Feature Scale Simulation of Selective Chemical Vapor Deposition Process

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ABSTRACT

The feature scale model for selective chemical vapor deposition process was proposed and the simulation was performed to study the selectivity and uniformity of deposited thin film using Monte Carlo method and string algorithm. The model was composed of direct deposition, re-emission, and surface diffusion mechanisms. The effect of model parameters such as sticking coefficient, aspect ratio, and surface diffusion coefficient on the deposited thin film pattern was investigated. The uniformity of selectively deposited thin film was improved for lower sticking coefficient and higher aspect ratio. It was revealed that the selectivity loss ascribes to the surface diffusion. Different values of sticking coefficients on Si and on SiO_2 surface greatly influenced the deposited thin film profile. In addition, as the lateral wall angle decreased, the selectively deposited film had improved uniformity except the vicinity of trench wall. The optimum condition for the most flat selective film deposition pattern is the case with low sticking coefficient and slightly increased surface diffusion coefficient.

1. INTRODUCTION

Selective chemical vapor deposition(CVD) has become one of the most promising process required for next-generation ULSI circuitry due to its potential advantages. The selective CVD process for metal or semiconductor material by using surface kinetics mechanisms provides a number of unique benefits. Filling vias or contact holes using selective tungsten(W)[1] or copper[2] deposition process offer process simplification and improved overall efficiency in manufacturing than conventional blanket deposition followed by etch-back process. And the selective epitaxial growth(SEG) technology of silicon by CVD process[3] as an alternative process over standard LOCOS(local oxidation of silicon) isolation technique has been widely studied because the SEG process can provide deep and shallow device isolation in submicron scale, which is impossible for conventional LOCOS isolation.

The selective W-CVD process using WF_6-SiH_4[4] or WF_6-H_2[5] chemistry and the SEG of silicon by CVD process using SiH_2Cl_2 / HCl / H_2[6], $SiCl_4$ / HCl / H_2[7], or SiH_4 / HCl / H_2[8] gas systems have been performed to find optimum operating condition. But the main problem which prevents the selective CVD process from being applied in the semiconductor industry is the selectivity loss phenomena that have been frequently observed in experimental results. Although the extensive effort to study the selectivity of CVD process, however, it is not well understood and controlled, since it mainly focuses on the experimental study to examine the effect of operating conditions and this only can show the effect of macroscopic process parameter. Therefore, the tool for investigating the behavior of reactant in the microstructure and understanding of selective CVD mechanism is needed urgently.

In this work, the simulation of the selective CVD process by using the microscopic feature scale model including direct deposition, re-emission, and surface diffusion mechanism was conducted using Monte Carlo method and string algorithm and effect of various model parameters on selectively deposited film pattern was examined and the cause of selectivity loss was clarified.

2. MODELING

A schematic diagram of a physical model for selective CVD process in a trench structure is illustrated in Fig. 1. Among the various mechanisms that consist in the selective CVD process, the representative behaviors of reactant in microstructure can be classified into three different mechanisms such as direct deposition, re-emission, and surface diffusion. The Monte Carlo method was employed in this study for the simulation of the selective deposition profile, which may give a good insight into the underlying physical priciples of the motion of gas particles and the interaction of them with the microscopic trench surfaces of the substrate to describe the selective deposition process. And transient profiles of selectively deposited film surfaces were traced by string algorithm. And the gas-gas collisions were ignored in this feature scale simulation because the mean free path of particles in low pressure CVD process is larger than the characteristic length of trench scale.

The re-emission mechanism used in this study is cosine re-emission which determines the direction of reactant from the surface if reactant is re-emit. In the cosine re-emission, there exists strong interaction between the incoming gas particle and solid surface so that it loses all its information of previous incoming trajectory. In this mechanism, the probability for a certain particle to re-emit with angle ϕ is proportional to cosine function, i.e., cos ϕ, where ϕ is defined as the angle from normal direction to the surface. The degree of re-emission is characterized by a sticking coefficient(η) which is the ratio of the number of the particles sticked onto the surface to the total number of the incident particles into trench.

The surface diffusion mechanism was considered to represent the motion of adatoms based on the unsteady surface diffusion equation with surface diffusion coefficient. Since the adatoms that sticks on the Si surface can move only along either Si or SiO_2 surface, the surface diffusion equation in two-dimensional trench structure can be transformed into one-dimensional equation. In this transformation, the distance between grid points should be precisely considered in the transformed one-dimensional equation. After solving the surface diffusion equation with appropriate boundary conditions by using the Crank-Nicolson method, the atomic number density of the adatoms on the surface after experiencing the surface diffusion of reactants was determined and then, the growth rate at each grid point was computed.

Only half of the two-dimensional trench structure schematically shown in Fig. 1 was considered as a system domain and the flow chart for selective thin film deposition simulation is represented in Fig. 2. For a number of particles (5 x 10^5), the trajectory of each particle was traced until it was finally sticked on the surface by the generation of random numbers, given sticking coefficients, and cosine re-emission mechanism. After the positions of given particle numbers were determined, the surface diffusion equation was then solved to obtain the atomic number densities of the adatoms on the surface after experiencing the migration of particles under the assumption that the surface mobility of adatoms on different material surface is same. And more or less dispersed atomic densities on the surface were smoothed. Finally, the surface evolution was carried out based on the string algorithm under the assumption that for the case of $\eta_{SiO_2} = 0.0$, the film deposited on both Si and SiO_2 surfaces has the original η_{Si} , while for the case of $\eta_{SiO_2} \neq 0.0$, the film deposited on the SiO_2 surface has the η_{SiO_2} and the film deposited on the Si surface has the η_{Si} as the deposition process goes on. Then each point on the string advances to next deposition front.

3. RESULTS AND DISCUSSION

The effect of sticking coefficient of silicon surface(η_{Si}) on the microscopic uniformity of the selectively deposited film for various aspect ratios(A.R.s) is shown in Fig. 3. The A.R., a geometrical parameter to describe the initial trench shape, is defined as the ratio of the height to the width of the trench. The deposited film thickness decreased with the decrease of η_{Si}, and this means the decrease of the finally attached number of particles for various A.R.s, at edge and center points of trench. But the gap between center and edge points in trench is reduced with the decrease of η_{Si} for various A.R.s implying that the uniformity of the selectively deposited film is better for lower η_{Si}. The difference of the film thicknesses between at center and at edge points in trench decreased with the increase of A.R.s for large value of η_{Si}, since the interaction between gas particle and SiO_2 surface is occurred more frequently finally to reach the Si surface with the increase of A.R. resulting in more uniform concentration distribution on Si surface.

Figure 4 shows the effect of the surface diffusion coefficient(D_S) on selectively deposited thin film pattern for various η_{Si}. From Fig. 4, the film thickness deposited at the center point of bottom side of the trench decreased but that at the center point of lateral wall side increased with the increase of D_S. This implies that the surface diffusion of the adatoms rather than the re-emission is the main reason of selectivity loss for the selective deposition process. The decreasing rate of film thickness at the center point of bottom side of the trench is more rapid for large η_{Si}, because the concentration gradient on Si surface is more larger for large value of η_{Si}. But the amount of surface diffusion is saturated for large D_S, since the near surface at center point on bottom side in trench is covered with Si film and resulting in the decrease of concentration gradient inside trench. The difference between the thickness at the center point of the bottom side and that at the center point of the lateral wall side in trench for low η_{Si} is reduced for large D_S.

As shown in Fig. 5(a), more uniform thin film patterns with decreasing of η_{Si} as described above. Figure 5(b) shows the effect of a little addition of surface diffusion on film deposition pattern for $\eta_{Si}=1.0$ and 0.1. The most flat film could be obtained for $\eta_{Si}=0.1$ with $D_S=5\times10^{-7}$ μm^2 / sec. However, it did not give the same result for $\eta_{Si}=1.0$ because the reduction of the concentration gradient bv surface diffusion had more dominant influence on the SiO_2 surface than on Si surface, which leads to the "creeping-up" phenomena of adatoms onto the SiO_2 surface. This means that η_{Si} should be kept low simultaneously with a little addition of surface diffusion in order to obtain uniformly selective thin film pattern. The thin film pattern with the selectivity lost is shown in Fig. 5(c). It was found out the selectivity loss occurs by the surface diffusion of adatoms and this phenomena appeares more severe for larger η_{Si}. Also, the initially nonzero value of η_{SiO_2}, though not clearly shown in Fig. 5(c), obviously made the selectivity loss to become worse.

The film deposition patterns with nonzero η_{Si} and η_{SiO_2} are shown in Fig. 6. As the η_{SiO_2} increased with η_{Si} fixed, the film thickness deposited on Si surface decreased by decreasing the width of entrance region of the trench and thus reducing the arrival angle on Si surface. This phenomena is extremely shown as compared with Fig. 6(c). As the η_{Si} increased with η_{SiO_2} fixed, the film thickness deposited on Si surface increased but the degree of increase is small compared with Fig. 6(a).

Figure 7 shows the effect of lateral wall slope angle(α) on the selectively deposited film pattern. The thicker and more uniform thin film pattern was obtained with the decrease of α. This is because the arrival angle increased and the relative difference of arrival angle inside the trench was reduced with the decrease of α.

4. CONCLUSIONS

Feature scale simulation for selective chemical vapor deposition process using the Monte Carlo method and string algorithm was conducted to investigate the effect of model parameters on the deposited film pattern.

The uniformity of selectively deposited thin film is improved for lower sticking coefficient and higher aspect ratio. The selectivity loss is originated from the surface diffusion of reactant initially adsorbed on Si surface. And the nonzero sticking coefficients of Si and SiO_2 surface have a greatly influenced on the deposited thin film pattern. More uniform thin film patterns were obtained except near trench wall side with the decrease of lateral wall slope angle. Therefore, the optimum condition to acquire the most selective and flat film pattern is the case with low sticking coefficient and slightly increased surface diffusion coefficient.

The ultimate goal of this research is to develop the combined macroscopic reactor and microscopic feature scale model and to predict deposition rate, uniformity, step coverage, selectivity for different operating conditions. This can be a powerful tool for design of reactor and analysis of LPCVD processes.

ACKNOWLEDGEMENT

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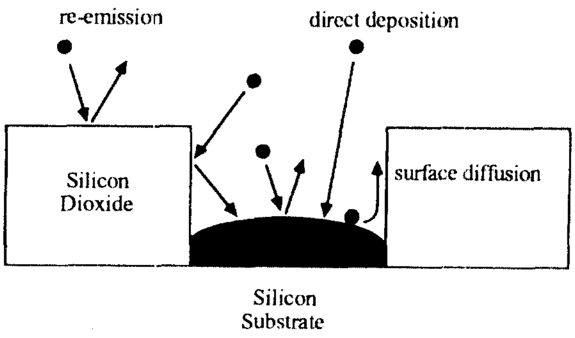


Fig. 1. Trench used to illustrate various selective deposition mechanisms.

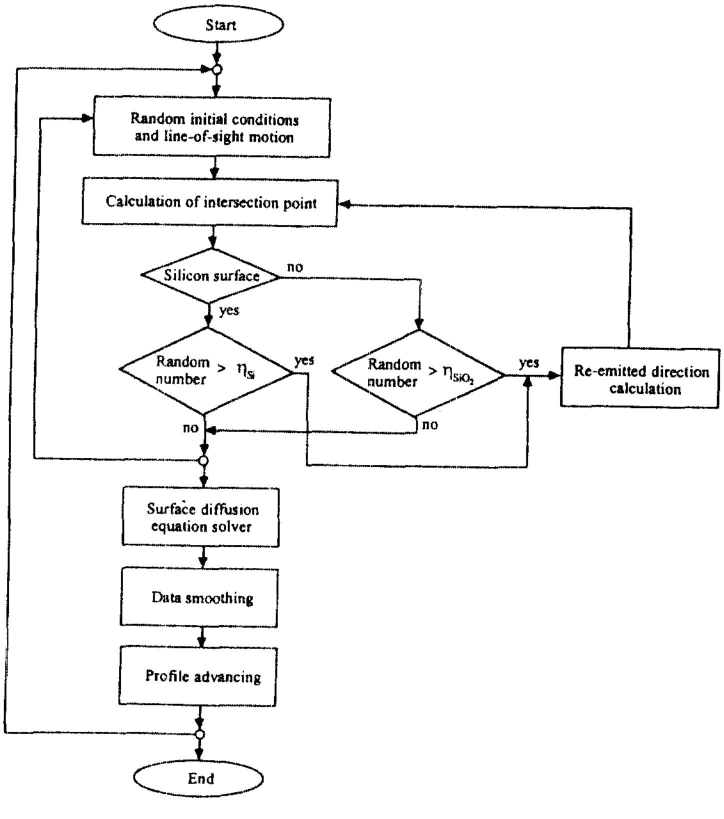


Fig. 2. Flow chart of feature scale simulation for selective chemical vapor deposition process using Monte Carlo method.

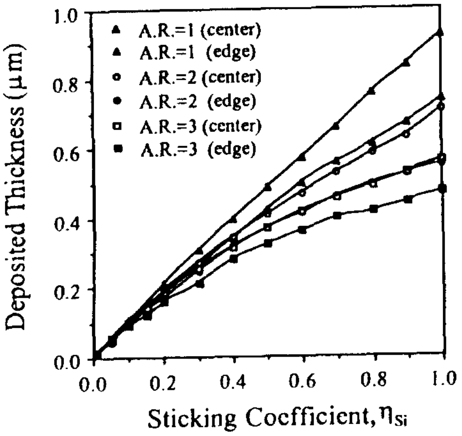


Fig. 3. Effect of sticking coefficient of silicon on the selectively deposited film thickness at the center point and edge point of trench bottom side for various A.R.s. at $\eta_{SiO_2} = 0.0$, $D_s = 0.0\ \mu m^2 sec^{-1}$, and $\alpha = 90°$.

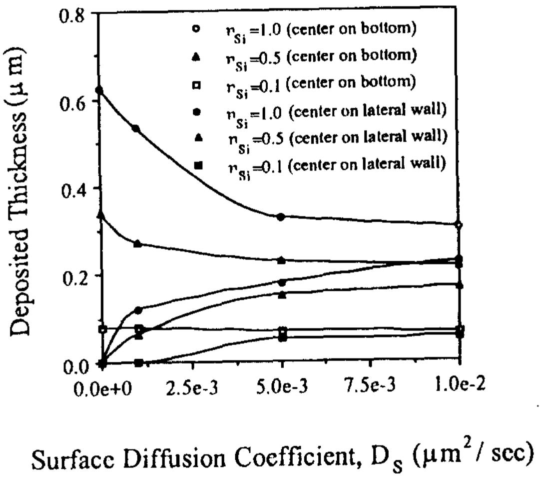


Fig. 4. Effect of surface diffusion coefficient on the deposited film thickness at the center point of trench bottom side and the center point of lateral wall side for various η_{Si} at $\eta_{SiO_2} = 0.0$, A.R. = 1.0, and $\alpha = 90°$.

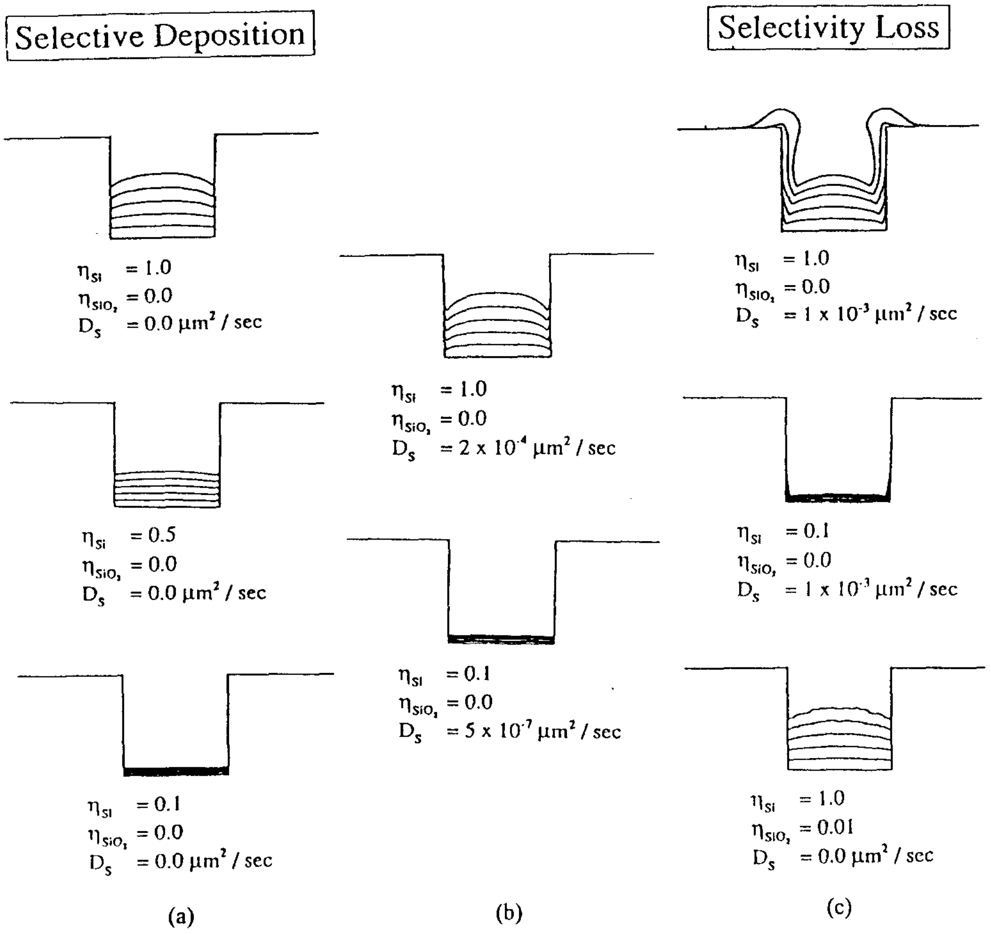
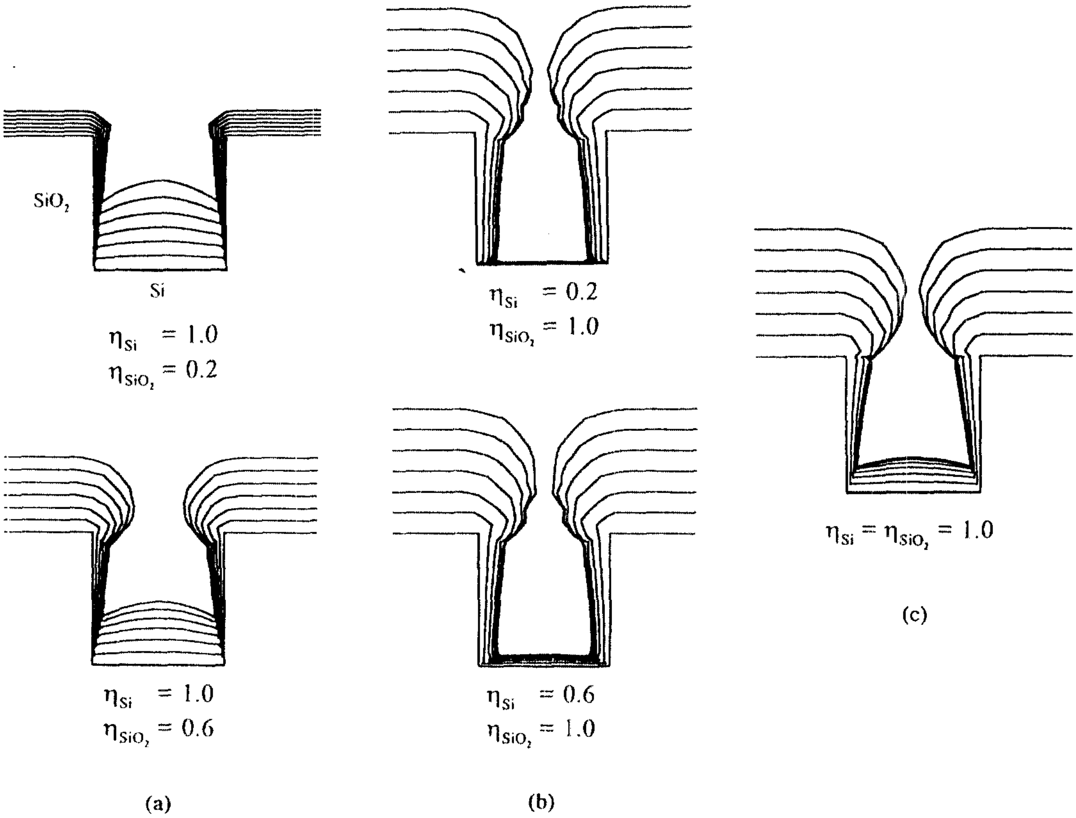


Fig. 5. Different deposited film patterns from selective deposition to selectivity loss phenomena appeared for various η_{Si}, η_{SiO_2}, and D_S at A.R. = 1.0 and $\alpha = 90°$.



$\eta_{Si} = 1.0$
$\eta_{SiO_2} = 0.2$

$\eta_{Si} = 1.0$
$\eta_{SiO_2} = 0.6$

(a)

$\eta_{Si} = 0.2$
$\eta_{SiO_2} = 1.0$

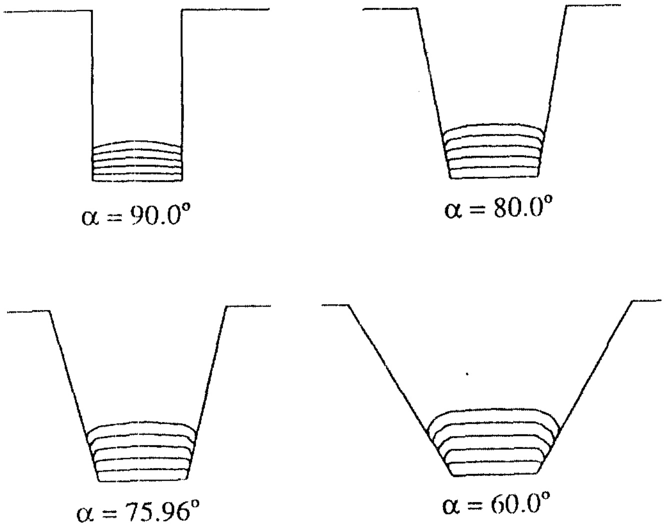
$\eta_{Si} = 0.6$
$\eta_{SiO_2} = 1.0$

(b)

$\eta_{Si} = \eta_{SiO_2} = 1.0$

(c)

Fig. 6. Deposited film patterns with nonzero η_{Si} and η_{SiO_2} at $D_S = 0.0\ \mu m^2\ sec^{-1}$, A.R. = 1.0, and $\alpha = 90°$.



$\alpha = 90.0°$

$\alpha = 80.0°$

$\alpha = 75.96°$

$\alpha = 60.0°$

Fig. 7. Effect of lateral wall slope angle on the selectively deposited thin film pattern at $\eta_{Si} = 1.0$, $\eta_{SiO_2} = 0.0$, and $D_S = 0.0\ \mu m^2\ sec^{-1}$.