

# Radical effect in a surface kinetic model of fluorocarbon plasma etching process

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**Abstract:** We propose a universal surface kinetic model developed with a self-consistent numerical algorithm verified under a wide range of fluorocarbon (FC) plasma conditions. The deposition or etch yield can be calculated by considering both the passivation layer and mixed layers simultaneously. This work incorporates neutral radical transport via the passivation layer into our proposed model. The internal model parameters such as deposition, sputtering, and consumption yield showed reasonable trends for various FC plasmas. Our model suggests that understanding radical transport will be critical to the next-generation semiconductor fabrication process.

**Keywords:** Plasma, Fluorocarbon, Simulation, Surface reaction.

## 1. Introduction

The fluorocarbon(FC) plasma etching process has been emerging as the most critical step in fabrication process of next-generation fabrication process such as NAND flash and sub-10 nm logic devices.[1] The development of plasma equipment and high aspect ratio(HAR) processes depends on empirical knowledge rather than a detailed understanding of these processes due to their inherent complexities.

The FC mixture plasma has been used for HAR etching processes to take the advantage of FC polymer passivation in the sidewalls of the nanoscale profiles.[2, 3] The successful utilization of these approaches is accompanied by a significant level of effort, owing to the presence of abnormal profiles such as randomly twisting, bowing, and bottom distortion.[4] Most of abnormal behaviors are strongly related to the surface etching characteristics. Therefore, An understanding of surface reaction mechanism is essential for the development of the next-generation fabrication field.

Frontier research groups have used a steady-state FC passivation layer (SPL) to understand these mechanisms[2, 3]. Subsequent studies have proposed various surface models including the detailed kinetic[5, 6], monte carlo kinetic[7, 8], and mixed kinetic models[9, 10]. Despite their contributions, most of developed plasma-surface models depend strongly on process-dependent fitting parameters with ad-hoc assumptions because of the inherent complexities of plasma etching. To address this issue, we present a universal surface reaction model in this work. Here, this model is verified through comparison studies with a wide range of experimental data reported in previous literature.

## 2. Theory

Our surface reaction model is based on a two-layer model consisting of an SPL and a mixed layer. As shown in Fig 1, ion and radical species from FC plasma generate

SPL and mixed layers simultaneously. This model consists of the deposition process on the top of SPL, the sputtering process occurring inside SPL, and consumption kinetic at the mixed layer. Based on this model, we can establish the following FC balance equation of SPL.

$$DR - CR_P(l) - CR_M(l) = 0 \quad (1)$$

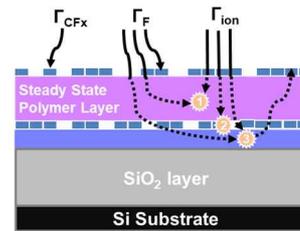


Fig. 1. Schematic diagram of surface reaction model.

First, the deposition rate(DR) can be derived from an active-site model that consists of the direct deposition and ion-enhanced deposition of the FC radical.[2] The sputtering rate  $CR_P(l)$  through the SPL layer is determined by integrating the physical sputtering equation with SPL thickness. For the incidence ion flux and energy( $\Gamma_i, E$ ) and the FC radical flux( $\Gamma_n$ ), the DR and  $CR_P(l)$  can be expressed as follows;

$$DR = \Gamma_n(0)S_p(1-\theta_A) + \Gamma_n(0)S_A\theta_A \quad (2)$$

$$CR_P(l) = \sum_i \int_1^0 d[Y_i(l) \Gamma_i(l)] \quad (3)$$

The consumption rate at the mixed layer( $CR_M(l)$ ) can be calculated by the surface reaction model developed in our previous work[11]. The  $CR_M(l)$  can be expressed as follows;

$$CR_M(l) = \sum_i \Gamma_i(l)Y_i(l)\theta_{SD-2-Polymer} \quad (4)$$

We considered the ion transport through an SPL, using the same approach of the mean-free path  $\lambda = 0.63E(0)^{0.6}$  nm as suggested by Abraham-Shrauner.[12] The  $E(0)$  and

$\Gamma_i(0)$  represent the incidence ion energy and ion flux on the top of the SPL. The  $E(l)$  and  $\Gamma_i(l)$  represent the ion energy and ion flux at the arbitrary SSPL.

$$\Gamma_i(l) = \Gamma_i(0) \exp\left(-\frac{l}{\lambda}\right), E(l) = E(0) \exp\left(-\frac{2l}{\lambda}\right) \quad (5)$$

In terms of radical transport through an SPL, we developed a diffusion model with the assumption of the continuum medium. Starting with Knudsen diffusion[13], we derive the diffusion equation including theoretical and experimental observations such as the directional ion sputtering effects, the porosity of the SPL, etc.

### 3. Results and discussion

Our surface reaction model is evaluated under the fixed conditions of ion and radical flux,  $1.5 \times 10^{15} \text{ cm}^2/\text{s}$  and  $1.5 \times 10^{17} \text{ cm}^2/\text{s}$ . The Figure 2 (a) represents deposition, sputtering and consumption yield according to the change in incidence ion energy. As the ion energy increases, deposition, sputtering, and consumption yields increase, and are balanced as shown in Fig. 2 (a). As shown in Fig 2 (b), the estimated SPL thickness decreases according to the ion energy.

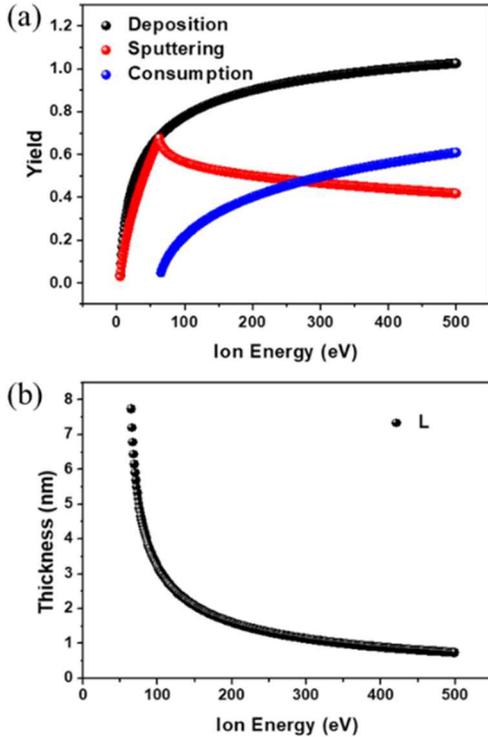


Fig. 2. Deposition, sputtering, and consumption yield as a function of ion energy (a), and the estimated SPL thickness in our model according to ion energy.

The plasma-generated radicals reach the mixed layer through the diffusion process. In the mixed layer, the arrived radicals play the role of the etchants. Figure 3 (a) represents a comparison between the experimental data and our modeling results. Experimental data with plasma

diagnostics were chosen for the  $\text{CF}_2$  beam[14],  $\text{C}_2\text{F}_6$ [2],  $\text{C}_4\text{F}_6$ [16] and  $\text{C}_4\text{F}_8$ [17] gases. Under the various experimental results of fluorocarbon plasma system, our modelling results showed good agreements with experimental data. The figure 3 (b) is the computed thickness of the SPL. In Fig. 3, the “Low SPL” and “High SPL” represents the surface reaction modeling results with and without considering the radical diffusion model. It is clear that the radical diffusion effect should be considered in the range of high ion energy and radical flux.

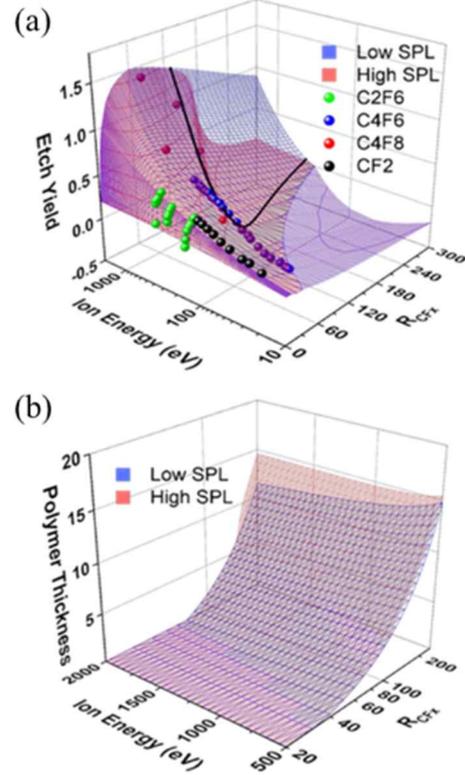


Fig. 3. Our modeling results and experimental data for etch yield and SPL thickness of under the wide range of plasma conditions.

### 4. Conclusion

We have developed a universal surface reaction model with the a self-consistent numerical algorithm. Therefore, we can calculate the deposition or etching rate according to plasma conditions without ad-hoc assumptions. Our model is verified through a comparison of experimental data for plasma of various FC gas species. We believe that our surface reaction model will be essential to understand specific abnormal behaviors under HAR etching process such as bowing, necking, and profile distortions. The coupling research with 3D topography simulation is underway and will be published. We believe that our surface reaction model will be useful for prediction and understanding the fabrication process conditions of sub-10nm devices.

## 5. References

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