INVERSE MODELING OF OXID DEPOSITION USING MEASUREMENTS OF A TEOS CVD PROCESS

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ABSTRACT

The goal of this paper is to identify simulation models for the deposition of silicon dioxide layers from TEOS (Tetraethoxysilane) in a CVD (Chemical Vapor Deposition) process and to calibrate the parameters of these models by comparing simulation results to SEM (Scanning Electron Microscope) images of deposited layers in trenches with different aspect ratios. We describe the three models used and the parameters which lead to the best results for each model which allows us to draw conclusions on the usefulness of the models.

1. INTRODUCTION

During the fabrication of an IC (Integrated Circuit) a wafer has to undergo many processes. Each process accomplishes a specific change in the state of the wafer. Some of these processes can be described using relatively simple models. However, many processes require more complex models to be developed reliably. Process modeling and simulation have been used generally for understanding and not for quantitative prediction of processes. Therefore, for more general prediction and analysis, a CVD topography model must use detailed descriptions of chemical reactions with chemical reaction rates and thermodynamic properties of species obtained by experiment and/or by calculation.

In spite of the complexity of these models, their quantitative predictability is still limited for processes of industrial interest. Therefore, the simpler calibrated sticking coefficient models provide good alternatives for process investigations and especially for time-consuming optimization and inverse modeling tasks. The simulations are performed by our topography simulator ELSA (Enhanced Level Set Applications) and the parameters are estimated using SIESTA (Simulation Environment for Semiconductor Technology Analysis) [1], [2].

The outline of this paper is as follows. First, we describe briefly the level set method which is used to track the moving boundaries in ELSA. Second, the different models used for the calibration of simulation results to measurements are presented. Finally, the simulation results are presented.

2. LEVEL SET METHOD

The level set method [3] provides means for describing the movement of boundaries, i.e., curves, surfaces or hypersurfaces in arbitrary dimensions, and their evolution in time which is caused by forces or fluxes normal to the surface. The basic idea is to view the curve or surface in question at a certain time t as the zero level set (with respect to the space variables) of a certain function $\phi(t, \mathbf{x})$, the so called level set function. Thus the initial surface is the set $\{\mathbf{x} \mid \phi(0, \mathbf{x}) = 0\}$.

Each point on the surface is moved with a certain speed normal to the surface and this determines the time evolution of the surface. The speed normal to the surface will be denoted by $F(t, \mathbf{x})$. For points on the zero level set $F(t, \mathbf{x})$ is usually determined by physical models and in our case by etching and deposition process models, or more precisely by the fluxes of certain gas species and subsequent surface reactions. The speed function $F(t, \mathbf{x})$ generally depends on time and the space variables.

After calculation of the initial level set function, the speed function values are used to update the level set function in a finite difference or finite element scheme. Usually the values of the speed function are not determined on the whole domain by the physical models and, therefore, have to be extrapolated suit-

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ably from the values provided on the boundary, i.e., the zero level set. This can be carried out iteratively by starting from the points nearest to the surface.

In order to extend the speed function, we use the fact that only the values of the level set function near its zero level set are essential, and thus only the values in a narrow band around the zero level set have to be calculated. Both improvements, extending the speed function and narrow banding, require the construction of the distance function from the zero level set in the order of increasing distance. Since calculating the exact distance function from a surface consisting of a large number of small surface elements is computationally expensive, it can be only justified for the initialization. Therefore, an approximation to the distance function by a special fast marching method is performed in [3], [4], [5].

3. THE MODELS

The transport model can be characterized by the ratio of the mean free path of the species to the characteristic length scale (the largest dimension of the feature). This ratio is called the Knudsen number. A high Knudsen number ($\gg 1$) implies that the frequency of particle-particle collisions is negligible relative to particle-surface collisions, i.e., the process is under free molecular regime. A small Knudsen number ($\ll 1$) implies that collisions between particles occur much more frequently than collisions between species and the feature surface. This is called continuum transport regime. A Knudsen number about one implies the transition regime where the order of magnitude of the particle-particle and particle-surface collisions are approximately the same [6].

Because of the low pressure condition of the TEOS process, the mean free path of the species is much higher than the feature dimensions and therefore the Knudsen number is $\gg 1$. The process is in the free molecular regime under which the radiosity model for the transport of the particles is used [3].

In our earliest attempts we successfully simulated a single trench. We used the so called point-shape source model, where the source of species is assumed to be a single point in the middle of the simulation domain above the trench. The flux distribution around the vertical axis follows a cosine form (this distribution is also assumed for the models presented in the next sections) and the direct flux received at the surface elements was assumed to be proportional to the inverse of the distance between the source and the middle point of a surface element. However, the optimum sticking factors showed a strong dependence on the aspect ratio [7].

3.1 Line source model

As mentioned above, the single-point shape model is not able to predictively simulate a set of trenches with different aspect ratios. There are additional problems as the model does not allow to simulate many trenches back to back (this is needed, e.g., for the deposition of silicon nitride into interconnect lines, e.g., for a backend process). The first idea for overcoming this problem was to set many point-shape sources along a source line above the wafer. However, one open question is in which distances the points must be set, i.e., how many source points and how long do we have to extend the source line outside of the simulation domain to obtain a reliable number of sources? To avoid the problem of asymmetry which happens by this solution, if one half of the trench may see one source point more than the other half due to discretization, the number of points has to be increased above a certain threshold value which is related to discretization. However, the simulation time is increased considerably because the number of visibility tests between the surface elements and point-shape sources increases significantly. The line source model presented in the following is a good alternative for overcoming these mentioned problems.

In this model the source consists of a line of continuous point-shape sources. Using this model, one of the expensive time consuming parts of the discrete set of point-shape source, namely, the visibility test is moderated and the computation time is therefore significantly reduced. As our experiences have shown, the visibility test in steps of one degree gives sufficient accuracy. Therefore, instead of separate visibility tests among a surface element and different sources, a complete visibility test is performed in maximum 180 steps, which is the case if a surface segment is on the flat open part of the trench. In this model the flux has been assumed to depend only on the visible angle between the surface elements and the line source. The two different sticking coefficients have been identified by calibration using SIESTA. The first coefficient denotes the probability of sticking the particles on the surface by first bouncing from the source and the second coefficient is for the probability of the reflection of the particles from the surface elements. Although the outline of the trench for a low aspect ratio is reproduced, predictively as shown in Fig. 1, it is difficult to reproduce both the upper and lower part of the trenches at the same time for a higher aspect ratio as shown in Fig. 4.

3.2 Flux dependent sticking coefficient model

Although in the previous model the sticking coefficients have been assumed to be constant, but in the reality they depend on temperature and on the local flux.

The overall sticking coefficient can be written as [8]

$$\beta(T, F(\mathbf{x})) = \frac{R(T)}{F(\mathbf{x})} \tag{1}$$

where R is the number of molecules per area and per time that become part of the film, and $F(\mathbf{x})$ denotes the position-dependent flux. If the reaction follows mth order kinetics, then

$$R = k(T)F(\mathbf{x})^m \tag{2}$$

where $k(T)$ is the rate parameter depending on temperature T. Substituting (2) into (1) results in:

$$\beta(T, F(\mathbf{x})) = k(T)F(\mathbf{x})^{m-1} \tag{3}$$

Based on (3) and two further assumptions we have developed a flux dependent sticking coefficient model. The first assumption is that the temperature T remains constant and the second one that the deposition of silicon dioxide from TEOS follows a half order reaction [8], i.e., $m = \frac{1}{2}$. Therefore, the sticking coefficient is $\beta = \beta_0 F(\mathbf{x})^{-1/2}$, where β_0 is a constant scaling factor to guarantee that sticking coefficients are always less or equal than one.

The results are in good agreement with the measurements of low aspect ratio trenches as shown in Fig. 2. For higher aspect ratios, however, the amount of material deposited on the side-walls is overestimated as shown in Fig. 5. This may result in spurious void formations.

3.3 Two species model

With the last two models we have reached the limits of models which only assume one species for the deposition of silicon dioxide from TEOS. In [9] it has been assumed that there may be two reaction paths in the LPCVD (Low Pressure CVD) of silicon dioxide from TEOS. One is the direct decomposition of TEOS on the surface, with a very low sticking coefficient, and the other is the formation of a very reactive intermediate, due to gas phase reactions, which reacts with the surface to form silicon dioxide [9]. The model considers two species but does not differentiate how they are formed. Therefore, the model is independent of the reaction path. The implementation of this model has been performed by Islamraja *et al.* [9]. Although a relative good agreement between the simulation results and measurement has been presented, the simulations have only been performed for a single trench [9].

Based on the idea of this model we have developed our two species model, where the second species is the by-product of the reaction of a particle of the first species with the surface. The flux of the second species is proportional to the flux of the first species, but the sticking probabilities of both species remain again constant. This model shows excellent agreement with SEM images as shown in Fig. 3 and Fig. 6.

4. CONCLUSION

A multitude of deposition models for TEOS processes and the calibration of simulation results to measurements have been proposed. In summary we find that a two-species model yields the best results among the three different deposition models investigated, both for high and low aspect ratio trenches. With this model we can avoid more complex deposition models.

5. REFERENCES

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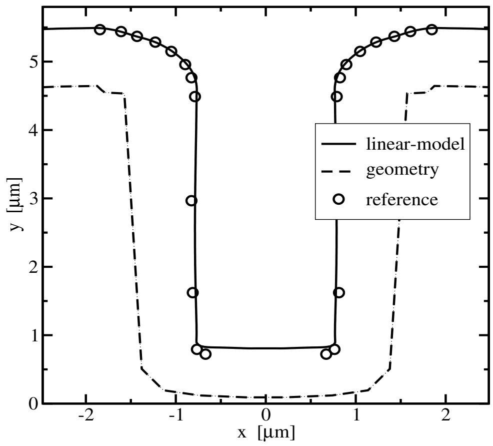

Fig. 1. Comparison between simulation and measurement for the continuous line-source model for a trench with a low aspect ratio.

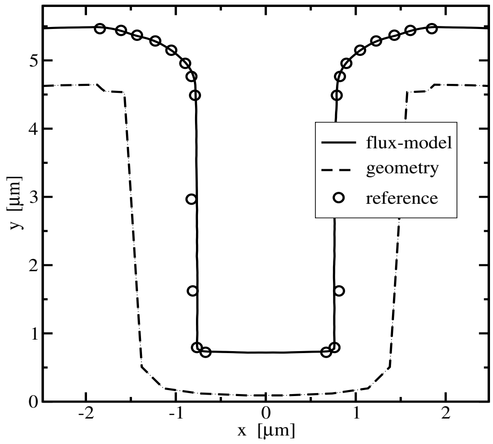

Fig. 2. Comparison between simulation and measurement for the flux-dependent sticking coefficient model for a trench with a low aspect ratio.

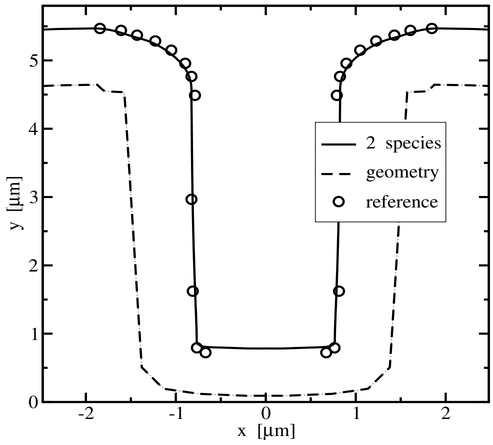

Fig. 3. Comparison between simulation and measurement for the two-species model for a trench with a low aspect ratio.

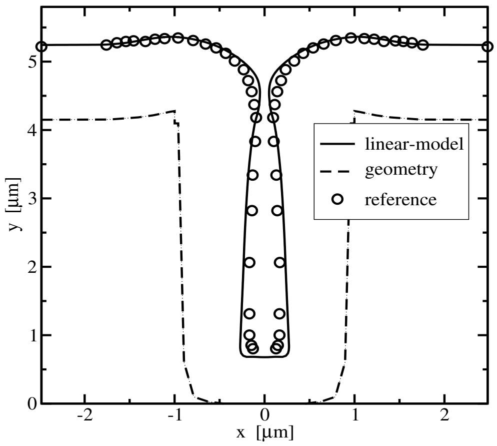

Fig. 4. Comparison between simulation and measurement for the continuous line-source model for a trench with a higher aspect ratio.

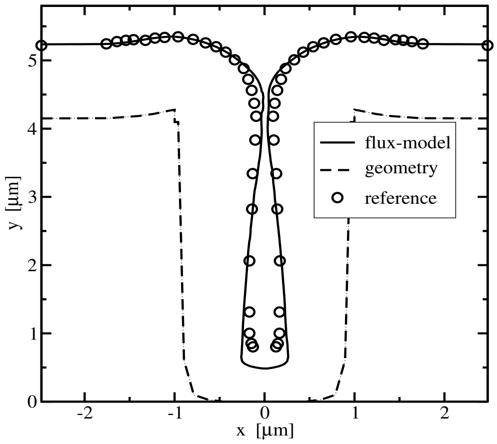

Fig. 5. Comparison between simulation and measurement for the flux-dependent sticking coefficient model for a trench with a higher aspect ratio.

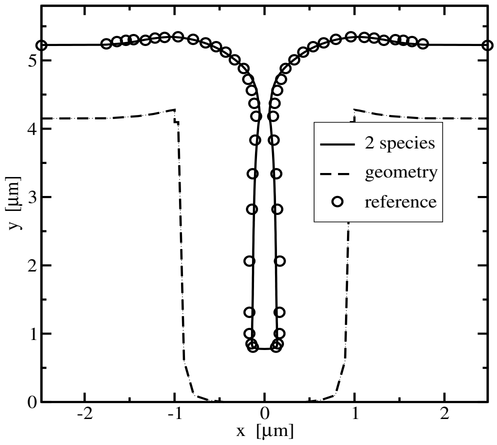

Fig. 6. Comparison between simulation and measurement for the two-species model for a higher aspect ratio.