Simulations for Surface Evolvement and Footing Effect in ICP DRIE Fabrications

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Abstract. Simulations of surface evolvement are performed using an ICP DRIE model, in which a new method is adopted for the material identification. The simulation and experimental results are shown in this paper, which indicate that the veracity provided by this modified model is satisfied. The high-efficiency of this model over other former ones are due to the ability of identification of different material by uniform algorithm, and accordingly, it has much shorter executing time. Furthermore, an approximate model is presented to simulate the footing effect in DRIE fabrications, with the simulation results of the surface affected by footing effect in accordance to the experiments.

1. Introduction

Deep reactive ion etching (DRIE) of silicon enables the microfabrication of high-aspect ratio structures for MEMS applications. To make the microstructures being etched deeper and avoid the slopes of sidewalls, a process named time multiplexed deep etching (TMDE) or Bosch process[1] is adopted in modern ICP etching equipments, which includes both etching and deposition steps. It is important to forecast the etched surface by processing simulations to reduce the testing costs and optimize the fabrication parameters. However, there is few researcher that develops the models or simulators for etching processes of this type. A novel ICP DRIE model based on time multiplexed deep etching has been developed[2]. The model couples the advanced plasma sheath approximation and has the simple structure based on string algorithm[3]. In spite of simple surface evolvement algorithm, this model has the ability to identify different types of etched materials efficiently. In the etching model, ion-assistant etching plus uniform etching is taken as whole etching part, and the deposition rate is set to be isotropic. The present work is to do some modifications to the algorithm of the material identification, and a more precise description is adopted. The simulation and experimental results are also shown in this paper, which indicate that the veracity provided by this modified model is satisfied.

Since Silicon-on-insulator (SOI) wafers are very frequently used for MEMS, and the footing effect may then take place at the silicon/insulator interface when the silicon is overetched, pilot study on simulation of footing effect has been made by an experimental fitting method. A simple expression for describing the undercut profile is proposed, with the primary parameters that can determine the shape of the undercut profile after these parameters are chosen by experimental data. The simulation results of the surface affected by footing effect are in quite accordance with the experimental ones.
2. Models

2.1. Sheath Mode
As for the ion transport from the plasma to substrate surface, scattering of ions within the sheath is negligible in ICP equipments. Thus, the directionality of ions striking the substrate may be primarily affected by the temperature or random motions of ions in the plasma. For simplicity, ions in bulk plasma enter a collisionless and time-independent sheath with an isotropic Maxwellian velocity distribution\[4\]. Then the ions are accelerated toward the substrate without collisions, and finally strike the substrate surface. As the distribution function is kept constant along a particle path, the velocity distribution on substrate surface is given by the distribution function, \( f(\vec{v}) \)[2], where \( \vec{v} = (v_x, v_y) \) is the ion velocity at the substrate surface. And then the incident ion flux onto the substrate can be got with \( f(\vec{v}) \)[2].

2.2. Etching model
In 2-D infinitely long trench etching, the incident ion flux is assumed to be governed by geometrical shadowing effects of the structure. The opening window \((\theta_1 \leq \theta \leq \theta_2)\) limits the trajectories of the ions traveling in straight lines toward the surface points in the feature. The etched boundary of substrate is approximately described with strings connecting the points of the surface. The boundary is advanced in small discrete time steps by moving each point \( P \) along an outer normal at the local surface with certain etch rate \( ER(P) \)[4], where the normal is approximated as the bisector of the angle formed by two strings connecting this point.

For ion-assistant etching, there is the expression elided the signs of \[5\]

\[
ER_i = \frac{1}{\rho_{Si}} Y_{Si} \cdot \Gamma_i \cdot \alpha = \frac{1}{\rho_{Si}} Y_{Si} \cdot \alpha \cdot \Gamma_{i0} \int_{\theta_1}^{\theta_2} G(\theta) \cos(\theta - \psi) \, d\theta
\]

(1)

where \( \rho_{Si} \) is the atomic density of Si substrate (\( \rho_{Si} = 5.0 \times 10^{22}\)cm\(^{-3}\)), \( \psi \) is the slope angle of the surface, \( \alpha \) is the surface coverage of adsorbed neutrals thereon, and \( Y_{Si} \) is the sputter yield (number of adsorbed neutrals removed per incident ion) for a saturated surface with \( \alpha = 1 \). For the model of this paper, \( \frac{1}{\rho_{Si}} Y_{Si} \cdot \alpha \cdot \Gamma_{i0} \) is substituted by a parameter \( eri \), which is proportional to the value of \( \Gamma_{i0} \) approximatively.

The other part of the etching model is uniform etching, which is reasonable based on the assumption of isotropic angular distribution of incident neutral flux. Being ignored the re-emission of neutrals in the microsubstrate, the uniform etching rate is given by

\[
ER_n = ern
\]

(2)

where \( ern \) is a constant. Then the total effect of etching is the linear addition of ion-assistant etching part and uniform etching part in the etching model

\[
ER = ER_i + ER_n
\]

(3)

2.3. Deposition model
The passivation during time multiplexed deep etching, which is actually a deposition process, can help to keep the vertical sidewalls. The small difference of deposition models has little influence on the simulation results since the polymer layer is very thin in practice. Therefore the isotropic deposition model is adopted, and the deposition rate \( DR \) is

\[
DR = dep
\]

(4)

where \( dep \) is a constant.

2.4. Time multiplexed deep etching
Time multiplexed deep etching (TMDE), which is a popular method to get high-aspect ratio structures, is very important in MEMS fabrications. It can be described as the repetition of etching cycle and
deposition cycle with the mentioned models, and it can obtain vertical sidewalls with high etching rate due to the passivation of sidewalls.

2.5. Material identification

Because the surface materials after etching or deposition step are different, and the surface component is ideally silicon after etching while polymer after deposition, the corresponding etching rates are different. To resolve this problem of material identification, some researchers adopted a string–cell hybrid method based on string structure and cell structure[6]. The subsequent disadvantage caused by the hybrid data structure is that the total executing time is determined by the slower algorithm, i.e. the cell algorithm. Because single string algorithm is used to achieve this material identification without any other type of structure in our model, the simulation efficiency can be improved greatly and the executing time will shorter than the cell algorithm or quasi cell algorithms by one order of magnitude in practice.

There is a status parameter \( S \) setting in the program for every point on the etched surface. If the material is judged to be silicon, \( S=S_s \), and if the material is judged to be polymer, \( S=S_p \). Recording the profile situation formed by \( S \), and comparing it with the profile formed by former \( S_p \) or \( S_s \), the type of material being etched can be identified. For example, when \( S_p<S<S_s \), the deposited polymer are being etched, but when \( S<S_p \), it indicates that the polymer formed by former depositions have been cleaned away and the silicon are being etched. The brief illumination is shown as Figure 1. After the first etching and deposition cycle, the surface (or interface) is formed by the points of \( S_s \) and \( S_p \) respectively, as shown as Figure 1(a). And after the second etching process, the new surface is made up of two kinds of points, as shown as Figure 1(b). The deposition will then take place based on the surface determined in Figure 1(b), as shown as Figure 1(c). Thus, the material identification can be achieved by these repeated cycles. The surfaces (or interfaces) figured by solid lines are formed by points of \( S_p \), and the surfaces (or interfaces) figured by dash lines are formed by points of \( S_s \) in figure 1.

![Figure 1. Schematic illustration of material identification by single algorithm](image)

2.6. Surface model of footing effect

Deep reactive ion etching through the silicon device layer is an essential step in microstructure fabrication. However, plasma etching the silicon over the insulator layer has long been recognized to result in a silicon footing problem at the silicon/insulator interface. There is not a canonical or classical theory that can explain and describe this important effect to the present. To simulate the etched profiles affected by footing effect, the experimental data is used here to abstract the relationship between the trench widths and the maximal undercutting depths. The graph of the trench widths and the maximal undercutting depths of certain DRIE process[7] is shown as Figure 2. The polynomial fit of four stages is performed to approximate the trend of the variety, which is also shown in Figure 2. Then an expression of profile characteristic is assumed as

\[
Y = \left(2/\sqrt{2\pi} \cdot \sigma\right) \cdot \exp\left(-X^2 / 2/\sigma^2 / 2.5^2\right)
\]

where \( Y \) is the coordinate of undercutting, \( X \) is the vertical depth of the trench.
When \( X \) equals to 0, \( Y \) will be the maximum \( Y_0 \). Then \( Y_0 \) is set to equal to the value of former polynomial, which is the function of trench width, the parameter of \( \sigma \) can then be determined. Therefore, the only parameter in current profile equation will be gotten under a certain fabrication condition.

![Figure 2. Polynomial fit for the experimental data of footing depth and trench width](image)

3. Simulation and experimental results

3.1. Simulations and Experiments of TMDE

The simulation results of TMDE are obtained using the aforementioned method with \( e_{ri}=0.09 \), \( e_{rn}=0.01(\mu m/s) \) and \( d_{ep}=0.004 \). Referring to a stable working status of ALCATEL adixen 601E ICP plasma etching system for MEMS with etching period of 7 seconds and deposition period of 2 seconds, 7 repetitions in the algorithm for single etching module and 2 repetitions for single deposition are made. To the deposited polymer, \( e_{ri} \) is set to be 0.25 and \( e_{rn} \) to be 0. The width of etched window is set to be 5\( \mu m \) with aspect ratio of 12:1 in Figure 3, and the width of etched window is 10\( \mu m \) with aspect ratio of 7:1 in Figure 4. The mask material is SiO\(_2\) and the thickness is 1\( \mu m \) in these two figures. At the same time, experiments have been done to validate the simulation results. The etching period of the equipment is just 7 seconds and the deposition one is 2 seconds, with some other autoregulative parameters of the system, which need not be considered by the current model. After comparing these simulation results with the experiments, the conclusion can be gotten that this model has applicability to general simulations for different aspect ratio structures, and it is visible to lateral etching effect and micro scallops under the masks.

![Figure 3. Simulation results of etched profiles for a trench structure by TMDE with etched window of 5\( \mu m \) and aspect ratio of 12:1 and experimental result (a)2-D simulation (b)corresponding SEM microphoto](image)

![Figure 4. Simulation results of etched profiles for a trench structure by TMDE with etched window of 10\( \mu m \) and aspect ratio of 7:1 and experimental result (a)2-D simulation (b)corresponding SEM microphoto](image)
3.2. Simulations and experiments of footing effect

The simulation of footing effect follows the three steps as described. Firstly, the polynomial fit is performed according to the experiment data of maximum footing depths and etched windows, so as to get the relationship of these two parameters. Secondly, the expression according to the surface character to describe the etched profiles of the footing region is assumed to be a quasi Gauss distribution as mentioned as Equation 5. Finally, the parameter in the expression will be determined by the polynomial. Based on the experimental data and corresponding SEM microphotos[7], the profile simulations are performed, and the simulated results are shown in Figure 5. The experimental results are shown in Figure 6 to validate the simulations, and the experimental condition is given by Li J., et al[7].

4. Conclusion

A new method to resolve the problem of material identification in the DRIE surface model is presented, thus the material identification in the model of single surface structure data is more accurate. Furthermore, a simple surface model of footing effect is proposed and validated. The simulations of normal DRIE and footing effect are in quite good accordance with the experimental results.

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