Comparison of Deposition Models for a TEOS CVD Process

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This paper focuses on the comparison of calibrated models for TEOS deposition in a CVD process according to SEM images of SiO_2 layers. We describe the applied models and the parameters which lead to the best results for each model. The simulations have been performed using our topography simulator ELSA (Enhanced Level Set Applications) which follows the surface evolution by solving the level set equation [1, 2]. The parameter calibration and optimization has been carried out with our simulation and optimization framework SIESTA (Simulation Environment for Semiconductor Technology Analysis) [3].

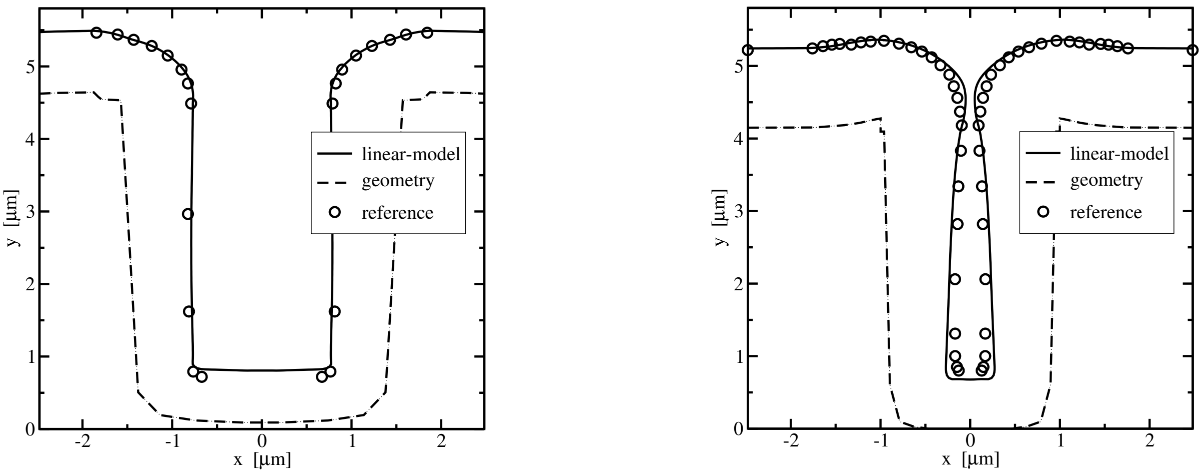
For accurate simulation of deposition processes it is frequently claimed that chemical reaction mechanisms should be used rather than sticking coefficients. However, the quantitative predictability of such fairly complex models is still limited for processes of industrial interest [4]. Thus, simple calibrated process models applying sticking coefficients are a good alternative for process investigations, especially for time-consuming optimization and inverse modeling tasks.

In an earlier attempt we considered a model based on a single point-shaped source of species [2]. Since this approach did not deliver satisfactorily results, we extended 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 the earlier attempt, the problem that the trench closes at its top with increasing AR (aspect ratio), is shifted to higher ARs, but the geometry at the bottom of the trench does still not satisfactorily agree with measurement as shown in Figure 1. The parameters calibrated by SIESTA were the sticking coefficients, β_1 and β_2, which describe the sticking probability for particles coming directly from the source and already reflected particles, respectively. The values obtained for these coefficients were $\beta_1 = 0.248$ and $\beta_2 = 0.267$.

The next approach we considered has been suggested in [5] and includes a single flux-dependent sticking. The deposition reaction follows the half order kinetics for a CVD process of TEOS. Hence, the sticking coefficient is proportional to the inverse of the square root of the local flux coming from the source $\beta = \beta_0 F(\mathbf{x})^{-1/2}$, where $\mathbf{x}$ is the space variable, $F(\mathbf{x})$ the local flux, and β_0 a constant scaling factor. The results obtained for $\beta_0 = 0.852$ are in good agreement with the measurements for low aspect ratios as shown in Figure 2-a. However, for higher aspect ratios (c.f. Figure 2-b) a significant overestimation of the material deposition on the walls is obtained which may result in spurious void formations.

With increased AR the overestimation of the wall thickness increases as shown in Figure 1-b and 2-b. Thus, we considered in another attempt a deposition model with two species which take part in a TEOS deposition reaction to overcome this spurious effect. The second species is a chemical product of a reaction from a particle of the first species with the surface where the flux of the second species is proportional to the flux of the first species but the sticking probability coefficients for both species remain constant. This new model shows excellent agreement with measurements for different geometries as shown in Figure 3-a and 3-b with the sticking parameters $\beta_1 = 0.581$ and $\beta_2 = 0.732$ for the first and the second species. In addition, this model requires only 80% of the CPU time than that of the flux-dependent model and overcomes the overestimation at the trench walls. Thus, the presented method enables efficient and accurate geometry optimizations. The hereby extracted sticking coefficients are already been applied to three-dimensional structures and have shown promising results.

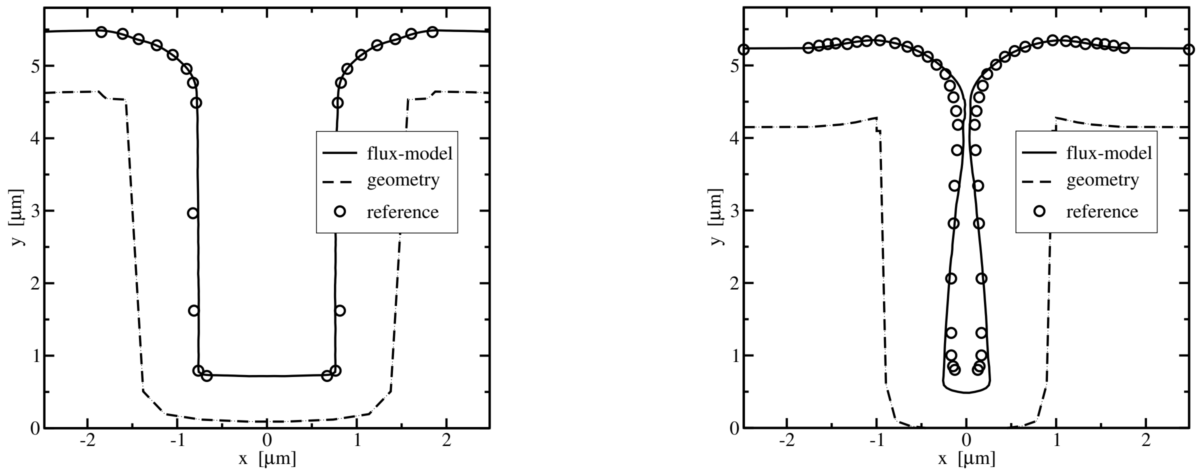
[1] J. Sethian, *Level Set Methods and Fast Marching Methods* (Cambridge University Press, Cambridge, 1999).
[2] C. Heitzinger *et al.*, in *Simulation of Semiconductor Processes and Devices* (Kobe, Japan, 2002), pp. 191–194.
[3] S. Holzer *et al.*, in *SNDT 2004, Symposium on Nano Devices Technology 2004* (Hsinchu, Taiwan, 2004), pp. 113–116.
[4] M. Coltrin *et al.*, Thin Solid Films **365**, 251 (2000).
[5] T. Cale and G. Raupp, J. Vac. Sci. Technol. B **8**, 1242 (1990).



(a) Trench with AR = 1.35.

(b) Trench with AR = 2.28.

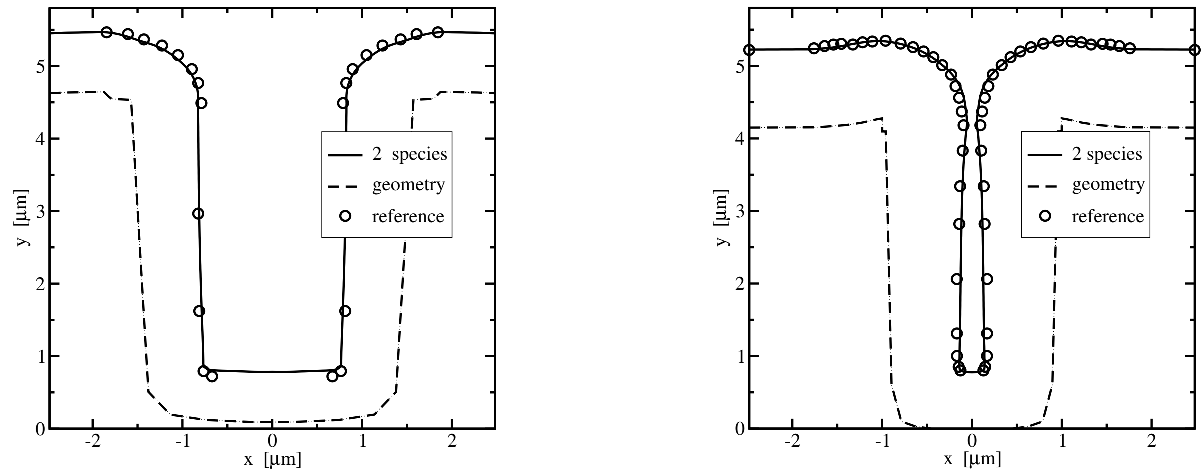
Figure 1: Comparison between simulation result and measurement for the continuous line-source model.



(a) Trench with AR = 1.35.

(b) Trench with AR = 2.28.

Figure 2: Comparison between simulation and measurement for the flux-dependent sticking model.



(a) Trench with AR = 1.35.

(b) Trench with AR = 2.28.

Figure 3: Comparison between simulation and measurement for the 2-species model.