ELSEVIER

Available online at www.sciencedirect.com
ScienceDirect

Microelectronics Reliability 47 (2007) 623–625

MICROELECTRONICS RELIABILITY

www.elsevier.com/locate/microrel

Comparison of deposition models for a TEOS LPCVD process

Stefan Holzer [a,*], Alireza Sheikholeslami [b], Markus Karner [b], Tibor Grasser [a], Siegfried Selberherr [b]

[a] *Christian Doppler Laboratory for TCAD in Microelectronics at the Institute for Microelectronics, TU Wien, Gußhausstraße 27–29/E360, 1040 Wien, Austria*

[b] *Institute for Microelectronics, TU Wien, Gusshausstrasse 27–29/E360, 1040 Wien, Austria*

Available online 2 March 2007

Abstract

We present a comparison of models describing the pyrolytic deposition of SiO_2 with a low pressure chemical vapor deposition process. In order to meet industrial simulation requirements, e.g. accuracy and fast delivery of results, we present an overview of established and new models, their use within TCAD applications, and their best results which have been obtained by calibrations according to SEM measurements.
© 2007 Elsevier Ltd. All rights reserved.

1. Introduction

Recent developments of semiconductor device structures require more accurate material deposition models. This is particularly true for embedded materials such as silicon dioxide which is used as a common dielectric or a hard mask material [1]. One widely applied process is oxide deposition with a TEOS (tetraethoxysilane) LPCVD (low pressure chemical vapor deposition) process. The rigorous description of oxide deposition with TEOS requires the consideration of more than 40 different chemical reactions [2,3], which increases the simulation time tremendously and offers at the current stage improvement for the insight into the rather complex pyrolytic deposition process only at high computational costs, which limits any industrial interest [2]. Industrial applications require fast and accurate simulation results for this fairly complex chemical process.

For reasonably accurate and fast simulation of deposition processes it is frequently claimed that chemical reaction mechanisms should be used rather than sticking coefficients. However, the quantitative predictability of such fairly complex models is still very limited for industry-related processes [2]. Thus, simple process models applying calibrated sticking coefficients are a good alternative for process investigations, especially for time-consuming optimizations, calibrations, and design of experiments.

We present several models which sufficiently describe the oxide deposition with TEOS within reasonable computation times to meet the industrial requirements.

2. Simulation method

To investigate the complex deposition process, a level-set algorithm [4] has been implemented into our topography simulator ELSA (Enhanced Level-Set Applications) [5]. This algorithm describes the evolution of a moving boundary by applying a speed function $F(\mathbf{x}, t)$ (normal to the boundary) to the level-set function $\varphi(\mathbf{x}, t)$:

$$\partial_t \varphi(\mathbf{x}, t) + F(\mathbf{x}, t)\|\nabla_{\mathbf{x}} \varphi\| = 0. \quad (1)$$

The initial condition for $\varphi(\mathbf{x}, 0)$ is the initial surface geometry. The speed function F represents the physical behavior (growth rate) during the deposition process which can be approximated to suit our demands. The current position of the evolving surface is determined by the zero values of the level-set function $\varphi(\mathbf{x}, t) = 0$. A particularly intriguing feature of the use of level-set algorithms is that the computational effort of tracking a three-dimensional surface

* Corresponding author. Tel.: +43 1 58801 36015; fax: +43 1 58801 36099.
E-mail address: Stefan.Holzer@ieee.org (S. Holzer).

0026-2714/$ - see front matter © 2007 Elsevier Ltd. All rights reserved.
doi:10.1016/j.microrel.2007.01.058

evolution is comparable with that of a two-dimensional one, when using a cell-based algorithm [4]. Hence, the order of the computational effort is dramatically reduced.

3. Model description

First, a model based on a single point-shaped source of species [5] is considered, which yields excellent results for wide rectangular trenches. When this model is applied to thinner trenches or trenches with non-rectangular shapes, it fails due to overestimation of the local fluxes at some parts of the trench surface.

Since this approach does not deliver satisfactory results, we extend the single source model into a continuous line-source model where the flux depends only on the visible angle between the surface elements and the source. Compared to our previous work [5,6], the problem that the trench closes at its top with increasing AR (aspect ratio, height to width ratio), is shifted to higher ARs, but the shape of the calculated surface at the bottom of the trench still does not reproduce the trends of the corresponding measurements, as shown in Fig. 1. However, for wide trenches with low ARs, this models is applicable and very fast.

In order to describe the deposition for trenches with large AR, we have implemented a flux-depended sticking coefficient model which considers the sticking coefficients as a function of the local material flux at the surface of the trench. The sticking probability of the incoming molecules follows a half-order kinetic law [3], where the sticking coefficient β is proportional to the inverse of the square root of the local material flux $\Gamma(\mathbf{x},t)$ coming from the TEOS material source

$$\beta = \beta_0 \Gamma^{-1/2}(\mathbf{x}, t), \tag{2}$$

where β_0 represents a constant scaling factor to guarantee that the sticking probability of β remains within the open interval]0,1[. This model produces results in good agreement with measurements for $\beta_0 = 0.852$, as presented in Fig. 2, in particular also at the top of the trench. Furthermore, a good accordance at the top of the trench is shown. However, as soon as the sidewalls grow towards each other, an overestimation of the sidewall growth is also clearly evident for this model. Hence, this model can be applied for deposition thicknesses $d < 0.5$ AR.

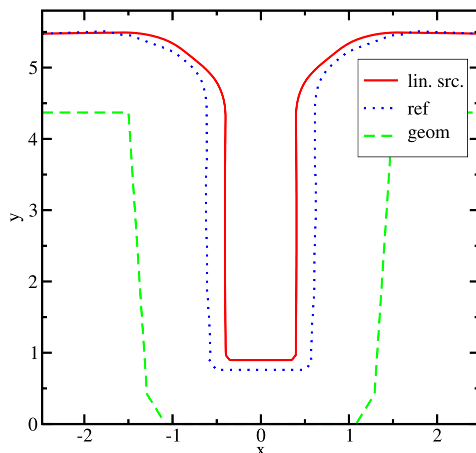

Fig. 1. Simulation using the linear source model compared with measurements.

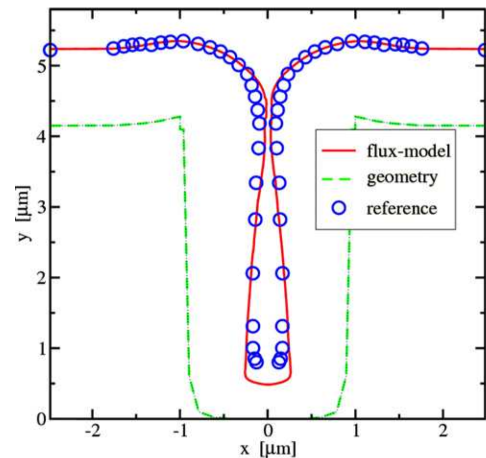

Fig. 2. Comparison of measurements and simulation result with the flux-dependent model using $\beta_0 = 0.852$.

To overcome this constraint, we have developed an improved model considering a main contribution of the material deposition and a second contribution that follows from the sum of the deposition of the by-products. We model these two processes as statistically independent processes, dealing with two independent sticking coefficients β_1 and β_2, which describe the sticking probabilities for particles coming directly from the source and already produced particles on the surface due to chemical surface reactions, respectively.

A calibration of this model yields the values for the two sticking probabilities as $\beta_1 = 0.581$ and $\beta_2 = 0.732$, which results in excellent agreement with experimental data.

4. Comparison

Each of the proposed models has been calibrated using the simulation and optimization framework SIESTA (simulation environment for semiconductor technology analysis) [6,7].

As a result of the calibration process we obtained technology-dependent coefficients for the linear source model and the flux-dependent sticking coefficient model, which affect only the speed of material growth. The calibration of the two-species model was more sensitive to the model parameters, because the variations of the sticking coefficients alters the shape of the surface of the deposited material, which can cause numerical shadowing effects and yields non-physical deposition results. This requires to renormalize the probabilities of the sticking coefficients as an equivalent to mass conservation which has also improved the numerical robustness of our model. Finally, we obtained the best values for the sticking coefficients of the two-species model as $\beta_1 = 0.581$ and $\beta_2 = 0.732$.

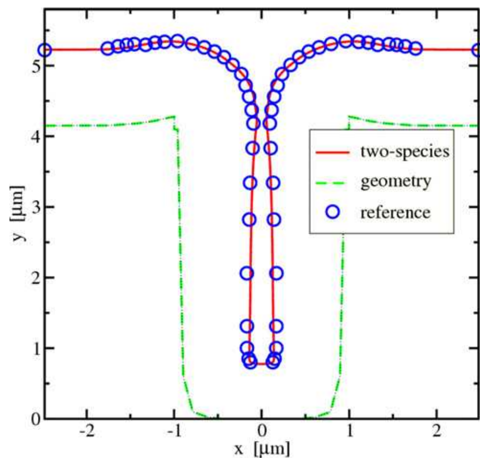

Fig. 3. Comparison of measurements and simulation results with the two-species model using $\beta_1 = 0.581$ and $\beta_2 = 0.732$.

Because the two-species model considers two different species for deposition, there is only a slight coupling between them. Instead of a numerical intensive calculation as for the flux-dependent sticking coefficient model, the two-species model uses the benefit of two independent coefficients, which speeds up simulation and demands only 80% of the CPU time compared to the flux-dependent sticking coefficient model. Furthermore, the two-species model overcomes the overestimation at the sidewalls of the trenches (cf. Fig. 3). Thus, the presented method enables efficient and accurate geometry optimizations.

5. Summary and conclusion

We have presented models for state-of-the-art algorithms to track the surface evolution during oxide deposition by a TEOS deposition process in two and three dimensions. The calibration and inverse modeling with SIESTA provides a fast and accurate calibration of the model parameters. However, for each new technology node the model parameters have to recalibrated to maintain the same accuracy and predictability of the simulations tools. For that purpose, SIESTA offers various features, e.g. design of experiments, statistical analysis, and different methods of calibrations, to improve the speed of model calibrations. Comparisons of the two-species model with measurements give a perfect agreement for arbitrarily shaped geometries.

References

[1] Arakawa S, Mizuno I, Ohoka Y, Nagahata K, Tabuchi K, Kanamura R, et al. Breakthrough integration of 32 nm-node Cu/ultra low-*k* SiOC ($k = 2.0$) interconnects by using advanced pore-sealing and low-*k* hard mask technologies. In: 2006 International interconnect technology conference, San Francisco: 2006. p. 210–2.

[2] Coltrin M, Ho P, Moffat H, Buss R. Chemical kinetics in chemical vapor deposition: growth of silicon dioxide from tetraethoxysilane (TEOS). Thin Solid Films 2000;365(2):251–63.

[3] Cale T, Raupp G. A unified line-of-sight model of deposition in rectangular trenches. J Vac Technol Sci B 1990;8(6):1242–8.

[4] Sethian J. Level set methods and fast marching methods. Cambridge: Cambridge University Press; 1999.

[5] Heitzinger C, Fugger J, Häberlen O, Selberherr S. Simulation and inverse modelling of teos deposition processes using a fast level set method. In: Simulation of semiconductor processes and devices, Kobe. Japan: 2002. p. 191–4.

[6] Holzer S, Sheikoleslami A, Wagner S, Heitzinger C, Grasser T, Selberherr S. Optimization and inverse modeling for TCAD applications. In: Symposium on nano devices technology 2004, Hsinchu. Taiwan: 2004. p. 113–6.

[7] Institute for Microelectronics, SIESTA – The simulation environment for semiconductor technology analysis, Technische Universität Wien, Austria 2003.