Modified Model for Sacrificial Layer Etching

Chang-ju Wu, Hui-lian Ma, Yue-lin Wang and Zhong-he Jin*
Department of Information & Electronic Engineering, Zhejiang University, Hangzhou, 310027, China

Abstract: Sacrificial layer etching with different structures is studied in this work. It is found that the existed model doesn’t match with the experimental data well. A modified model is proposed by considering the diffusion coefficient of HF as a function of temperature and concentration in the solution. In the modified model, the decrease of the HF concentration will cause the increase of the HF diffusion coefficient, which will partly compensate the decrease of the concentration caused by the long diffusion distance. In this way, the modified model matches with the experimental data very well both for channel structure and bubble structure. Combined structures are also studied in this work. Some interesting phenomena are observed during the etching of the combined structure, including the etching rate jumps down or up near the joint area. The proposed model can explain these phenomena well.

0 Introduction
HF etching of sacrificial layer is an important process in surface micro-electro-mechanical systems (surface MEMS). In fabrication process of many important surface MEMS devices, over etching is harmful to the structure layer[1]. Therefore, precise prediction of the etching process will save process time and protect the structure layer from over etching as well. Some models have been proposed to describe the etching process, such as Monk’s[1,2,3] and Liu’s[4] combined first-and-second order release-etching model. For short etching time at room temperature, these models fit the etching process well. However, it is still not clear whether the model could fit the extended etching process at different temperatures.

On the other hand, the structures used in MEMS are various. Channel (or port), bubble and joint of channel are the most general structures. The etching behavior in the joint structures is more complex than that in the single one. Eaton et al[5] proposed a model to calculate the etching rate in the joint channel. The model predicts the etching rate decreasing quickly when the etching proceeded from a narrow channel to a wide channel, because the etching front area increasing rapidly. However, no experimental results are observed to support this phenomenon[6] till now. On the other hand, it is still not clear what will happen if the etching proceeds from a wide channel to a narrow one.

In this paper, sacrificial layer etching in the channel, bubble and joint channel structures is studied in detail. A modified model to predict the etching process in these structures is proposed and compared with existed model and experimental data.

1 Model of sacrificial layer’s etching
For etching in a single channel, Liu[4] and Eaton[5] proposed,

$$\nu = \frac{d\delta}{dt} = -\frac{D M \frac{\partial C}{\partial x}}{\rho \delta}|_{x=\delta(t)}$$  \hspace{1cm} (1)

$$J_d = -D \frac{\partial C}{\partial x} = D \frac{(C_b - C)}{\delta}$$  \hspace{1cm} (2)

$$J_{HF} = k_1 C + k_2 C^2$$  \hspace{1cm} (3)

$$J_d = J_{HF}$$  \hspace{1cm} (4)

Where $\nu$ is the etching rate, $D$ is diffusion coefficient, $M$ and $\rho$ are the molecular weight and density of $\text{SiO}_2$, $J_d$ and $J_{HF}$ are the diffusion flux and reactive flux of HF, $C_b$ is the bulk concentration of the solution, $C$ is the concentration of etching front, $k_1$ and $k_2$ are the etching rate coefficients.

The diffusion coefficient in the model is assumed as a constant during the whole etching process [4,5,6]. However, studies by many chemical researchers have already shown that the diffusion...
coefficient is a function of concentration and temperature[7,8,9]. For HF solution, it could be expressed as,
\[
D(T) = \frac{RT^2}{334\eta_p F^2} \frac{n_+ + n_-}{n_n} \frac{\lambda^0_n}{\lambda^0_n + \lambda^0_{\infty}} \left(1 - \frac{0.02C}{d}\right)
\]
(5)

Where \(D(T)\) is the diffusion coefficient, \(T\) is temperature, \(d\) is density of solution.

Etching rate coefficients are function of temperature, which is given by the Arrhenius Equation[10],
\[
k_{1,2} = A_{1,2} \exp \left(-\frac{E_a}{RT}\right)
\]
(6)

Where \(A_{1,2}\) is constant, \(E_a\) is the activation energy, \(R\) is the gas constant. The values of \(A_i\) and \(E_a\) can be determined by three experiments. The etching time for all three experiments is in short time, about ten minutes, ensuring the diffusion limitation ignorable.

For bubble etching, radical system is used. Then Eq. (2) becomes,
\[
J_d = D \frac{(C_b - C)}{r \ln(r - \ln r_0)}
\]
(7)

Where \(r\) and \(r_0\) are the radii of etched disk and etching window, respectively. Other equations are the same as the channel structure.

For a joint channel structure, when the etching reaches the joint, the diffusion flux of the second channel can be evaluated by applying a total mass flux boundary condition[5].
\[
J_1 \cdot S_1 = J_2 \cdot S_2
\]
(8)

Where \(J_1\) and \(S_1\) are the diffusion flux and cross-section area of the first channel. And \(J_2\) and \(S_2\) are the diffusion flux and etching front area at the second channel. The widths of the two channels are \(W_1\) and \(W_2\), respectively. The thickness of the two channels can be set equal and marked with the letter \(H\). So \(S_1\) is the product of the \(W_1\) and \(H\). In previous model, the etching front is considered as a straight line with joint channel structure, so \(S_2\) is the product of the \(W_2\) and \(H\). This is true according to many experiments when the etching process begins from the wide channel. However, if the etching begins from the narrow one, the etching front will be an arc rather than a straight line when the etching front reaches the joint. According many experiments, it is found that the radius of the arc can be calculated as,
\[
\begin{align*}
& r^2 = \left(\frac{x + W_1}{2}\right)^2 + (r - x)^2 & x \leq \frac{W_2 - W_1}{2} \\
& r = r' + \left(\frac{x - \frac{W_2 - W_1}{2}}{2}\right) & x > \frac{W_2 - W_1}{2}
\end{align*}
\]
(9)

Where \(r'\) is the radius of the arc when \(x = (W_2 - W_1)/2\). From Eq. (9), \(S_2\) can be expressed as,
\[
\begin{align*}
& S_2 = \frac{r \pi H}{90} \sin^{-1} \left(\frac{x + W_1}{r / 2}\right) & x \leq \frac{W_2 - W_1}{2} \\
& S_2 = \frac{r \pi H}{90} \sin^{-1} \left(\frac{W_2}{2r}\right) & x > \frac{W_2 - W_1}{2}
\end{align*}
\]
(10)

So when the etching runs in the second channel, the etching length is the sum of \(x\) and the length of the narrow channel.

Eqs. (1)-(4) and (12) can be used to predict the etching process. For Eaton’s model, \(D\), \(k_1\), \(k_2\) are assumed constant for all etching processes. And \(S_2\) always equals with \(W_2 H\). In the modified model, \(D\) is a function of the temperature and HF concentration as indicated by Eq. (5), \(k_1\) and \(k_2\) are functions of temperature as equation (6). For the narrow-wide channel process, Eq. (10) is used to calculate \(S_2\). Visual C++ is employed to help the calculation of the whole etching process.

2 Experimental
The fabrication process of the samples begins from a 4-inch silicon wafer. First, a phosphosilicate-glass (PSG) layer is deposited by low-pressure chemical vapour deposition (LPCVD). The PSG layer is then patterned to form the etching structures and the rulers to indicate the etching length. A low-stress poly-silicon layer is deposited by LPCVD. The etching windows are opened by SF$_6$ plasma on the poly-Si layer. Then the wafer is cut into 5mm×5mm small samples for the etching process.

Figure 1 shows different structures’ etching photos. Figure 1(a) is the channel structure and 1(b) is bubble structures. For these two structures, the thickness of the PSG is 2.1µm, and concentration of phosphorus in PSG is 5wt%. Figure 1(c) shows the wide-to-narrow structure and Figure 1(d) shows the narrow-to-wide structure. For (c) and (d), the thickness of the PSG is 0.6µm, and concentration of phosphorus is 8wt%.

3 Results and Discussion

Figure 2, Figure 3 and Figure 4 shows etching length, etching rate and HF concentrations at the etching front as a function of etching time, respectively. The etching solution is 24, 16 and 12mol/l HF at 25°C. The sample is channel structure as shown in Figure 1a. Etching rate of experiment is obtained by difference between the neighbor data of etching length. It can be seen from Figure 2 that the etching length increases with the etching time for all three HF concentrations. And for the same etching time, the etching length increases with HF concentration. But for all three HF concentrations, the etching rate decrease with etching time as shown in Figure 3. The initial etching rate is 7.74, 3.70 and 2.22 µm/min at 24, 16, 12mol/l HF solution as indicated by both models. After etching of 1000µm, the previous model indicates that the etching rates decrease to 3.69, 2.07 and 1.37µm/min. The reduction is 52.3%, 44.1% and 38.3%, respectively. But both the experimental and the modified model indicate that the etching rates decrease not as seriously as the previous model. The ended etching rates are 4.92, 2.63, and 1.68µm/min. The reduction is 36.4%, 28.9% and 24.3%. The rates obtained by modified model are 33.3%, 27.1% and 22.6% higher than those by previous model at the etching length of 1000µm, respectively.

The etching rate decreases with etching time could be explained that the etchant concentration at etching front drops gradually during the etching process because of diffusion limitation. For both models, the HF concentration at etching front decreases with etching time as shown in Figure 4, resulting in the etching rate decreasing. However, the diffusion coefficient increases with the decrease of the concentration as indicated by Equation (5). So the etchant can diffuse to the etching front more quickly, resulting in the concentration decreasing not as quickly as prediction by the previous model.
In this way, increasing of the diffusion coefficient partly compensate the diffusion limitation. In previous model, the diffusion coefficient is considered as constant in different concentrations. So the etchant concentration of etching front in previous model drops more quickly than that in modified model. The etching length increases with the etching time quickly, according to the experimental and both models. The rate of the modified model is quicker than that of the previous one obviously. For example, to etch 1000μm, in modified model, the etching time is 806, 1432 and 2141 minutes when the HF concentration is 12, 8 and 6mol/l, respectively. In previous model, the etching time is 1091, 1857 and 2701 minutes, which are 35.4%, 29.7%, and 26.2% longer than those by the modified model, respectively.

The etching rate decreases with etching time as shown in Figure 6. For both models, the initial etching rate is 2.12, 1.06 and 0.67 μm/min at 12, 8, 6mol/l HF solution, respectively. After etching 1000μm, the etching rates decrease to 0.57, 0.35 and 0.25 μm/min in previous model. The reduction is 73.1%, 67.0% and 62.7%, respectively. But the ended etching rates according the modified model are 0.86, 0.51 and 0.35 μm/min. The reduction is 59.4%, 51.8% and 47.8%, respectively. The ended rates obtained by the modified model are 50.9%, 45.7% and 40.0% higher than those by the previous model at the extended etching process, respectively.

Comparing Figure 3 with Figure 6, the reduction of etching rate in bubble structure is larger than that at channel structure. For example, when the bulk concentration is 12mol/l, after etching 1000μm, the etching rate decreases to 0.57, 0.35 and 0.25 μm/min in previous model. The reduction is 73.1%, 67.0% and 62.7%, respectively. But the ended etching rates according the modified model are 0.86, 0.51 and 0.35 μm/min. The reduction is 59.4%, 51.8% and 47.8%, respectively. The ended rates obtained by the modified model are 50.9%, 45.7% and 40.0% higher than those by the previous model at the extended etching process, respectively.

As shown in Figure 7, the etching process can be separated to 4 stages, (1) the first 1000μm, (2)1000μm-1038μm, (3)1038μm-1140μm, and (4)the rest 160μm. At the first 1000μm, the etching length increases with the etching time quickly, according to the experimental and both models. The
initial etching rate is about 76.95μm/min for both models. The etching rate decreases quickly, indicating diffusion limited of the etching process. After 20min etching, the etching length predicted by the previous model is significant larger than that obtained by the experiment. With previous model, the first 1000μm can be etched in 70.6min. However, the actual time is about 100min according to the experiment. The difference between them reaches above 40%. The modified model can predict the etching time precisely. The error of length by modified model is less than 3.05% for the first 1000μm.

At this stage, the etching rate decrease quickly. With previous model, the etching rate at the end of the first 1000μm is about 8.11μm/min, which is about 10.54% of the initial etching rate. However, this rate is still much higher than that predicted by the modified model. With the modified model, the etching rate at the end of the first 1000μm is about 4.89μm/min. This is only about 6.35% of the initial etching rate. The decrease of the etching rate indicates the decrease of HF concentration. Figure 8 shows the HF concentration as a function of the etching time. The etching front area as a function of the etching time is also shown in the figure. The HF concentration at the etching front decreases from 22.64mol/l to 5.08mol/l, or 3.81mol/l according the previous model or the modified model, respectively.

At the second stage, the etching rate decrease suddenly in a very short time. For the previous model, the etching rate decreases from 8.11 to 2.39μm/min in seconds. This is mainly due to the etching front area increase suddenly from 15 to 60μm² as shown in Figure 8. For the modified model, the etching front at the beginning of the second channel is an arc, and the etching front area increases gradually as shown in Figure 8 and Figure 1d. The etching front area at this stage increases from 15 to 60μm² and further to 80.4μm². The etching front area could be larger than the cross section area of the channel, since the etching front is an arc. The area increase to 5.36 times of the initial 15μm², resulting in the HF concentration decreasing from 3.81 to 1.02mol/l. These further results in the etching rate decreasing gradually from 4.89 to 1.01μm/min in 19min. At this time, the etching length is about 1038μm.

For previous model, after the suddenly jumping down, the etching rate further decrease slightly during etching the second channel. For example, as the etching length reaches 1300μm, the etching rate is about 2.23μm/min. Compared with 2.39μm/min, the etching rate decreases about 6.69%. For the modified model, the etching front area decreases gradually from 80.4 to 60μm² again. This is the third stage of the etching process. In this stage, the etching rate will increase slightly, much different from the previous model. At time 190min in Figure 7, the etching rate reaches the maximum 1.49μm/min, which is 40% higher than 1.01μm/min. At this time, the etching front area decreases to 63.2μm², and the etching length reaches 1140μm. After that, the etching process goes into the 4th stage. Since the etching front area becomes stable as 60μm² again, the etching is controlled by the diffusion limited again. At the end of the total 1300μm etching length, the etching rate decreases down to 1.46μm/min, which is only 2% lower than 1.49μm/min.

Figure 9 shows the etching length and rate as a function of etching time for the wide-narrow joint channel. The length of the narrow and wide channel is 1000μm and 500μm, respectively. The concentration of the solution is 22.64mol/l. The temperature is 10°C. The etching time for the first 1000μm channel is 69min according previous model, which is 34.8% shorter than the time by experimental or the modified model. With previous model, the etching rate decrease to 11.0μm/min at the end of the first 1000μm. This value is about 13.3% of initial etching rate, 83.0μm/min. However, with the modified model, the etching rate is only about 7.9μm/min at the end of the first 1000μm, which is about 9.5% of the initial etching rate. The quick decreasing of the etching rate is again due to the diffusion limited as shown in Figure 10. The HF concentrations decrease to 4.8 and 3.8mol/l at the end of the first 1000μm with previous model and the modified model, respectively.

As soon as the etching front reaches the narrow channel, the etching rate jumps up suddenly. According to previous model, the etching rate jump to 23.1μm/min, which is 2.1 times of the value
11 μm/min. This is comparable with the etching front area jump down to 15 μm², which is 1/4 of the first channel’s section area 60 μm². For the modified model, the etching rate jump to 17.8 μm/min, which is about 2.3 times of the value 7.9 μm/min.

Then the etching rate decreases again due to the diffusion limited. Interesting is that the etching rate decrease quickly even in the second channel. This is much different from the phenomenon of the narrow-wide structure. For example, the etching rate at 1300 μm is 9.8 μm/min, which is 14.9% lower than that at 1200 μm, 11.5 μm/min, with modified model for the wide-narrow channel. However, for the narrow-wide channel, the etching rate at 1300 μm is 1.46 μm/min, which is only 1.4% lower than the etching rate at 1200 μm, 1.48 μm/min. This could be explained by the diffusion limited. For narrow-wide structure, the diffusion limited is mainly due to the diffusion in the first narrow channel. Therefore, as the diffusion length increase in the wide channel, the decreasing of the HF concentration is not significant. But for wide-narrow structure, the situation is different. The diffusion limited is mainly due to the second narrow channel. As the diffusion length increases in the second narrow channel, the HF concentration decreases significantly.

In Figure 7 and 9, one can notice that the modified model matches with the experimental data much better than previous model. However, it could be noticed that the error increases as the etching length increases even in the modified model. In figure 7, the relative error of the etching length reaches 4.8% at the end of 1300 μm. In figure 9, the error is about 5.77%. In the modified model, the diffusion coefficient in the etching front is used to calculate the whole diffusion process. Since the HF concentration at the etching front is lower than other place, the diffusion coefficient used in the model may a little higher than the actual value. This results in the overestimation of HF diffusion in the model. So the etching rate by the model will be somewhat higher than that by the experiments. But it is too difficult to consider the diffusion coefficient as a function of the location and the time. Fortunately, 5% error is acceptable for most case.

In Figure 3 and 6, one can noticed that the etching rate obtained by previous model is lower than that by modified model, as the etching temperature is above 20°C. However, in Figure 7 and 9, as temperature lower than 10°C, the etching rate by previous model is lager than that by the modified model. This phenomenon is mainly due to the diffusion coefficient used in the previous model. In previous model, D is a constant and the value used is measured by experiment at room temperature, which is about 20°C. For Figure 3 and 6, D used in the previous model is approximately equal with the initial value used in the modified model. As the etching process going on, the diffusion coefficient in the modified model will be larger than that used in previous model, because the HF concentration decreases during the etching process. So the HF concentration at the etching front and the etching rate by the modified model are larger than those by previous model. For the etching process at temperature lower than 10°C, the diffusion coefficient used in the previous model is still the value at room temperature, which is much higher than the value used in the modified model. So the etching rate by previous model would be much higher than the modified model.

4 Conclusions

The diffusion coefficient is considered as a constant in previous model. However, the difference of etching rate between the experimental and the model becomes very high at the extended etching process. A modified model is proposed to explain this phenomenon by considering the diffusion
coefficient of HF as a function of temperature and concentration in the solution. Combined structures are also studied in this work. Comparing to the previous model, the etching front of combined structures is also modified besides the diffusion coefficient. Some interesting phenomena are also observed during the etching of the combined structure. For wide-to-narrow channel, the etching front is a straight line during the whole etching process and the etching rate increases quickly near the joint area and decreases gradually after that. For narrow-to-wide channel, the etching front will be an arc rather than a straight line as the etching front reaches the wide channel and the etching rate decreases suddenly near the joint area. The sharp change of the etching rate is found mainly due to the sudden change of etching area, which results in the sudden change of the HF concentration near the joint area.

Acknowledgment
The author would thanks the Institute of Microelectronic, Beijing University, and the Shanghai Institute of Microsystems and Information Technology, CAS, Hong Kong University of Science & Technology, for the fabrication of the samples. This work is supported by National Natural Science Foundation of China (60476033) and National High Technology Research and Development Program of China (2003AA404012, 2005AA404240).

References
[1] Monk D J 1993 Controlled structure release for silicon surface micromachining, Ph. D Dissertation (California University at Berkeley, Department of Chemical Engineering)
[2] Monk D J, Soane D S and Howe R T 1991 Int. Con. on Solid-State Sensors and Actuators 647
[3] Monk D J, Soane D S and Howe R T 1992 Solid-State Sensor and Actuator Workshop, IEEE 46
[4] Liu J Q, Tai Y C, Lee J, Pong K C, Zohar Y, and Ho C H 1993 Proc. of Micro Mechanical Systems, IEEE 71
[5] Eaton W P, Smith J H, and Jarecki R L 1996 Micromachined Devices and Components, Proc. of the SPIE 2882 1
[6] Eaton W P, Jarecki R L, and Smith J H 1997 Int. Con. on Solid-State Sensors and Actuators 249
[7] Reid R C, Prausnitz J M, and Poling B E 1977 The properties of gases & liquids (New York: McGraw-Hill) 566-595
[8] Gordon A R 1937 J. Chem. Phys 5 522
[9] Harned H S, and Owen B B 1950 The physical chemistry of electrolytic solutions N.Y, Reinhold publishing Corporation 12
[10] Judge J S 1976 Proc. of the Symp. on Etching for Pattern Definition H G Hughes and M J Rand, Eds. Princeton (New Jersey) 19