Simulation and Inverse Modeling of TEOS Deposition Processes Using a Fast Level Set Method

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Abstract **– Deposition and etching of Silicon trenches is an important manufacturing step for state of the art memory cells. Understanding and simulating the transport of gas species and surface evolution enables to achieve void-less filling of deep trenches, to predict the resulting profiles, and thus to optimize process parameters with respect to manufacturing throughput and the quality of the resulting memory cells. For the simulation of the SiO_2 deposition process from TEOS (Tetraethoxysilane), the level set method was used in addition to physical models. The level set algorithm devised minimizes computational effort while ensuring high accuracy by intertwining narrow banding and extending the speed function. In order to make the predictions of the simulation more accurate, model parameters were extracted by comparing the step coverages of the deposited layers in the simulation with those of SEM (scanning electron microscope) images.**

I. INTRODUCTION

The level set method is based on representing surfaces as the zero level set of a function $u(t, \mathbf{x})$ and solving the partial differential equation

$$u_t + F(t, \mathbf{x})\|\nabla_{\mathbf{x}} u\| = 0,$$
$$u(0, \mathbf{x}) \text{ given},$$

where $F(t, \mathbf{x})$ is the speed function determining the speed points of the surface move in direction normal to it. The advantages of the level set method are twofold: The resolution achieved is higher than the resolution of the grid where calculations takes place, and hence higher than the resolution achieved using a cellular format on a grid of the same size [1]. Furthermore, calculating surface normals is more precise than when using a cellular format.

As part of a general simulator for etching and deposition processes, an advanced level set algorithm was devised and implemented. Its features are presented in the next section. Then the transport of species above the wafer surface and a method for speeding up and thus increasing the accuracy of radiosity calculations are discussed. Finally simulation results and examples of narrow bands and extended speed functions are shown. The simulation flow for etching and deposition processes as it is implemented in the simulator is depicted in Figure 1.

II. NARROW BANDS AND EXTENDING THE SPEED FUNCTION

For the first time narrow banding and extending the speed function were combined into one algorithm. This algorithm provides several benefits. First, the speed function is retained as the signed distance function throughout the simulation, which assures good accuracy till the end of the simulation. Second, narrow banding reduces the number of active points that have to be updated from $O(n^2)$ to $O(n)$. By retaining the signed distance function the width of the narrow band is kept down to two points on each side (cf. Figure 4) without decreasing accuracy. Third, time consuming calculations (cf. [2]) are reduced to a minimum by intertwining the computations necessary for narrow banding and extending the speed function. Finally, it is noted that the width of the narrow band can be adjusted if desired.

An outline of the algorithm is as follows. First the initial points near the zero level set, where the speed function is known, and the neighboring trial points are determined. In the main loop it is checked if there is still a trial point to be considered in the narrow band. All trial points are stored in a heap ordered by their distance to the zero level set. If there is a point to be considered, both its distance is approximated and its extension speed calculated, and its neighbors are updated accordingly. Finally after the main loop, bookkeeping information for the narrow band points is updated using distance information just computed. The computation

time consumed by this algorithm is negligible compared to that required for the physical models, while it provides high accuracy.

The details of the algorithm that performs narrow banding and extending the speed function are as follows.

1. Tag all points neighboring the current zero level set as *known*. Compute their distance to the zero level set. Tag the rest of the points as *far*. (All points are partitioned into three sets: *far*, *known*, and *trial*.) Initialize the speed function at the known points from the results of the simulation of transport.
2. Find the *trial* points, i.e., the neighbors of the *known* points, and compute their tentative distance from the zero level set. Store the *trial* points in a heap.
3. **Loop** while there are *trial* points: let a be the *trial* point with the smallest distance value. Remove a from the heap. If the distance of a from the zero level set is larger than the width of the narrow band, return from the loop. Tag a as a known point. Do the following for all neighbors b of a: if b is a *far* point, tag it as *trial*, insert it into the *trial* heap, and compute and set its distance and extension speed; after that, if b now is a *trial* point, compute and set its distance and extension speed.
4. Finally, sign the distance function accordingly. Use the distance function just computed for keeping track of the narrow band. Use the extended speed function for the level set iteration.

III. MODELING OF TRANSPORT AND THE DEPOSITION REACTION

Under the process conditions applied in one of the examples (cf. Figure 2), the transport of TEOS in the boundary layer above the wafer happens in the diffusion regime and thus is governed by the diffusion equation. The boundary conditions are as follows: at the top of the simulation domain a Dirichlet boundary condition is assumed, i.e., a constant concentration is supplied from the convective zone in the reactor; on the left and right hand side a Neumann boundary concentration is assumed, i.e., the fluxes are zero; and finally the fluxes at the wafer surface are determined by the amount of particles deposited.

In order to calculate the thickness Δd of the film deposited during a time interval of length Δt, we observe that Δd is proportional to Δt, to an Arrhenius term, and to the deposition rate R_i corresponding to the deposition model chosen. This implies

$$\Delta d = \Delta t \cdot k_e \mathrm{e}^{-E/kT} \cdot R_i.$$

Here $k_e \mathrm{e}^{-E/kT}$ is the Arrhenius term with activation energy E, absolute temperature T, and preexponential constant k_e. R_i is the deposition rate of the deposition model

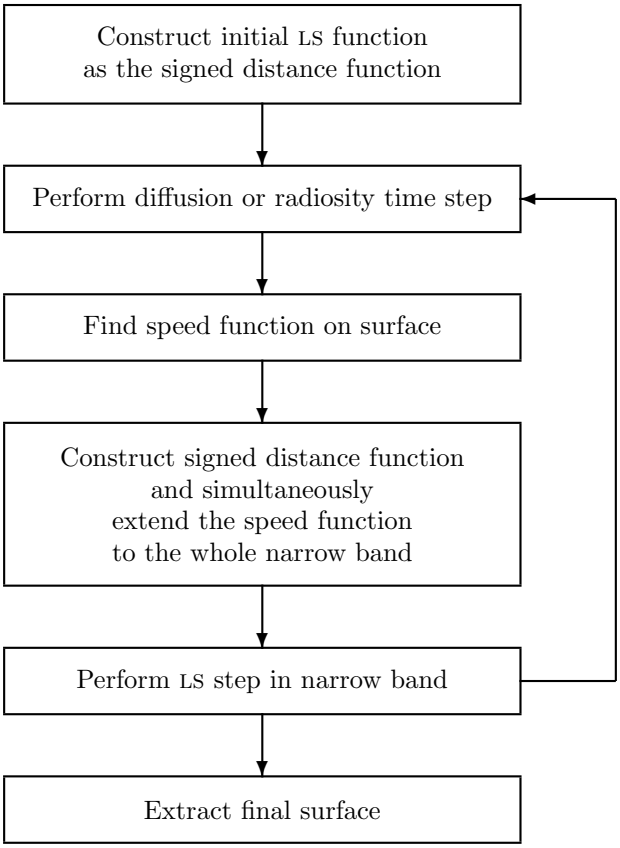

Figure 1: Overview of the simulation flow combining transport by diffusion or radiosity and surface evolution using the level set (LS) method. The simulation stops when a prescribed time is reached on when a layer of prescribed thickness has been deposited.

chosen, where two heterogeneous deposition models, a homogeneous intermediate-mediated deposition model, and a heterogeneous deposition with byproduct inhibition model are available [3]. This setup also provides a way to determine the actual chemical reaction, which is a non-trivial problem and can only be done indirectly by comparing measurements and simulation results.

IV. RADIOSITY AND COALESCING SURFACE ELEMENTS

For simulations where the transport of the particles happens in the radiosity regime, the simulator uses the formulation of radiosity for particles of low energy, where luminescent reflection is assumed, that can be found, e.g., in [4]. In the case of multiple, low energy species the calculation of the visibility matrix and the inverse T only depends on topographic information and thus is not repeated for each species.

When using radiosity models, two operations consume most of the computation time. The first operation is determining the visibility between all surface elements,

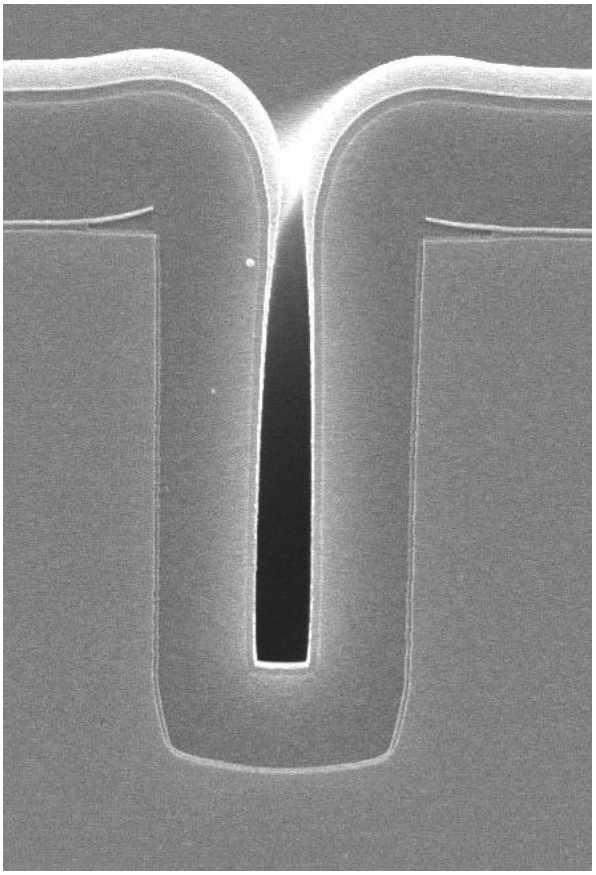

Figure 2: SEM (scanning electron microscope) image of a cross section through a trench about $4\,\mu$m deep and $2\,\mu$m wide. The white layer is a protection layer.

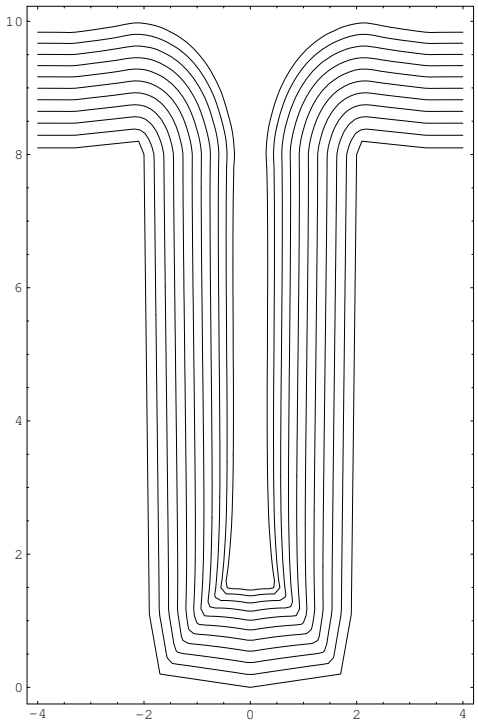

Figure 3: Simulation result and intermediate zero level sets of the simulation of the deposition process corresponding to the image shown in Figure 2.

which is an $O(n^2)$ operation where n denotes the number of surface elements extracted from the level set grid. The second operation is solving a certain system of linear equations, which leads to calculating the inverse of a matrix with n^2 elements, which is an $O(n^3)$ operation.

Obviously increasing the number of surface elements is not a remedy in cases where high resolution is required. High resolution is needed, e.g., near the trench opening, and the bottom of the trench, and for the simulation of microtrenching and side wall push back. One approach is to devise a refinement and coarsening strategy for unstructured grids on which the level set equation is numerically solved. This, however, complicates the fast marching algorithm necessary for extending the speed function. A different approach was taken here by coarsening the surfaces after having been extracted from the level set grid.

The algorithm works by walking down the list of surface elements extracted as the zero level set and calculating the angle α between two neighboring surface elements. Whenever $|\pi - \alpha|$ is below a certain threshold value of a few degrees, the neighboring elements are coalesced into one. After one sweep through the list, the algorithm can be reapplied for further coarsening. After k coarsening sweeps, at most 2^k surface elements are coalesced into one. The resulting longer surface elements are used for the radiosity calculation, after which the fluxes are translated back from the coarsened elements to the original ones.

V. SIMULATION RESULTS AND INVERSE MODELING

Several SEM images of trenches about $4\,\mu$m deep and $2\,\mu$m wide were used for comparing the step coverages of simulated deposition processes with reality. Since three-dimensional simulations are still too computationally expensive for inverse modeling problems, the two-dimensional simulation module was used in combination with the optimization framework SIESTA [5] for determining the parameters of the model. Hence extracting the model parameters is done automatically and can be immediately applied to different measurements and structures produced under different process conditions. A simulation result is shown in Figure 3. For all the processes and trenches simulated, very good agreement was found. Typical simulation times are in the range of a few minutes.

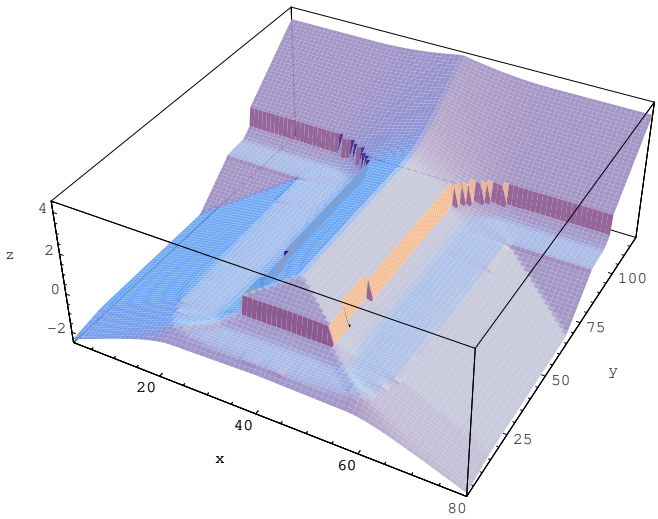

Figure 4: The level set function during the simulation whose results are shown in Figure 3. The active narrow band around the zero level set is very small and retained the signed distance function, whereas other grid points have not been updated.

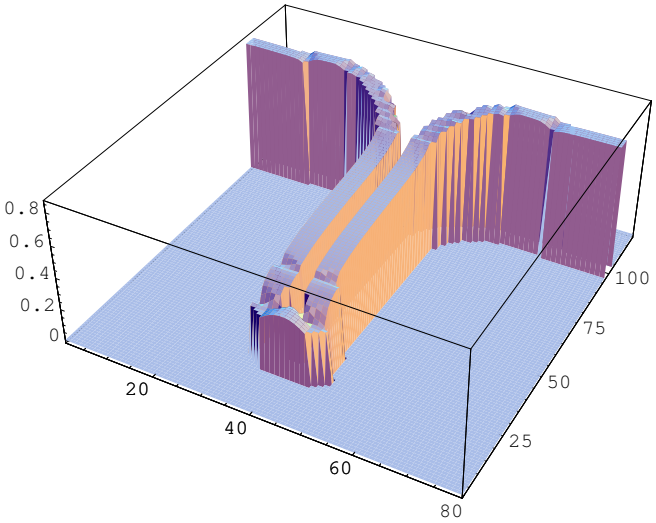

Figure 5: Example of an extended speed function during the simulation whose results are shown in Figure 3.

VI. CONCLUSION

For simulating etching and deposition processes, a general simulator was developed. It consists of three independent modules, namely the level set module, a reaction module, and a transport module for diffusion and radiosity simulations, and can be used for simulating all common deposition and etching processes. For tracking surface evolution, a fast and accurate level set algorithm including narrow banding and extending the speed function was devised and implemented.

In practice the simulator was applied to the simulation of SiO_2 deposition from TEOS in different Silicon trenches under different process conditions. To that end step coverages measured in several SEM images were used for extracting model parameters, where good quantitative agreement was achieved. All observed effects match well comparing the SEM pictures and the simulation results. Thus the process conditions could be optimized with respect to the quality of the trenches and manufacturing throughput.

Additionally, two strategies for increasing the accuracy of radiosity simulations are presented and compared to measurements of a deposition process. The first method is the algorithm which performs three level set computations in parallel: calculating the signed distance function via a fast marching algorithm, extending the speed function so that the signed distance function is retained throught the simulation, and moving the narrow band according to the new zero level set. This gives rise to a fast and accurate level set algorithm.

The second method is a coarsening algorithm which ensures fine resolution of the surface in parts of the boundary with relatively high curvature, i.e., where it is needed most. These parts are typically the opening of the trench, its bottom, and places where microtrenching and side wall push back take place. At the same time the resolution is lowered where possible which reduces the demand on computational resources significantly. Typically radiosity simulations run five to ten times faster, when this algorithm is employed.

ACKNOWLEDGMENT

The authors acknowledge support from the “Christian Doppler Forschungsgesellschaft,” Vienna, Austria.

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