the polymer layer, amongst others. It was shown that this model reproduces reasonable etching geometry. According to Takagi et al. [1], by including plasma sheath simulations, the relationship between the reactor conditions and model parameters can be obtained and calibrated.

As for the dependence of etching profile on reactor conditions, please refer to the original paper [1].

Acknowledgment

We deeply appreciate Dr. Takagi for his essential contribution to practical application of MC Plasma Etch Model. We also appreciate very much to Jpn. J. Appl. Phys. for giving us permission to reprinting figures.

References

[1] S. Takagi, et al., "Topography Simulation of Reactive Ion Etching Combined with Plasma Simulation, Sheath Model, and Surface Reaction Model", Jpn. J. Appl. Phys., Vol. 41 (2002), pp. 3947-3954, Pt. 1, No. 6A,

[2] SILVACO Simulation Standard, August 1998, p6-9, "Simulating Redeposition During Etch Using Monte Carlo Plasma Etch Model"

[3] SILVACO *ATHENA User's Manual*