Feature Scale Simulation for Advanced Processing

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***Abstract*— Feature-scale profile-evolution simulator, FPS3D is used to simulate an advanced processing method of atomic layer deposition. Two SiN ALD cases are considered for comparison as they lead to different deposition rates, namely about 0.5 ML and 1 ML of deposition per cycle. Steric hindrance was found to be an important factor. The results of simulations are compared with experimental data. The effect of aspect ratio of features is investigated.**

Keywords— plasma processing, simulation, feature-scale, ALD, surface interactions.

I. Introduction

Semiconductor industry overcomes many challenges by advancing materials processing to new levels of precision, accuracy, manufacturability, and reliability. Experimental methods have always been, and probably will be so in the foreseeable future, a leading approach in that. However, ever growing and more stringent requirements on processing for semiconductor industry require additional tools helping in finding optimal parameters, predicting the output of processing, and understanding the details of processes. Without such an understanding, any further progress is hindered or becomes ineffective.

Here we present new results on Monte Carlo feature-scale simulations. Features with scales of 10-1000 nm cannot yet be addressed by any other simulation technique such, for example, as molecular dynamics or quantum-chemistry methods, on the small-scale end, or by equipment modelling approaches, on the large-scale end. We are using a Monte Carlo feature-scale profile-evolution simulator, FPS3D [1-3], to model various gas-surface and plasma-surface interactions and to simulate the resulting profiles obtained due to etching and/or deposition processes.

There is a significant advantage in carrying out simulations based on modelling of actual physical and chemical processes of interactions with the surface, and not just drawing the profiles that look similar to the experimental ones. Such physics-based approach provides a path to better understanding of involved processes as well as their dependence on various parameters of experiments.

FPS3D is a general software package applicable to any chemistry or any materials and is capable of simulating etching, deposition and implantation processes. The only difference in obtained results is thus due to differences in physical and chemical properties of used solid materials and that of incoming species. If those species are energetic, then their energy and angle of incidence become important factors as well.

The scope of this article is limited and is focused on consideration of atomic layer processing, such as Atomic Layer Deposition (ALD). The ALD processes are often complex, involving large molecules and, to our knowledge, have not been addressed by other feature-scale simulations except via FPS3D [3-4]. ALD has a potential for conformal and precise deposition. However it requires definite conditions for being successful, and those conditions are very important to understand and satisfy.

The ALD processing comprises a quickly expanding set of applications and could be foreseen as becoming one of the leading semiconductor technologies of the future. The main factor of all of ALD schemes is the cyclic change of flux parameters and the corresponding chemistry. In traditional approach, that produces a single monolayer (or a fraction of a monolayer) of the deposited film after application of a cycle.

II. Results of Calculations

A. SiN ALD with Si_2Cl_6 and N_2H_4, precursors

Here we consider a case of silicon nitride ALD with cycles of alternating fluxes of hexachlorodisilane and hydrazine [6]. This seems to be the simplest possible ALD case, not only because the set of reactions might be very simple, but rather because those reactions corresponds to deposition of 1ML of the film per cycle. In a typical ALD case, two or more cycles are required to produce 1ML of the film and thus building reaction steps is typically more difficult. The following reactions were used in our simulations:

$$2SiNH(s) + Si_2Cl_6 \rightarrow 2SiN(s) + 2SiCl_2(s) + 2HCl \quad (1)$$
$$2SiCl_2(s) + N_2H_4 \rightarrow 2SiNH(s) + 2HCl + Cl2 \quad (2)$$

We use (s) at the end of some molecules to denote surface, while gaseous molecules do not have it. The reaction (1) represents two effects: (a) a conversion of SiNH into SiN by bonding H with Cl into a non-reactive volatile HCl, and (b) a deposition of $SiCl_2$. The reaction (2) represents a nitridation step with N_2H_4 converting $SiCl_2$ into SiNH and producing two non-reactive gases HCl and Cl_2, so the new cycle could start the same way as the first one.

Fig. 1 shows instantaneous deposition rate, which could reach up to 0.7A/s but for very short periods of time, while the average deposition rate was only slightly above 0.02A/s. Fig 2 shows the TiN film grown during those 10 cycles.

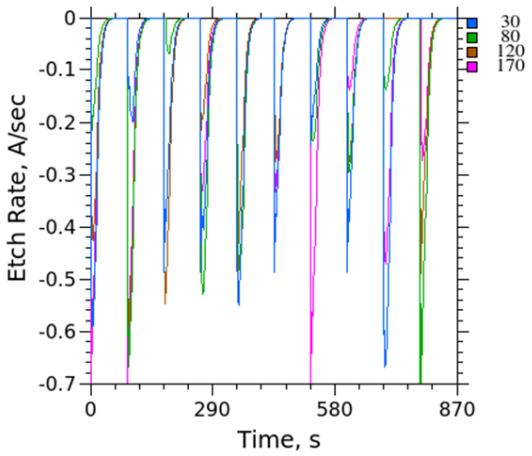

Fig. 1. Instantaneous deposition rate (shown as negative etch rate) during the first 10 cycles of Si_2Cl_6/N_2H_4 ALD.

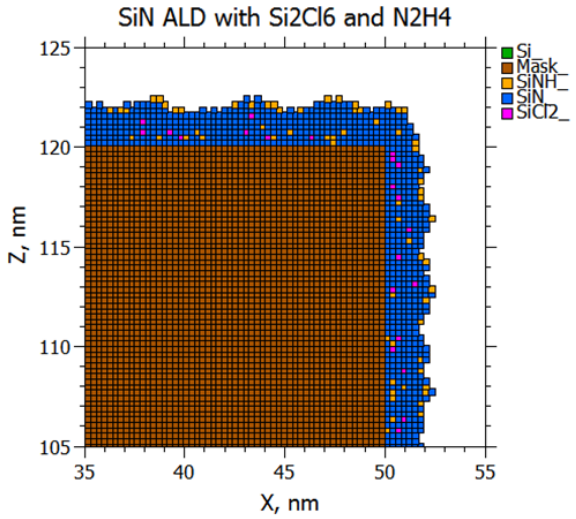

Fig 2. SiN film deposited during the first 10 ALD cycles of Si_2Cl_6 and N_2H_4.

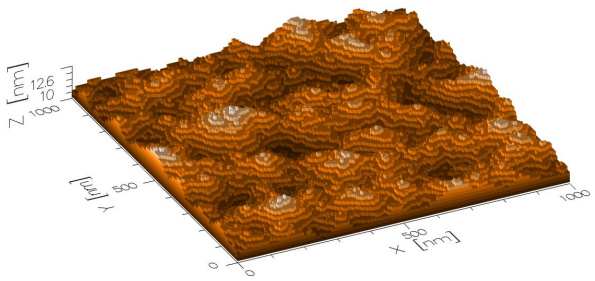

Fig. 3. Roughness of SiN film, as calculated after 100 ALD Si_2Cl_6/N_2H_4 cycles.

Experiments [6] provide data on the roughness of the grown film after 100 ALD cycles. Fig 3 shows the corresponding results of calculations. Calculated RMS roughness was about 5 A and close to that reported in experiments.

B. SiN ALD with SiH_2Cl_2 and NH_2 precursors

This case was considered in experiments [3-5] and corresponds to the deposition of about 0.5 ML of SiN film per cycle. Once again, we have chosen to start from the hydrogenated surface, and our set of reactions was the following:

$$SiNH(s) + SiH_2Cl_2 > SiN(s) + SiH_2Cl(s) + HCl \quad (3)$$
$$SiH_2Cl(s) + NH_2 > SiNH(s) + H_2 + HCl \quad (4)$$

In this case, the deposited SiH_2Cl molecule is counted by FPS3D as large enough to cover two surface sites, which results in the reaction (3) acting only on half of available SiNH molecules, thus requiring two cycles to deposit a new SiN layer. The corresponding deposition profile in the area of a corner in shown in Fig. 4, so it could be easily compared with Fig. 3.

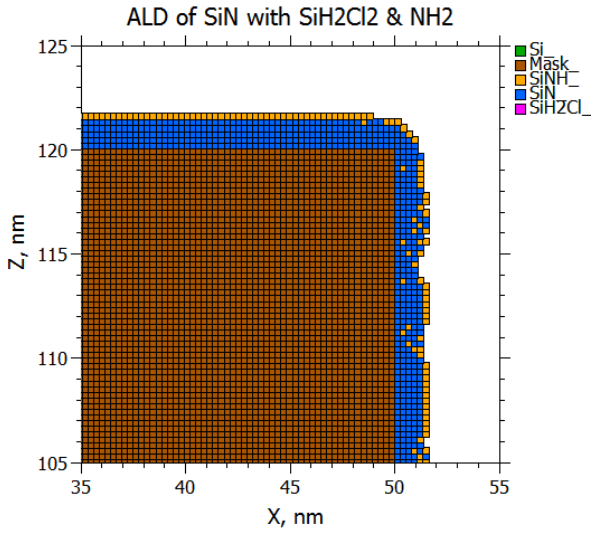

Fig 4. SiN film deposited during the first 10 ALD cycles of SiH_2Cl_2 and NH_2.

C. SiN ALD for High Aspect Ratio feeatures

In simulations, we also considered the cases of SiN ALD for low-aspect-ratio (LAR) and for high-aspect-ratio (HAR) features. For the same durations of time-steps in a cycle and same incident fluxes, we observed a difference in deposition profiles for features with different aspect ratios. The deposition profiles for the LAR features were smooth and almost conformal, except rounded corners. On the other hand, ALD profiles for the HAR features demonstrated non-

conformity in conditions when self-limitation of surface reactions was broken. In addition, the roughness of obtained profiles was also increased. Some results of simulations are shown in Figs. 5 and 6.

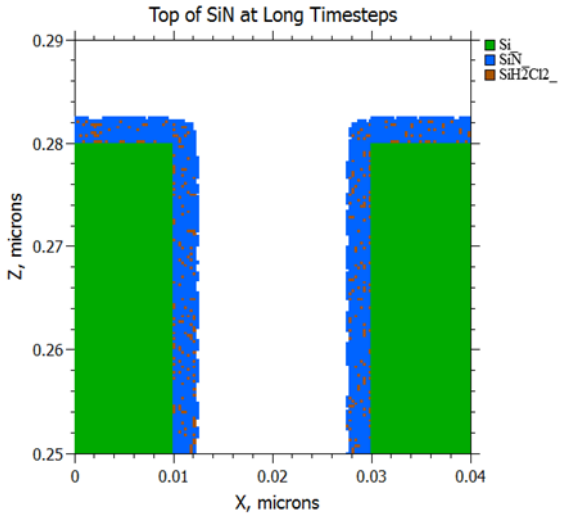

Fig. 5. Conformal SiN ALD profile for high aspect ratio feature and long timesteps. Only the top part is shown.

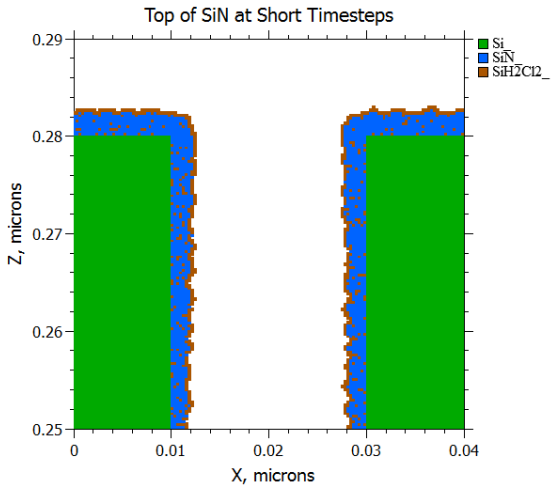

Fig. 6. Non-conformal SiN ALD profile for high aspect ratio feature and short timesteps. The roughness of the profile is also increased. Only the top part is shown.

III. Discussion and Conclusions

Numerical simulations provide valuable details and insight into involved processes and reactions and could lead to understanding of main factors for efficient materials processing. Atomic layer processing such as ALD is especially challenging to properly simulate, and to our knowledge FPS3D is so far the only feature-scale simulator capable of doing that.

We considered two different cases of SiN deposition to demonstrate the effect of steric hindrance of large molecules often used for ALD processing on resulting deposition rate. The first case corresponded to ALD cycle with application of hexachlorodisilane, Si_2Cl_6, and hydrazine, N_2H_4, precursors, while the second case utilized the cycle of dichlorosilane, SiH_2Cl_2, precursor and remote ammonia plasma for which we suggested NH_2 radical as being the most chemically active species.

The effect of steric hindrance was apparent only in the second case, as large SiH_2Cl_2 molecules were covering two surface sites upon adsorption. As a result, the deposition rate was only about half a monolayer of SiN per ALD cycle. During the first case, however, the large precursor molecules of Si_2Cl_6 and N_2H_4, were interacting differently with the surface. They split into two smaller radicals of $SiCl_3$ and NH_2 upon adsorption and surface interaction. Each of those smaller radicals was interacting with only a single surface site. Correspondingly, the steric hindrance effect was not involved, and the resulting deposition rate was about one SiN monolayer per cycle.

The results of SiN ALD simulations were found to be in good agreement with experiments [3-6].

ALD is especially important for deposition in the HAR features, where theoretically it should provide uniform deposition and good step coverage. However, ALD works well only when the duration of its time-steps is large enough for the self-limitation of reactive processes to occur. Because the fluxes of active species are reduced deeper inside a HAR feature, the time required for the self-limitation is growing. As only the self-limitation breaks somewhere at the depth, the local surface becomes underexposed, and that, according to FPS3D simulations, could result in a number of negative effects such as reduced deposition rate, increased surface roughness, and increased impurity content of the film.

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