Modeling of Deep Reactive Ion Etching in a Three-Dimensional Simulation Environment

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Abstract

The deep reactive ion etching process (DRIE) [1] is a time multiplexed process where a fast chemical etching and a passivation processes are applied alternatively. It is very popular in surface micro-machined MEMS processing to obtain trench structures with high aspect ratios. The presence of a thin passivation layer makes it a very challenging process, especially for the three-dimensional simulation analysis. In this work we present a modeling approach for the simulation of DRIE processes. The model has been implemented in the three dimensional process simulation framework *Victory-Process*. When varying the etching / deposition cycles' time ratios, the DRIE process shows three different regimes. These regimes are as well represented by the developed model. The simulation results obtained are compared with the corresponding REM images of trench etching experiments.

1 Simulation Environment

To model the DRIE process the three-dimensional process simulator *Victory-Process* has been used. The model has been implemented via the C-Interpreter based modeling interface of the simulator [2]. The primary particle mode of the ballistic transport engine of the etching / deposition module of *Victory-Process* can be applied for the simulation of the DRIE process because the mean free path of the reactants is significantly larger than the feature size, which is typically few micrometers.
In this model equation (1) is used to calculated the etch / deposition rate for all surface points,

$$R(\vec{x}) = \iint\limits_{\Omega} S(\vec{x},\theta,\phi,\vec{F}(\theta,\phi)) \cdot \cos(\alpha(\vec{x},\theta,\phi)) \cdot \sin(\theta)\, d\theta\, d\phi \tag{1}$$

where R is the rate, S is the surface reaction function, $\vec{F}$ are the reactant flux functions (one for each reactant considered) and α is the angle to the surface normal. $\vec{F}$ and S, which are configurable C-Interpreter based functions, have been developed for the DRIE process' model for both cycles of the DRIE process.
Victory-Process uses implicit representations of the geometry [3] and moving surface. The etching/deposition rate is calculated at surface points. From those surface values a continous velocity function in the whole computational domain is derived using extension techniques [4]. The Level-Set equation [5] is solved to propagate the top interface (front) during the etching and deposition cycles. Between the etching and deposition cycles the multi-layer representation of a geometry is updated: boolean operations of the front and the multi-layer representation of the geometry are performed.

2 The Deep Reactive Ion Etching Model

In this work we have modeled and calibrated the DRIE process of silicon, but the model is applicable to other materials. As already mentioned the DRIE process consists of repeating the sequences of passivation and etching cycles, which can be treated independently.

2.1 The Etching Cycle

The process gas SF_6 dissociates inside the reactor plasma, and the ionized $S_xF_y^{(ion)}$ and the neutral $F^{\bullet}$ atoms, which predominantly contribute to the surface reactions, are generated. Only these particles are considered in our model.
The neutral $F^{\bullet}$ radicals show a homogeneous velocity distribution within the reactor, while the $S_xF_y{}^{(ion)}$ ions are accelerated by an electrical fields towards the wafer surface. The $F^{\bullet}$ radicals attack the silicon wafer surface by a fast selective chemical process. The $S_xF_y{}^{(ion)}$ ions interact with the surface by a slow non-selective sputter reaction, which also attacks the passivation layer.
The flux of the $F^{\bullet}$ radicals is modeled by assuming an isotropic particle distribution inside the reactor. In contrast to this, the ions show a preferential direction towards the wafer surface. Therefore a Von-Mises distribution function has been applied to model the ion flux. This function allows to tune any divergences of the ion flux.
Both particles' reactions with the surface are of the first order, and the rates are linear functions of the flux. It makes $S(\vec{x},\theta,\phi,\vec{F})$ in equation (1) a linear function of the flux for each reactant.
We have simplified the model to the case of one reactant by introducing the material dependent flux, material dependent efficiency ratio $\varepsilon(\vec{x})$ measuring the contribution of the ions and neutrals to the total etch rate, and an effective material dependent plane wafer etch rate $R_{0eff}(\vec{x})$. The resulting modeling functions (2) and (3) for equation (1) are:

$$F_{eff}(\vec{x}) = \frac{F^{(neutral)}(\vec{x}) + \varepsilon(\vec{x}) \cdot F^{(ion)}(\vec{x})}{1+\varepsilon(\vec{x})} \qquad (2)$$

$$S_{eff}(\vec{x}) = R_{0eff}(\vec{x}) \cdot F_{eff}(\vec{x}) \qquad (3)$$

This approach is not only a simplification to speed up calculations, but actually the effective material dependent plane wafer etch rate $R_{0-eff}(\vec{x})$ can be measured more easily than the ion etch rate and the chemical etch rate. The efficiency ratio can be considered as a material dependent calibration constant.

2.2 The Passivation Cycle

The passivation cycle is also modeled by applying a single particle approach. A homogenous velocity distribution for reactant is assumed, as in a case for the neutral radicals in the etching cycle. Therefore, the flux and surface reaction functions are identical to the flux and surface reaction functions of the $F^{\bullet}$ radicals in the etching cycle.

3 Results

Using the implementation of the previously described DRIE model three different regimes of the DRIE process were simulated and the results were compared with the experimental data. Those regimes are characterized by the ratio of the etching and passivation cycle's times.

If the duration of the etching cycle is short, the ions either cannot penetrate the passivation layer formed during the passivation cycle, or only a very small part of the trench at the bottom and near the corners can be freed of passivation layer material by the sputtering reaction. The consequence is that no proper trench shape can be formed because the chemical etching process never attacks the whole structure at the trench' bottom. The resulting trench shape obtained by simulation is shown in figure 1, and the corresponding experimental result (REM image) is shown in 2.

If the passivation time is reduced, the overall passivation layer's thickness is also reduced, and the chemical etching process can attack the whole area at the bottom of the trench. Nevertheless the shape at the bottom of the trench is still strongly influenced by the duration of the passivation cycle. For a ratio 1:1 of passivation over etch time, the resulting trench' bottom is shown in figure 3, and the corresponding experimental result is shown in figure 4.

Finally if the passivation time is further reduced, the etching process dominated which can be seen at the bottom of the trench and also on the side walls. The shape of the trench' bottom when the ratio passivation over etch time was 1:2 is shown in figure 5 (simulation) and figure 6 (experiment).

4 Conclusion

In this work we have presented a numerical model for the simulation of DRIE processes. The model has been implemented into the three-dimensional simulation environment of *Victory-Process* via its open modeling interface and has been successfully calibrated on the basis of a series of trench etching experiments.

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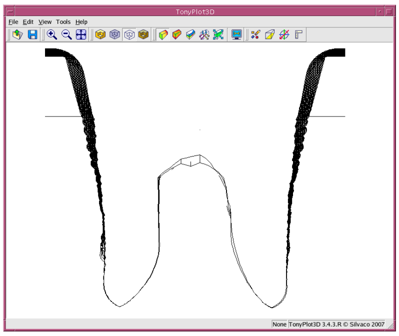

Figure 1: Simulation result obtained when applying the DRIE model with long passivation cycle times (2:1)

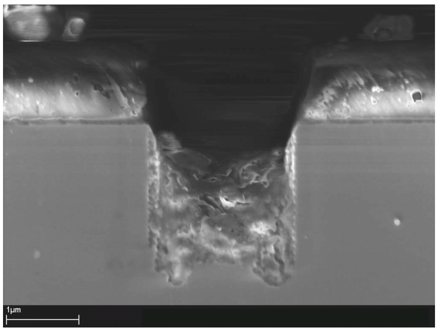

Figure 2: REM image of a trench obtained by DRIE processing with a passivation/etch time ratio of 2:1

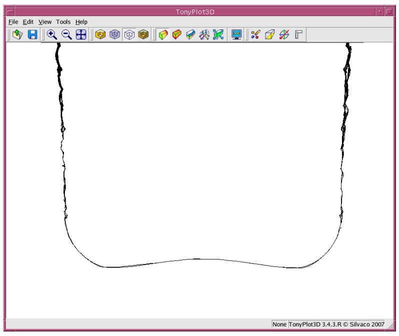

Figure 3: Simulation result obtained when applying the DRIE model with passivation cycle times of the order of the etching cycle times (1:1)

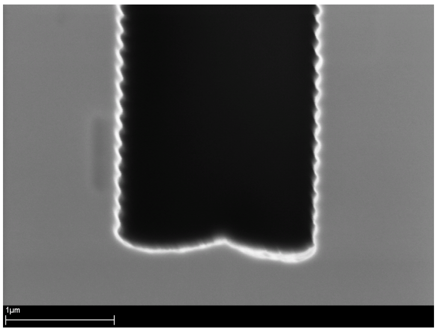

Figure 4: REM image of the bottom of a trench obtained by DRIE processing with a passivation/etch time ratio of 1:1

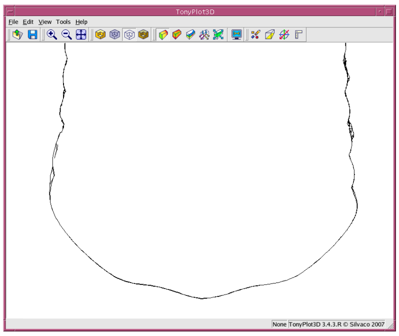

Figure 5: Simulation result obtained when applying the DRIE model with passivation cycle times shorter than the etching cycle times (1:2)

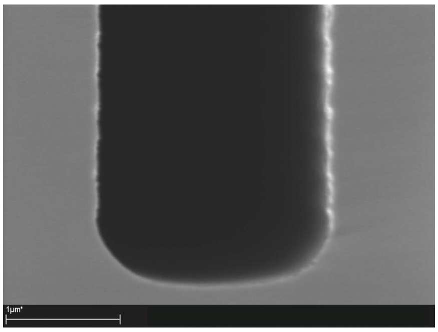

Figure 6: REM image of the bottom of a trench obtained by DRIE processing with a passivation/etch time ratio of 1:2