SIMULATION OF SEMICONDUCTOR PROCESSES AND DEVICES Vol. 12 Edited by T. Grasser and S. Selberherr - September 2007

Modeling of Deposition During C₅F₈/CO/O₂/Ar Plasma Etching Using Topography and Composition Simulation

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Abstract

We proposed a simple model to simulate topography and composition of deposited films. Our model described topography and composition of deposited fluorocarbon films in $C_5F_8/CO/O_2/Ar$ plasma etching. Analysis of compositions facilitated making of the reactor and surface models, and our model could treat the gas flow and open width dependency of the SiO₂ etching. It was very useful in designing devices for easy manufacturing.

1 Introduction

In semiconductor processes, a topography simulation model is becoming increasingly important for designing devices reflecting process considerations and the need to reduce trial production costs. Also, topography depending on open width or size of contact hole is particularly important.

To simulate topography in dry etching processes, it is important to model deposition, which has the dominant effect on the final shapes. It is well known that there are many kinds of deposition precursors, which have different sticking coefficients and form different deposition films [1-3]. So, in some cases, we should consider not only topography but also composition of deposition films.

In this study, we propose a simple model to simulate topography and composition of deposited films during the $C_5F_8/CO/O_2/Ar$ plasma etching and we investigate the mechanism of the deposition. Then we simulate the topography of SiO₂ etching by using the model.



Figure 1: Test structures etched in C₅F₈/CO/O₂/Ar plasma for 5 minutes.

2 Modeling

To develop the deposition model, we analyzed the characteristics of test structures, which were etched in $C_5F_8/CO/O_2/Ar$ plasma for 5 minutes (Fig.1.). From the analysis, we modeled two deposition precursors, namely, C atom and C_5F_8 molecule in excited states.

Gas phase reactions

$$CO_{gas} + e^{-} \longrightarrow C_{gas} + O_{gas} + e^{-}$$
(1)

$$C_5 F_{8gas} + e^- \longrightarrow C_5 F_{8gas}^* + e^-$$
(2)

Surface reactions

$$C_{gas} \xrightarrow{\eta_{c}=1} C_{bulk}$$
(3)

$$C_{5}F_{8\,gas}^{*} \xrightarrow{\eta_{C_{5}F_{8}^{*}}=0.3} C_{5}F_{8bulk}$$

$$\tag{4}$$

where $_{gas}$ and $_{bulk}$ represent gas phase species and deposited species, respectively. Comparison of results for test structures etched with and without CO (presented in Fig.1(c).) led to the understanding that the deposition precursor having large sticking coefficient may increase. So we considered C_{gas} as a precursor with sticking coefficient of 1. Flux of C_{gas} at CO=50[sccm] was determined with reference to the change in topography from CO=0[sccm]. Estimated flux of C_{gas} is reasonable, since the reaction rate of equation(1) is approximately equal to the rate estimated from the cross-section [4]. We considered $C_5F_8^*_{gas}$ as another deposition precursor on the basis of research reports available in the open literature [1-2]. Sticking coefficient of $C_5F_8^*_{gas}$ is determined by analyzing topography etched in C_5F_8 plasma [1]. Fluxes of $C_5F_8^*_{gas}$ remain constant irrespective of the change in CO flow rates. Obtained sticking coefficients and fluxes are presented in Table 1.

	Sticking	Bulk	Flux on flat surface		
	Coefficients	density	[mol/m ³ /sec]		
		$[g/cm^3]$	CO=0[sccm]	CO=50[sccm]	
С	$\eta_{\rm C} = 1$	2.25	0	1.39×10 ⁻⁴	
C_5F_8	$\eta_{C_5F_8^*} = 0.3$	2.15	3.19×10 ⁻⁵	3.19×10 ⁻⁵	

Table 1: Parameters for topography simulation

To simulate the topography of the etching process, local growth rates are calculated in each time step and the level set functions are evolved by using the local growth rates [5]. Local growth rate of a deposition film is given as

$$GR_{depo} = \frac{\eta_C \Gamma_C}{\rho_C} + \frac{\eta_{C_s F_8^*} \Gamma_{C_s F_8^*}}{\rho_{C_s F_8}} - ER_{depo}$$
(5)

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where ρ represents bulk density, Γ represents local flux, and \mathbf{ER}_{depo} is etching rate by other species (Ar⁺, O^{*}, O₂, whose fluxes and sticking coefficients remain constant irrespective of the change in CO flow rates). If $\mathbf{GR}_{depo} > 0$, deposition films grow, whose composition of C atom is given as

$$R_{\rm C} = \frac{[\rm C]}{[\rm C] + [\rm F]} = \frac{\eta_{\rm C} \Gamma_{\rm C} + 5 \times \eta_{\rm C_5 F_8^*} \Gamma_{\rm C_5 F_8^*}}{\eta_{\rm C} \Gamma_{\rm C} + 13 \times \eta_{\rm C_5 F_8^*} \Gamma_{\rm C_5 F_8^*}} [atomic\%]$$
(6).

If $\mathbf{GR}_{depo} < 0$, we modeled 2 patterns. When we calculate the etch rates of the deposition films, we use the \mathbf{GR}_{depo} as the surface growth rate. When we calculate the etch rates of SiO₂, we use the \mathbf{GR}_{siO2} as the surface growth rate.

$$GR_{SiO_2} = -ER_{SiO_2} \left(\frac{GR_{depo}}{ER_{depo}} \right)$$
(7).

where \mathbf{ER}_{siO2} is etching rate of SiO₂ by ion species (Ar⁺ and CF₃+, whose fluxes and sticking coefficients remain constant irrespective of the change in CO flow rates). Eq.(7) expresses that the ions, which are not used for removing deposition films, can etch the SiO₂ substrate.



(a) CO=0[sccm]

(b)CO=50[sccm]





Figure 3: Calculated *R*_C in deposited fluorocarbon films (CO=50[sccm]).

	Α	В	С	D
Experimental (SEM-EDS analysis) [atomic%]	38%	32%	48%	50%
Calculated (Topography simulation) [atomic%]		38%	45%	49%

Table 2: Comparison between exp. and calc. results of $R_{\rm C}$ (composition of C atom) in
deposited fluorocarbon films at spot in Fig.3. (CO=50[sccm])

3 Result

Calculated topography and $R_{\rm C}$ is shown in Fig.2 and 3, and comparison of computed and experimental EDS analysis of $R_{\rm C}$ is presented in Table.2. Our model describes topography and composition of deposited fluorocarbon films. Large composition of C atom at bottom of the test structures is expected due to $C_{\rm gas}$ direct flux.

Also, we calculate the topography of SiO2 etching while changing the CO gas flow rate by using the same reactor and surface model for CO_{gas} and C_{gas} . Fig.4 shows the topography of computed and experimental results, respectively. Our model describes the taper angle depending on CO gas flow and open width.



Figure 4: Calc. and exp. structure of SiO₂ etched in C₄F₈/CO/O₂/Ar plasma.

4 Conclusions

A simple model to simulate topography and composition of deposited films has been described. Analysis of compositions facilitates making of the deposition models, and our model can treat the gas flow and open width dependency of the etching. It is very useful in designing devices for easy manufacturing.

In the future modeling of topography behavior including the depletion of deposited films, the composition of the films should be used.

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