Flux based modeling and simulation of dry etching for fabrication of silicon deep trench structures

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Abstract

Deep reactive ion etching (DRIE) process is a key growth for fabrication of micro-electromechanical system (MEMS) devices. Due to complexity of this process, including interaction of the process steps, full analytical modeling is complex. Plasma process holds deficiency of understanding because it is very easy to measure the results empirically. However, as device parameters shrink, this issue is more critical. In this paper, our process was modeled qualitatively based on “High Density Plasma Etch Model”. Deep trench solutions of etch rate based on continuity equation were successfully generated first time through mathematical analysis. It was also proved that the product of fluorine and gas phase concentration in SF₆ remains identical during both deposition and etching stages. The etching process was treated as a combination of isotropic, directional and angle-dependent component parts. It exploited a synergistic balance of chemical as well as physical etching for promoting silicon trenches and high aspect ratio structures. Simulations were performed for comprehensive analysis of fluxes coming towards the surface during chemical reaction of gas. It is observed that near the surface, the distribution of the arrival flux follows a cosine distribution. Our model is feasible to analyze various parameters like gas delivery, reactor volume and temperature that help to assert large scale effects and to optimize equipment design.

Keywords: DRIE, Plasma modeling, Silicon deep trench, MEMS

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1. INTRODUCTION

The dry etching of deep trenches and contact holes in single crystal silicon is valuable for an ample variety of applications in micro-electromechanical systems (MEMS). Wet chemical etching was dually replaced in the late 1970s by a dry etching using reactive plasma in semiconductor processing technology field [1]. Reactive ion etching (RIE) that realized a directional etches profile without an undercut for excellent line delineation was established [2]. In the last 20 years, to endorse the auxiliary shrinkage and precision etching, low-pressure and higher density plasma generation were developed such as magnetron RIE [3], electron cyclotron resonance (ECR) and inductive-coupled plasma (ICP) sources. The plasma etching is especially beneficial in microfluidics because the hydrophilicity of the etched surfaces is regulated with $O_2$ plasma exposure after etching [4-5]. The design of the majority of micro-electro-mechanical systems (MEMS) requires silicon-etch step at some stage in production sequence because MEMS/ NEMS devices are being created commencing silicon due to sticking coefficient $S_e$ inherent properties like material strength, miniaturization, integration, low electric power and low cost [6]. Therefore, polysilicon is used as a mature manufacturing material and to develop high aspect ratio and etch rate. As plasma etching of deep structures is complex because the etch rate depends on feature size, etch time and aspect ratio so dry etching of silicon oxide is one of the key steps not only in silicon integrated circuit (IC) fabrication but also in other applications such as the fabrication of optical wave guides [7-8]. Standard RIE of Si, used in the IC industry, utilizes a synergistic balance of chemical and physical etching to produce silicon trenches and structures with aspect ratios on the order of 5:1 [9-10]. Currently chlorine and fluorine based gases are being extensively used in plasma etching. To improve the device performance and yield, silicon etching requires a high etch rate, a vertical profile, surface morphology and low etch induced smash up. As the
MEMS devices entail extremely elevated structures or extremely deep trenches, now often on the order of 35:1 for which standard RIE is incapable of meeting this requirement. Only DRIE is handy for deep trenches. Previously, \(SF_6\) and the \((c-C_4F_8)\) plasma reactions by themselves have been modeled extensively [11-12].

In this paper, we selected \(SF_6\) gas for etching because it releases six fluorine atoms with more than 16 eV energy. These fluorine atoms then spontaneously retort with the \(Si\) material, forming volatile \(SiF_4\). In this switching process, \(SF_6\) etches the silicon substrate in the etch cycle and the sidewall will be coated by \(C_4F_8\) in the passivation cycle to prevent undercutting. Modeling of the DRIE is to be involved into the integration of two models (deposition and etch models) and include a mechanism to remove the polymer from the trench bottom during each cycle. Our followed process is modeled on the bases of “High Density Plasma Etch Model” as this model is capable of specifying different etch rates or depositions for different materials. This model assumes that the etching is composed of isotropical and anisotropical conditions. Comprehensive analysis of fluxes towards the surface during chemical reaction of gas is obtained by using simulation software tool named as “Taurus Topography”, in which numerical methods are used to describe fully the fluxes at the wafer surface for particular equipment and topographical configurations.

2. PROCESS MODELING

The deposition and etch steps are performed separately on \(Si\) wafer surface to analyze the percentage of fluorine and sulphur contents during chemical reaction of \(SF_6\) with surface. Two steps are considered at this time for derivation. In the deposition step, plasma splits apart the strained cyclic hydrocarbon \((c-C_4F_8)\) into extremely excited fragments. The individual fragments react with one another on the exposed surface and build up a more or less strongly cross-linked layer of polymer. Although many neutral and ionic species are
generated, the highest fluxes of species at the surface during deposition are measured to be $CF_2$ and $C_2F_4$. The general chemical reactions are

$$c - C^* F_3 + e^- \rightarrow \text{gas-phase} \rightarrow C^*, F_2, C* F_2, C* F_3, C* F_4 + \xi^{SP}$$

$$C* F_2, C* F_4 + \xi^{SP} \rightarrow \text{adsorbed & polymerize at surface} \rightarrow (C* F)_n \xi^{SP}$$

Where the deposited polymer $(C*F)_n$ is Teflon and is $\xi^{SP}$ the sum of neutral and ionic species. Here “*” sign is denoted to keep the concentration point of view closely in mind. Sidewalls are passivated by this layer of polymer during deposition step and then both polymer and silicon are etched from the base of the structure during etching step. Accurate control of anisotropy is achieved by a fine stability between etching and passivation [13]. The deposition of the polymer film is affected by both etching and plasma characteristics [14-15]. Deposited polymer protects sidewalls as the etch step attacks on $Si$ surface. The main chemical reactions occur in the gas phases of the $SF_6$ are

$$SF_6 + e^- \xrightarrow{k_1} SF_4 + 3F + e^- (\text{PhaseI})$$

$$SF_6 + e^- \xrightarrow{k_2} SF_4 + 4F + e^- (\text{PhaseII})$$

Where $k_1$ and $k_2$ are phase constants in two phases (deposition and etching). At the wafer surface, $Si$ is etched by the following reaction

$$F_{gas} \xrightarrow{k_i} F_{ads}$$

$$Si_{solid} + 4F_{ads} \rightarrow (SiF_4)_{gas}$$

Where $k_i$ is the surface constant after two segments. Ion fluxes at the $Si$ wafer surface are relatively low as compared to the $F$ flux; therefore, $SiF_6$ is producing an isotropic profile. By continuity equation at the surface we obtain an analytical appearance for the etch rate of equation (1) by differentiating with $\partial t$, as follows
Plasma consist of several reactions, but it is renowned that the one producing $SF_3$ according to equation (1) accounts for about $2/3$ and that producing $SF_2$ accounts for $1/3$ of the released etching species of $F$ [16]. During chemical reaction it is very vital to keep an eye on gas phase concentration of $SF_6$ and $F$ that can be obtained from equation (3) as \( \frac{\partial SF_6}{\partial t} = 0 \), so

\[
C^*_E = \frac{FC^*_r}{V} \quad \text{and} \quad n = \frac{FC^*_r - SC^*_r}{VC^*_r (k_1 + k_2)}
\]

Where $n$ and $V$ denote the number of deposition / etch species and total volume of $SF_6$ respectively. The energy supplied to the surface during etch step in the form of fluorine concentration removes the passivation from the base of the features thus exposing silicon for spontaneous etching. It can be calculated as

\[
C^*_r = -\frac{V}{S} (3k_1 n + 4k_2 n) \cdot \frac{FC^*_r}{V} \quad \text{and} \quad \frac{S}{V} + \frac{FC^*_r - SC^*_r}{VC^*_r (k_1 + k_2)}
\]

Product of fluorine and gas phase concentration in $SF_6$ remains identical is derived by putting value of $n$ in equation (6)
\[ C_{SR_s}^* = \frac{FC_{SR_s}^*}{V} \left( S + \frac{FC_{SR_s}^* - SC_{SR_s}^*}{VC_{SR_s}^* (k_1 + k_2)} \right) \]  

(7)

\[ C_{SR_s}^* FC_{SR_s} = C_{SR_s}^* FC_{SR_s} \]  

(8)

\textit{Phase I (deposition) = Phase II (etching)}

On the basis of silicon surface resistance coefficient “Ω” and gas phase concentration of fluorine, etch rate is \( \frac{\Omega_{Si}}{4} k_3 C_r^* \)

\[ Etch\ Rate = -\frac{\Omega_{Si}}{4} k_3 \frac{V}{S} (3k_1n + 4k_2n) \left( \frac{FC_{SR_s}^*}{S} \right) \left( \frac{FC_{SR_s}^* - SC_{SR_s}^*}{VC_{SR_s}^* (k_1 + k_2)} \right) \]  

(9)

Putting value of “n” from Eq. (5),

\[ Etch\ Rate = -\frac{\Omega_{Si}}{4} k_3 \frac{V}{S} \left( \frac{FC_{SR_s}^* - SC_{SR_s}^*}{VC_{SR_s}^* (k_1 + k_2)} \right) \left( 3k_1n + 4k_2n \right) \]  

(10)

Where \( \Omega_{Si} \), \( k_3 \), \( V/S \), \( FC_{SF6}^* \), \( SC_{SF6}^* \) and \( VC_{SF6}^* \) symbolize resistance of Silicon material, silicon surface constant, ratio of total gas volume to sulphur contents, fluorine concentration in \( SF_6 \), sulphur concentration in \( SF_6 \), Volume concentration of both \( F \) and \( S \) in \( SF_6 \). The negative sign in equation (10) presents evolving species during reaction.

3. SURFACE FLUX DISTRIBUTION MODELS
Etching process modeling of the trench bottom compared to its sides is divided into two models such as reactor as well as cosine distribution model explained beneath.

### 3.1. Reactor Modeling

A plasma-enhanced reactor model, neglecting the gas boundary layer near the surface is shown in Figure 1. The physical processes of deposition and etch are a function of the material fluxes of reactants at the wafer’s surface.

![Fig. 1. Distribution of the arrival fluxes at the surface](image)

Summation of all fluxes acting at the surface is

$$\gamma_{NET} = \gamma_{direct(neutrals)} + \gamma_{direct(ions)} - \gamma_{emitted} + \gamma_{redeposited} - \gamma_{sputtered}$$  \hspace{1cm} (11)

Since plasma processing is performed at relatively low temperature, therefore, a diffusion flux expression is neglected here.

### 3.2. Cosine distribution model

The first two expressions in etch rate describe fluxes of species arriving directly from the reactor to the wafer surface. These can be calculated from the concentration and velocity of gas at the surface [9-10]. There are several models for describing the direct flux arrival with
time [9]. A simple method with good results for most cases is the cosine distribution of flux model, shown in Figure 2.

![Cosine distribution model](image_url)

**Fig. 2.** Cosine distribution model

Surface modification rate at an arbitrary point $M$ on the wafer surface depends on the normal component, or the cosine of the angle of incoming flux to the surface. Near the surface, the distribution of the arrival flux follows a cosine distribution. If $\gamma_s$ is the flux toward the surface, and $\gamma_n$ is the flux normal to the surface at point $M$, then

$$
\gamma_s = \frac{\gamma_n}{2} \left(1 + \cos \theta \right). \begin{cases} 
\gamma_n, \theta = 0^\circ \\
\gamma_n, \theta = 90^\circ
\end{cases}
$$

(12)

Therefore, point $M$ seems to have maximum incoming flux at $\theta = 0^\circ$. As $\theta$ increases, flux decreases until a minimum is observed at $\theta = 90^\circ$. Actually in plasma systems, the incident flux becomes more directional than cosine distribution. So, the generalized flux expression by using $\cos^n(\theta)$ distribution becomes $\gamma_{\text{direct}}(\theta) = \gamma_n \cos^n(\theta)$. The third expression in equation (11), the emitted flux expression, considers the fact that not all molecules stick where they arrive at the surface, and those which do not stick are re-emitted. The emitted flux expression is $\gamma_{\text{emitted}} = (1 - Sc) \gamma^e$, where $Sc$ (modeled as a constant for a
particular system) is the ratio of the number of incident atoms stick on the surface to the total number of incident atoms. Figure 3 illustrates the $Sc$ concepts as,

![Image of Fig. 3](image)

**Fig. 3.** Sticking coefficient effects on profile evolution (a) high Sc. (b) low Sc. (c) deposition. (d) etch.

Figure 3(a) presents that incident species with a high sticking coefficient react where they strike. In Figure 3(b), species with a low sticking coefficient don’t “stick” where they first strike but re-emitted to re-deposit elsewhere. Emission/re-deposition occurs multiple times. Deposition and Emission are shown in Figure 3(c) And 3(d). Generally, ions stick at $Sc = 1$ and chemically reactive neutrals have $Sc < 1$. The fourth expression in Eq. (11) is the re-deposition flux, describes that species which do not stick and re-emit lands elsewhere on the surface. This is described with emitted flux expression $(1 - Sc)\gamma_{emitted}^{x'}$ as

$$\gamma_{redeposited}^{x} = g^{x'x} * \gamma_{emitted}^{x'} = g^{x'x} * (1 - Sc)\gamma_{emitted}^{x'}$$  \hspace{1cm} (13)$$

Where, the term $g^{x'x}$ represents the blocking effects of local topography, which limit the probability that the emitted flux from any point $x'$ is able to be re-deposited at any point $x$ on
the surface. The redeposit flux also dependants on the sticking coefficient. The re-emitted flux is generally assumed to be re-emitted with a \( \cos^n(\theta) \) distribution angle similar to that derived for direct fluxes, with no memory of the arrival angle at that point. The final term in equation (11) is the sputtered flux (energetic incoming ions). \( Y_s \) is the sputtering yield that is angle sensitive. The sputtered molecules re-deposited elsewhere, and enhance the deposition rate by supplying energy that modifies the surface or drives the chemical reaction to overcome a rate-limiting step given as

\[
\gamma^{sputtered} = \text{grind-rate} \times Y_s \times \gamma^{ions}
\]  

(14)

4. SIMULATION RESULTS AND DISCUSSION

Comprehensive solutions of etch rate are obtained by using “Taurus Topography” software. In our simulations, the etch rate for photoresist is set much smaller than that for either polysilicon or polymer. The machine changes the polymer deposition at the same time as it changes polysilicon etching in any desired combination. The basic structure is presented by ideal depositions of polysilicon and photoresist on top of a silicon wafer, as shown in Figure 4(a). A photoresist coating of 1.5 \( \mu \text{m} \) over a small 3.5 \( \mu \text{m} \) polysilicon layer is used. We assume that each cycle will etch only about 0.6 \( \mu \text{m} \) to create a trench with a 35:1 aspect ratio. The photoresist layer is etched in the center to create opening in the mask of exactly 1.5 \( \mu \text{m} \).

The first etch perspective used is the Dry Etch Model. Etching of photoresist, etching of polysilicon, and deposition of polymer are shown in Table 1. It is observed that only polymer is re-deposited during etching and so needed a defined sticking coefficient and re-emission rate. This simulation shows anisotropic etch profile, as can be seen in Figure 4(b).
parameters are adjusted to produce an isotropic profile. The first two sputtering yield parameters, Sput.$Y_1$ and Sput.$Y_2$, are kept same throughout simulations. Reducing the sputter yield widens the view angle, reduces the overall etching rate and increases the deposition rate. Therefore, reducing the Sput.$Y_4$, sputtering yield for the polysilicon produces an anisotropic profile. Unfortunately, by increasing it does not produce any perceptible difference to the etch profile, no altering the view angle. Reducing the view angle for polymer deposition, however, gives result in more sidewall deposition. Reducing the etch rate of polysilicon results in a extra rounded bottom to the trench profile. Adding a lower rate for the polysilicon with a lesser sputtering term for the polymer greatly increases the overall etch rate.

**Fig. 4.** (a) Basic simulation structure. (b) Dry etch model with polymer deposition. (c) Initial etch plus first deposition.

**Table I**

| Initial dry etch model and second etch cycle machine parameters |  |  |
|---|---|---|

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Next step is to define polymer deposition perspective. In this model, the polymer is only defined for the deposition machine, not for the etch machine. The original parameters are given in Table II. Figure 4(c) show that the initial deposition process results in more polymer coating on the sidewalls than on the horizontal surfaces. This is the result of a balance between the deposition and etching parameters chosen for the deposition machine. The etching parameters are the grind-rate and the sputtering yield coefficients, $Y_1$, $Y_2$, and $Y_4$. The deposition parameters are characterized by the flat, un-shadowed, surface rate, the re-deposition rate, the sticking coefficient and the anisotropy. Increasing the grind-rate and decreasing the re-deposition rate decreases the overall deposition on the horizontal surfaces. Initially, the re-deposition rate is set close to zero and the grind-rate close to one. This results that almost no polymer is deposited on the trench floor. Some deposition on the horizontal surfaces is needed for the next etch step and so the grind-rate is reduced and the re-deposition rate is increased until an unbroken layer of polymer covered the trench floor.
The polymer on the sidewalls needs to stay, while the polysilicon below needs to be etched isotropically. This is accomplished by separating this step into two separate etch machines and etch times. The first etch machine etches the polymer more than the polysilicon, while the second machine etches only the polysilicon. The first machine removes the polymer from the entire floor of the trench, and leaves a good coating on the trench sidewalls. A set of time-lapse snapshots of this etch step are shown in Figure 5. Table II outlines the parameters chosen for this etch machine. It is noted that the anisotropy is set to a negative value. This indicates that the polymer etches more laterally than vertically called a “super-isotropic” profile. This is necessary in order to remove the polymer from the bottom corners of the trench. Figure 5 presents that the polymer at the bottom of the trench is etched first. In reality, by 0.03 minutes, the polymer is almost completely gone. The corners of the trench, however, do not show appreciable etching until 0.09 minutes and the trench floor is not completely clear until 1.2 minutes.
The second etch perspective is designed to perform a super-isotropic etch of polysilicon below the left-over polymer. The parameters chosen are shown in Table II. The anisotropy is set to 1.1 to indicate that the polysilicon is etched more laterally than vertically. The second deposition machine parameters remained the same. The resulting profile is shown in Figure 6.

The etch machine parameters are given in Table I. Two parameters are changed from the first deposition/etch cycle, the polysilicon etch rate and the polymer sputter yield. Reducing
the polysilicon etch rate allows a corresponding increase in time and thus more control over the etching profile. We need the polysilicon sidewalls below the left-over polymer to bow out to allow room for the next polymer deposition. Leaving the polysilicon etch rate high for this etch machine does not give this profile. This machine is used primarily to etch through the polymer at the bottom of the trench so that the next machine could reach the polysilicon just beneath the polymer.

5. CONCLUSIONS

In summary, important chemical reactions are derived mathematically in which it is proved that the product of fluorine and gas phase concentration in $\text{SF}_6$ remains same during deposition and etching phases. First time, a simplified flux cosine distribution reaction rate model based on continuity equation is established. In this model, it is observed that silicon etch step requires a highly isotropic component and the polymer deposition process needs a simultaneous sputtering component. This is composed of equal parts of physical etch and sputtering re-deposition. We observed that a highly directional physical etch is also required to break through the thin polymer at the bottom of the trench in order to bare silicon for the fluorinated chemical etch. A fascinating correlation is realized between deposition and etching species presents that deposition species with a high $Sc$, generate less conformal films and vice versa while etching species with a high $Sc$ generate more anisotropic etch and with a low $Sc$ result in a more isotropic etch. It is also analyzed that ions are sticky when $Sc = 1$ and chemically reactive neutrals are originated at $Sc < 1$. Comprehensive clarification of etch rate is attained by using simulation software tool Taurus Topography. It predicts the feasibility of process changes, in which numerical methods are used to describe the fluxes at the wafer surface for particular equipment and topographical configurations.
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