Modeling of Deep Si Etching in Two-Frequency Capacitively Coupled Plasma in SF$_6$/O$_2$

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Abstract. We developed the simulation model of deep Si etching for MEMS fabrication. This model includes the physical effect of ions under the presence of plasma molding, chemical etching by radicals, and the formation of a passivation layer on the wafer. The simulation was carried out in SF$_6$/O$_2$ in two-frequency capacitively coupled plasma using an extended vertically integrated computer aided design for device processing (VicAddress). We estimated the local characteristics of plasma structures (such as potential distribution, ion velocity distribution) near an artificial microscale hole pattern on the wafer. In this case, the sheath thickness is comparable to or even smaller than the size of the hole. Thus, the sheath tends to wrap around the hole on the wafer. The distorted sheath field directly affects the incident flux and velocity distributions of ions. The angular distribution of ions at the edge of the hole is strongly distorted from the normal incidence. The ion flux becomes radially nonuniform in the vicinity of the hole pattern. That is, the etching profile is distorted particularly at the bottom corner because of the removal of the passivation layer by energetic ion under the presence of plasma molding.

1. Introduction
Micro-electro-mechanical systems (MEMS) has been developed on the basis of the technique utilized in micro fabrication of semiconductor device. Deep Si etching for MEMS fabrication with several tens or hundreds $\mu$m in width and depth strongly requires a high speed, high selectivity and high anisotropy. Fluorine-containing plasma, such as SF$_6$, are widely used in deep reactive ion etching (Deep-RIE) of large-scale Si that used in MEMS fabrication. In order to perform Deep-RIE, it is important to control a balance between sidewall passivation and bottom etching caused by reactants such as ions, radicals. For example, Bosch process is based on a cycle of etching and passivation processes under different gas chemistries in a room temperature[1]. Another approach is the plasma etching of Si substrate with bias voltage under cryogenic temperatures, where the sidewall will be protected by forming an passivation layer[2, 3]. F radicals incident on the Si surface saturate the dangling bond and insert into the Si-Si bond, resulting in an ejection of volatile particles, SiF$_4$, as the major etching product. The spontaneous etching of Si by F radical with a very high etching rate causes an isotropic etching profile. Thus, O$_2$ is added to SF$_6$ in order to protect the sidewall by forming the SiO$_x$F$_y$ (siliconoxyfluoride) layer[4, 5]. In addition, SF$_6^+$ ions remove the passivation layer and are responsible for the RIE of Si on the bottom, resulting in the increment of etching anisotropy. Especially in large-scale etching, plasma molding is one of the important issues[6]. The sheath tends to wrap around the micro-scale structure on a wafer because the sheath thickness will be
comparable or even smaller as compared with the size of the structure. The distorted electric field in the sheath will have a direct influence on the flux and velocity distribution of ions incident on the wafer. As a result, the ion angle distribution deviates from the normal incidence. The ion flux toward the trench surface becomes highly nonuniform as a function of radial position, resulting in less anisotropy of etch profile. That is, in the case of the large-scale etching, it is possible that positive ions incident on the wafer surface in the distorted sheath field make a contribution to removing the passivation layer on the sidewall as well as bottom. This implies less anisotropy of etch profile. These phenomena are intrinsic to a large-scale etching in MEMS fabrication and are not observed in a nano-scale etching in ultra-large scale integrated (ULSI) process.

In our previous study, the influence of the ion transport under the distorted electric field on the anisotropic etching of Si was discussed in [7]. Then, we numerically investigated feature profile evolution of deep Si etching under the presence of plasma molding in a two-frequency capacitively coupled plasma (2f-CCP) in SF$_6$/O$_2$. We focused on ion transport by plasma molding and the effects of neutral reactions, including the spontaneous etching and the mechanism of inhibiting the sidewall etching by forming the passivation layer, on the etching profile on the size of MEMS [8]. These investigation are based on the two-dimensional time-dependent (2D-t) plasma structure using an extended vertically integrated computer aided design for device processing (VicAddress) [9].

2. Model Description
A procedure of the simulation is structured as follows (see Fig. 1): (1) The time varying two-dimensional cm-scale plasma structure in the 2f-CCP reactor is calculated by using the Relaxation Continuum (RCT) model [9]. (2) By using the whole plasma structure in the reactor, we recalculate the mm-scale plasma structure near the artificial hole pattern. (3) The trajectory of the positive ions incident on the Si wafer is traced using the Monte Carlo technique under the distorted electric field in the sheath. (4) Feature profile evolution of deep Si etching is estimated by the Level Set method under the presence of the plasma molding.

2.1. 2D-t Plasma Structure in 2f-CCP Reactor
The plasma characteristics in the narrow-gap 2f-CCP are calculated by using the RCT model. A schematic diagram of the 2f-CCP reactor and the external conditions considered in this study are shown in Fig. 2(a). The reactor is assumed to be axisymmetric with respect to the z-axis and has two parallel-plate electrodes with a diameter of 80 mm and a separation of 20 mm; the upper electrode, driven by a very high frequency of 100 MHz and an amplitude of 300 V, is responsible for the production of high density plasma, whereas the lower bias electrode, driven by 1 MHz and 100 V, is for the supply of energetic ions to the wafer surface. In this study, a Si wafer is set on the biased metallic electrode through a blocking capacitor of 500 pF to the bias rf source. The operating feed gas and the pressure are SF$_6$ (83%)/O$_2$ at 300 mTorr in Si etching. The charged particles considered in this study are SF$_5^+$, SF$_6^+$, SF$_5^-$, F$^-$, O$_2^+$, O$^+$, O$_2^-$, and an electron. And the neutral particles are F, SF$_2$ (x = 3 ~ 5), F$_2$, O($^1D$), O$_2$(a$^1D_x$), SO$_2$ (x = 2 ~ 4), and SO$_2$F$_2$. The time constants for diffusion of electrons, ions, and neutral species are $\tau_{e,i} \leq \mu$s and $\tau_N \sim$ ms. Thus, the numerical calculation of the governing equations based on the RCT model is performed self-consistently in a manner having different time steps, $\Delta x_i t = 10^{-11}$ s and $\Delta N t = 10^{-8}$ s. The computational time to simulate a plasma structure in the reactor in a periodic steady state is improved by a factor of 10. The reaction set for SF$_6$/O$_2$ plasma is shown in [8]. The electron impact cross sections of SF$_6$ and O$_2$ are those used in our previous studies [7, 8, 10, 11, 12, 13]. The rate coefficients of electron impact with SF$_6$ and O$_2$ are given from the analysis of the Boltzmann equation [14], and the other rate coefficients, such
as ion-ion, ion-molecule, molecule-molecule reactions, are the same as those used in our previous study[8].

2.2. Plasma Structure near Hole Pattern

In order to estimate the effects of plasma molding during etching, we will evaluate the phenomena associated with a hole having a 250~300 μm radius and a 100~500 μm depth on the Si wafer located on the lower bias electrode. We recalculate the plasma profile in the vicinity of the hole pattern to reduce the computational time[7, 8]. The artificial hole pattern and the recalculation region are shown in Fig. 2(b). In the first step, the whole plasma profile in the reactor in a periodic steady state is calculated without considering the effect of the microscale hole pattern. In the next step, in order to investigate the effect of the structure on the sheath (i.e., plasma molding), we calculate the plasma profile near the hole pattern with fine Δt, Δr, and Δz as compared to those of the first step, by using the cm-scale plasma structure as boundary conditions at the top and the right hand side of the recalculation region. The self-bias voltage can be given from the radial flux profile on the entire surface of the Si wafer. As is well known, the area where the hole pattern has possible influence on the plasma structure is limited to the sheath region in front of the biased electrode. In our model, the recalculation region is at least twice wider than the sheath area. The ratio of the computational volume between in the first
and the second step is more than $10^2$, and the plasma structure except for the limited region in the second step is unchanged.

2.3. Ion Velocity Distribution
The positive ion trajectory incident on the structured Si wafer from the plasma/sheath boundary is traced using the Monte Carlo technique[15] under the distorted potential distribution, i.e., plasma molding. In this study, we consider the main positive ion SF$_5^+$ as the ion affecting the wafer reaction, and the collision between SF$_5^+$ and SF$_6$ in the gas phase is considered as the interaction of 9-4-6 potential[16].
2.4. Feature Profile Evolution

The temporal evolution of the etching profile is estimated according to a competitive process between etching and deposition by the Level Set method\[17, 18\] under the presence of plasma molding. That is, the surface evolution is expressed by a Hamilton-Jacobi type of equation,

$$\frac{\partial \Phi(x, z, t)}{\partial t} - R_{\text{eff}}(x, z, t) |\nabla \Phi(x, z, t)| = 0,$$

where $\Phi(x, z, t)$ is a level set function and $R_{\text{eff}}(x, z, t)$ is the effective etch rate. We will construct a feature profile model of Si etching exposed to SF$_6$/O$_2$ plasmas by considering a two-layer film mode\[18\], i.e., a film consisting of a bare Si layer and overlaying SiO$_x$F$_y$ layer. The detailed calculation model for the Deep-RIE of Si in SF$_6$/O$_2$ is described in \[8\].

3. Results and Discussion

The axial density distribution of the charged particles at the center of the reactor, $r = 0$, is shown in Fig. 3(a) in a time-averaged form. The density of negative ions, such as F$^-$, SF$_6^-$, SF$_5^-$, is much higher than that of electron. Typical characteristics of negative ion plasma are formed in SF$_6$(83%)/O$_2$ at 300 mTorr. The flux of the charged and neutral particles incident on the Si wafer is shown in Fig. 3(b) in a time-averaged form. As a result, we consider the SF$_5^+$ ion and F radical as main etchant of Si etching in this study. In addition, SF$_6$ radical contributes to the chemical etching of Si with F and is considered to the effective flux of F radical. The ground state of the atomic oxygen, O($^3P$), forms the passivation (SiO$_x$F$_y$) layer on the Si wafer in order to protect the sidewall. The flux of SF$_5^+$ is responsible for removing the passivation layer on the bottom and contributes to the RIE with F radicals on a partially oxidized Si in this case.

Figure 4 shows the comparison of the potential distribution close to the hole surface at different hole radii. In the case of the smaller hole radius as shown in Fig. 4(a), plasma molding is observed only near the top-corner of the hole. On the other hand, in the case of the larger hole radius as shown in Fig. 4(b), the potential distribution wraps around the hole. The sheath thickness (\(\approx 1\) mm) is smaller than the hole diameter, and the plasma molding is also observed at the bottom. The penetration of the potential into the hole also depends on the hole diameter. Thus, when the size of the hole diameter is comparable or greater as compared with the sheath thickness, the electric field at the hole bottom is strengthened similar to the case in the flat wafer surface.

The SF$_5^+$ flux ion velocity distribution incident on a hole with 250 µm in radius and 500 µm in depth at $z = 0$ is shown in Fig. 5 in a time-averaged form. The positive value of the angle corresponds to the ion from the inside to the outside of the wafer, and the negative value from the outside to the inside of the wafer. At the center of the hole the normal incidence of the ions is dominant. In contrast, at the edge the ion energy distribution is shifted to the higher side due to the self-bias voltage and the ion angler distribution is distorted especially at the low-energy region. In the LF-biased process, the temporal and spatial change of the potential and ion velocity distribution in the vicinity of the hole causes anomalous etch profile by energetic ions in large-scale etching used in MEMS fabrication. That is, this result implies that ions incident on the wafer under the presence of plasma molding removes the passivation (SiO$_x$F$_y$) layer on the sidewall or bottom corner, resulting in the decrement of the etch anisotropy.

Through a series of modeling of the 2D-t plasma structure in the whole reactor and near the artificial hole pattern, we predict the feature profile evolution of Si exposed to the 2f-CCP in SF$_6$/O$_2$ under the flux velocity distribution of ions and neutral radicals characterized as a function of radial position at the top of the wafer, $z = 0$. One example of the feature profile evolution is shown in Fig. 6 to estimate the effect of plasma molding during the Deep-RIE of Si under the distorted ion velocity distribution as a function of radial position at the top of the structure. Figure 6(c) shows the feature profile evolution by RIE caused by both SF$_5^+$ ions and
Figure 3. Time-averaged profiles of number density of charged particles as a function of axial position at $r = 0$ (a), and flux of charged (solid line) and neutral (dotted line) particles incident on the wafer (b) in 2f-CCP in SF$_6$(83%)/O$_2$ at 300 mTorr[8]. The external conditions are shown in Fig. 2.

F radicals without the mechanism of inhabiting the sidewall. Due to a much higher etching rate of Si by F radicals than that by considering physical effect of SF$_5^+$, the influence of the plasma molding on the feature profile is not observed. In addition, the bowed and undercut profiles appear significantly at the sidewall and near the silicon-mask interface because of the chemical etching [see Fig. 6(b)]. The feature profile evolution of Si by RIE with the passivation layer formed by O radicals is shown in Fig 6(d) under the presence of the plasma molding. For physical ion etching under the presence of the plasma molding, the etching profile characterizes the direct effect of ions incident on each of local positions [see Fig. 6(a)]. As shown in Fig. 5(c) in
Figure 4. Time-averaged potential distribution in vicinity of structural hole of 500 µm in depth and with different radii of 250 (a) and 1000 µm (b) in 2f-CCP in SF<sub>6</sub>(83%)/O<sub>2</sub> at 300 mTorr[8]. The external conditions are shown in Fig. 2.

The vicinity of the edge, the incident angle of the ion shifts 10° toward the sidewall. That is, the removal of the passivation (SiO<sub>x</sub>F<sub>y</sub>) layer by energetic ions at the bottom corner is strengthened by the effect of excess ion flux with distorted angular distribution. On the other hand, an insufficient amount of ions leads to less efficient removing the passivation layer at the center of the bottom. In this study, we assume that the effective chemical etching yield of Si layer for F radicals is higher than that of passivation, SiO<sub>x</sub>F<sub>y</sub>, layer by a factor of 10<sup>3</sup>[8]. Thus, when the passivation layer is removed by SF<sub>y</sub><sup>6</sup> ion impact, the etching of Si is enhanced by addition of F radicals. As a result, this indicates that anisotropy of the etching profile is not achieved especially at the bottom under the effect of the plasma molding.
Figure 5. Flux ion velocity distribution of SF$_5^+$ incident on hole of 250 $\mu$m radius and 200 $\mu$m depth on Si-wafer (a) at center and (b) edge of hole[8]. The external conditions are shown in Fig. 2.

Figure 6. Feature profile evolution under presence of plasma molding: only by considering physical effect of SF$_5^+$ ions (a), only by F radicals (b), by RIE caused by both SF$_5^+$ ions and F radicals (c), and by RIE with passivation layer formed by O radicals (d)[8]. The external conditions are shown in Fig. 2.

4. Summary
We developed the simulation model of deep Si etching under the presence of plasma molding for MEMS fabrication, including physical ion etching, chemical etching by radicals, and passivation layer formation on the wafer. The numerical investigation of Deep-RIE of Si with several
hundreds of micrometers was carried out in SF$_6$(83%)/O$_2$ at 300 mTorr in 2f-CCP by using the extended VicAddress[9]. The influence of the ion transport under the presence of the plasma molding on the feature profile was investigated and discussed. Then, the influence of ions, neutral radicals and the mixture of ions and radicals was also discussed in terms of the feature profile of Si. In the deep Si etching, the sheath thickness will be comparable to or even smaller than the size of the structure. Due to the effects of the plasma molding, a distorted electric field in the sheath directly affects the flux and velocity distribution of ions incident on the wafer. That is, the ion trajectory is distorted toward the bottom edge. The ions incident on the wafer under the distorted sheath field remove the passivation (SiO$_x$F$_y$) layer on the bottom corner, whereas an insufficient amount of ions leads to less efficient removing the passivation layer at the center. Thus, the feature profile evolution indicates that etching is enhanced particularly at the bottom corner with time, resulting in the suppression of anisotropy of the etch profile.

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