

Physically Based Modelling of High-Density-Plasma-CVD on Different Scales

G. Schulze Icking-Konert* and A. Kersch
Infineon Technologies AG, Munich, Germany

A. Knorr
Infineon Technologies, East Fishkill, NY, USA

J. Radecker and A. Hausmann
Infineon Technologies, Dresden, Germany
 (Dated: September 30, 2002)

Simulations of SiO₂ HDP-CVD on both the reactor and the feature scale are presented. On the macroscopic scale "well mixed" reactor simulations using a literature chemistry model have been performed. Additionally the temporal evolution of sub- μ features has been studied using a custom simulator and a physically based microscopic model. A comparison with experimental data shows that the surface model presented here readily describes HDP-CVD over a wide range of process conditions.

I. INTRODUCTION

The continuously decreasing feature sizes in microelectronics call for more advanced isolation techniques. Today high density plasma chemical vapor deposition (HDP-CVD) of SiO₂ is widely used to electrically isolate neighbouring structures, e.g. metal lines and devices. Compared to thermal CVD this process exhibits superior gap fill properties, high deposition rates, and a low thermal budget. To support the development of advanced HDP-CVD processes we have performed an in-depth simulation study of the HDP-CVD process both on the reactor and the feature scale. Using the derived physically based microscopic model we are now able to consistently reproduce the temporal evolution of structures over a wide range of process conditions.

This paper is organized as follows. To obtain boundary conditions for the feature scale simulations we have performed "well mixed" reactor simulations using a literature model. These simulations are presented and discussed in section II. The obtained neutral/ionic fluxes and sheath voltages have been used for feature scale simulations which are described and discussed in section III. The paper concludes with a summary and an outlook.

II. REACTOR SCALE SIMULATIONS

The plasma properties inside a HDP-CVD reactor crucially depend on external process parameters like pressure or inductively coupled source power. In order to account for this in our feature scale simulations we first have performed "well mixed" reactor simulations. For this purpose we have used the commercially available *Aurora* simulator [1] and a chemistry model published

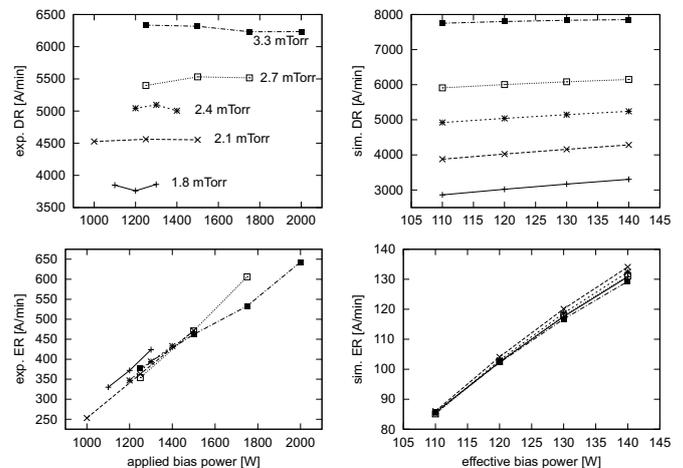


FIG. 1: Comparison of measured and simulated planar deposition and sputter rate as a function of applied bias power for various reactor pressures.

by Meeks et al. [2]. While we will not discuss this rather complex model here it is useful to point out its basic idea since our microscopic model is quite similar.

The key aspect of the surface chemistry proposed in [2] is that of an ion-enhanced deposition. Rather than depositing bulk material, ions (besides sputtering) merely activate passivated surface sites where subsequently neutral ballistic precursors can adsorb. After the deposition of neutrals the previously activated surface site becomes passivated again. In general, the surface activation depends on the kinetic energy of the incident ions which is controlled via the externally applied bias power.

Using this model we have performed well mixed reactor simulations over a wide range of process conditions. In figure 1 the calculated *planar* deposition (DR) and sputter rates (ER) are compared to experiments performed in an Applied Materials Ultima ICP reactor. Note that in the simulations the *effective* source and bias powers have been adapted to fit the data.

*Electronic address: georg.schulze-icking@infineon.com

As you can see the pressure and bias power dependence of both the DR and ER is reproduced well even though the absolute numbers differ noticeably. Besides pressure and bias power we have also varied the *effective* source power in the simulation. While not shown here the calculated trends agree well with those published by Nishimura et al. [3]. Therefore we are confident that our reactor scale simulations account for all dependencies relevant for the feature scale simulations presented below.

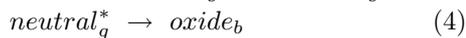
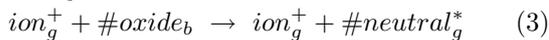
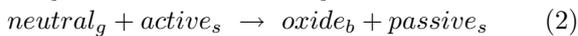
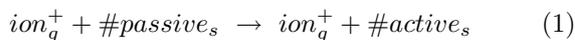
The measured dependencies in figure 1 fit well into the model of ion activated deposition:

- If the surface activation is high and only weakly depends on ion energy the DR mainly depends on the surface flux of the neutral precursors. This is consistent with the observed pressure dependence of the DR.
- In lowest order the ion loss does not depend on bias or reactor pressure. Under this assumption the ER is given by the (constant) ion flux times the sputter yield (which depends on bias power). This agrees well with the measured trends in the ER.

III. FEATURE SCALE SIMULATIONS

The reactor simulations presented above provide the input data for our custom feature scale simulator *Topsi*. This simulator works as follows. For fixed ionic/neutral fluxes and sheath voltage the flux distribution inside a microscopic structure is calculated via ballistic Monte-Carlo. From the sampled fluxes and energetic quantities (e.g. yield, see below) a surface chemistry solver computes the local deposition and etch rates. These are then used to propagate the surface via a levelset algorithm [4]. This procedure is re-iterated until the target film thickness is reached. Typically 10^5 MC particles are traced per time-step which takes approximately 1 s. Currently *Topsi* is limited to ballistic transport (Knudsen limit) which however is a reasonable assumption for HDP-CVD into sub- μ structures.

The effective surface chemistry model used for our HDP-CVD feature scale simulations has already been described in [5] and is inspired by that in [2]. Specifically the considered surface reactions are



with the subscripts g , s , and b denoting ballistic, surface, and bulk species, respectively. An '#' indicates an ion energy and angle dependent reaction multiplier (yield factor). In this model the first two reactions describe the surface activation by ions and the subsequent deposition

of neutral gas phase precursors. The next two reactions account for ion milling and redeposition of sputtered material. The last reaction describes the ion energy loss under reflection.

For each of the above reactions the respective probability prefactor, E/α -dependent probability and multiplicity ('#' reactions only), and velocity distribution of ballistic products have to be specified. Using well mixed reactor simulations, molecular dynamics calculations by Abrams et al. [6], and experimental data we have been able to determine a *single parameter set* which consistently describes the feature evolution over a wide range of HDP-CVD process conditions. The reaction parameters used for the simulations are characterized as following:

- For the surface activation by ions we assume a reaction probability which depends on the local angle of incidence like $\cos^{1.5}$ and increases with energy.
- Neutral gas phase precursors (*neutral_g*) are assumed to stick with unit probability on activated sites and zero probability on passivated sites. This results in an effective sticking coefficient which is equal to the activated surface fraction.
- The sputter yield used is mainly based on the MD data in [6]. It increases with impact energy and exhibits a pronounced maximum at large angles. With increasing ion kinetic energy this maximum shifts towards smaller angles while the ratio of maximum to planar ER decreases.
- Sputtered material is assumed to stick with unit probability (independent of activation).
- In all reactions ions are scattered diffusively and loose most of their kinetic energy for normal incidence or low impact energy. For grazing incidence ions are reflected almost specularly with little energy loss.

The above presented model contains the crucial reaction steps of the complex chemistry model in [2], namely ion assisted deposition and sputtering. On the other hand the number of parameters is sufficiently small to be fitted to experimental data. In contrast to simpler models (e.g. [7]) this model allows to predict the evolution of sub- μ under HDP-CVD of SiO_2 over a wide range of process conditions.

A. Results and Comparison to Experiment

To study the gap fill behaviour of HDP-CVD we have performed a variety of experiments under different conditions. Corresponding simulations have been performed using the above chemistry model. In this section some of the obtained results are compared to scanning electron microscopy (SEM) images.

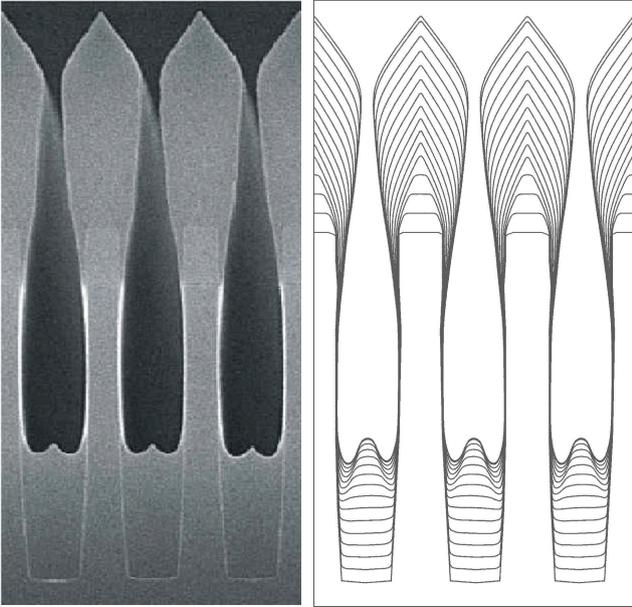


FIG. 2: Deposition into a trench test structure at extremely low bias. The SEM image is approximately 600 nm wide.

1. Low Bias Power

For very low bias powers the ion energy is below the sputter threshold. Therefore a measurement under these conditions allows a fit of the low-energy regime of reactions 1 and 5, independent of reactions 3+4. Figure 2 shows the SEM image of a test structure after HDP-CVD at low bias and the corresponding simulation. The simulation reproduces all features of the SEM image, namely the peaked shape, the low sidewall coverage, and the slight overhang. Note that at low bias the overhang is caused by *reflected* ions activating the surface and not by redeposition of sputtered material.

2. Pressure & Bias Variation

Under typical HDP-CVD conditions the sheath voltage is generally higher than the sputter threshold. In this case ion-assisted deposition and sputtering occur simultaneously which leads to a more complicated situation than in figure 2. In order to study this behaviour we have performed deposition experiments and simulations for different pressures and bias powers. For a "high" pressure of 3.5 mTorr and increasing planar DR/ER (bias power) the obtained results are shown in figure 3. The experimentally observed trends are reproduced by the simulation. At low bias (left image) only little sputtering is observed while sputtering leads to more redeposit (\rightarrow deeper voids) at higher sheath voltages (right image). Note also that by decreasing DR/ER the final surface becomes more planarized both in the experiments and the simulations.

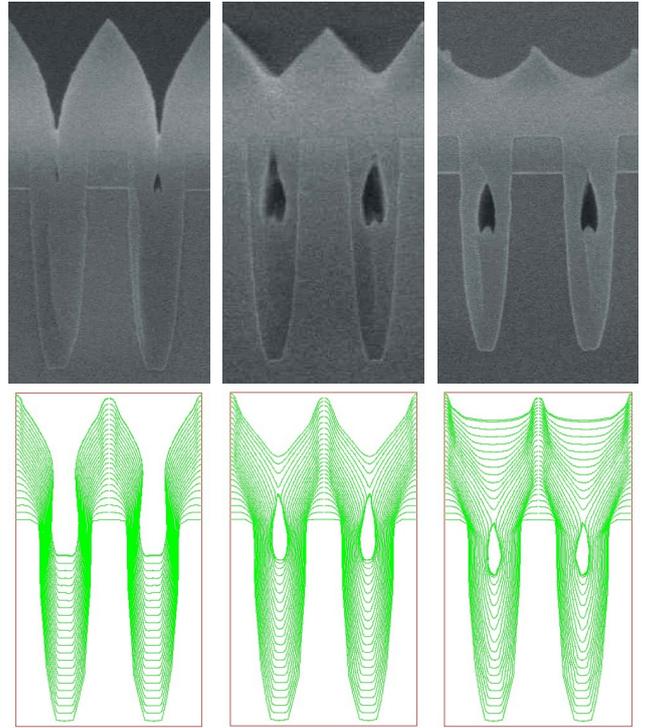


FIG. 3: Deposition into test structures at high pressure. The planar DR/ER decreases (bias increases) from left to right (20, 12, and 10). Each image is approximately 500 nm wide.

In figure 4 the SEM images and simulations are shown for a reduced pressure of 1.5 mTorr. However, the measured *planar* DR/ER ratios are identical to those in figure 3. Again, all experimentally observed trends are readily reproduced by the simulation. Specifically the simulated downward shift of the remaining voids, the clipped corners, and the faster planarization of the final surface agree well with the experiments. Comparing figures 3 and 4, it is evident that lowering the pressure increases the impact of ion milling, even at constant *planar* DR/ER.

3. Aspect Ratio Dependence

It has previously been shown that the HDP-CVD gap fill crucially depends on the initial geometry [8]. To further test our simulations we have therefore studied the evolution of test structures with different aspect ratios (AR). The obtained SEM images and the corresponding simulations are shown in figure 5. As can be expected the experimentally observed gap fill improves with AR. This behaviour is readily reproduced in the simulations: both the decreasing void size and its upward shift are correctly simulated.

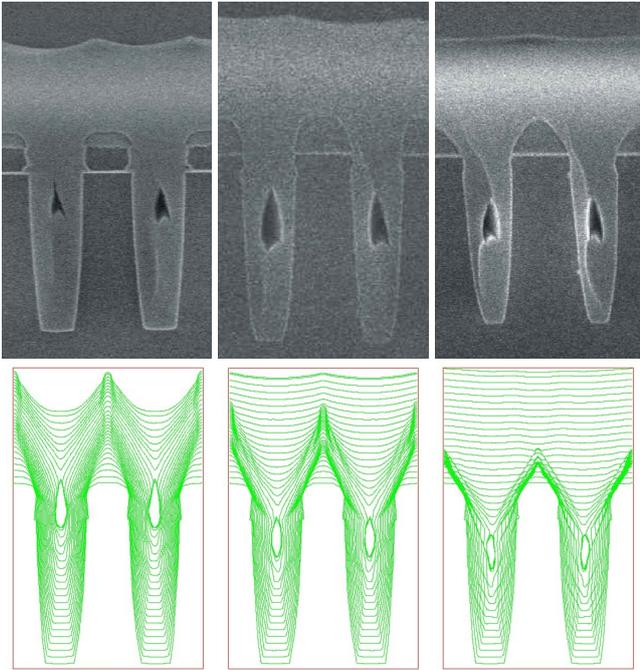


FIG. 4: Deposition into test structures at low pressure. The planar DR/ER decreases (bias increases) from left to right and are equal to those in figure 3. Note the clipped corners of the rightmost structure. Each image is approximately 500 nm wide.

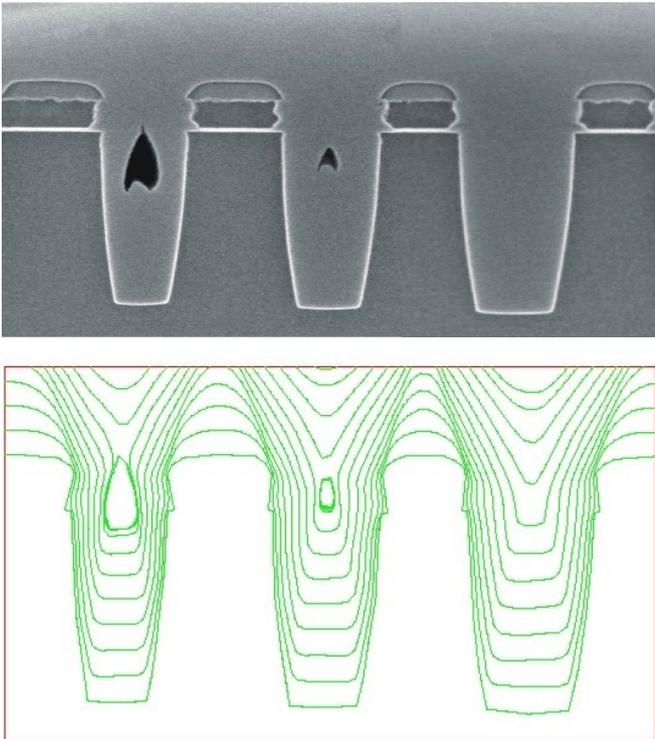


FIG. 5: Deposition into test structures with different aspect ratios. The AR from left to right are 4.6, 3.9, and 3.3. The image is approximately 1300 nm wide.

B. Discussion

The above presented experimental results contain some very interesting details which have been incorporated into our physical surface model.

One of the main features of the model is the assumption that the actual SiO_2 deposition in HDP-CVD is not directly ionic, but rather ion-activated. This assumption agrees well with [2] and also with the strong pressure dependence of the DR in figure 1. As we have seen in figure 2 this ion-activation leads to a pronounced peak structure, even at low bias. To account for this we have introduced a $\cos^{1.5}$ dependence of the surface activation (see model description). Together with the neutral deposition from the gas phase (reaction 2) this behaviour correctly describes the experimental observations.

As already pointed out the strong pressure dependence of the planar DR in figure 1 indicates that the planar deposition is limited by the flux of neutral precursors. This in turn implies that the planar surface is activated to a large extend since otherwise the neutrals could not react. However, if the surface activation was nearly perfect the differences between differently oriented surface patches would disappear. In this case no peak structure like that in figure 2 could evolve by mere ion activation. Together these two observations imply that the activation of a *planar* surface is of the order of several 10%. This estimate agrees well with our reactor simulations which typically yield 30% activation for the planar surface.

In process development the *planar* DR/ER ratio is commonly used to characterize the gap fill property of a process. However, as we have seen in figures 3 and 4, the DR/ER ratio is no suitable quantity for this purpose since it does not account for the pressure dependence of the HDP-CVD gap fill. The reason for this rather strong dependence lies in the energy dependence of the sputter yield in reaction 3: If the pressure is decreased at constant plasma source power the ratio of ions to neutrals increases. Consequently the bias power has to be decreased in order to keep the *planar* DR/ER constant. However, while the ER decreases with lower bias voltage, the *maximum shifts* to larger angles [6] where it eventually exceeds the growth rate (reaction 1 and 2) at this angle. Thus, a corner which was safe at higher pressure (*local DR > ER*) is clipped at lower pressure (*local DR < ER*).

IV. SUMMARY

In this paper we presented improved SiO_2 HDP-CVD simulations on the reactor and feature scale (with emphasis on the latter). The results show that our feature scale simulations reproduce the experimentally observed trends over a wide range of process conditions. We are confident that the proposed physically based surface chemistry model already accounts for the relevant mechanisms in the HDP-CVD of SiO_2 . Compared to sim-

pler models (e.g. [7]) our approach allows to predict the gap fill properties of different processes. This is a major

progress compared to the rules-of-thumb which are still common in todays HDP-CVD process development.

-
- [1] E. Meeks, *Aurora Manual*, Reaction Design (<http://www.reactiondesign.com>) (2000).
 - [2] E. Meeks, R. Larson, P. Ho, C. Applett, S. Han, E. Edelberg, and E. Aydil, *J.Vac.Sci.Technol.A* **2**, 544 (1998).
 - [3] H. Nishimura, S. Tagaki, M. Fujino, and N. Nishi, *Jpn.J.Appl.Phys.* **41**, 2886 (2002).
 - [4] J. Sethian, *Level Set Methods and Fast Marching Methods* (Cambridge University Press, 1999).
 - [5] A. Kersch and G. S. Icking-Konert, IEDM Proceedings (2000).
 - [6] C. Abrams and D. Graves, *J.Vac.Sci.Technol.A* **16**, 3006 (1998).
 - [7] R. Conti, L. Economikos, G. Papasouliotis, A. Knorr, and T. Ivers, DUMIC Conference Proceedings (1999).
 - [8] S. Kinoshita, S. Tagaki, H. Yabuhara, H. Nishimura, H. Kawaguchi, and N. Shigyo, *Jpn.J.Appl.Phys.* **41**, 1974 (2002).