Simulation of void formation in interconnect lines

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ABSTRACT

The predictive simulation of the formation of voids in interconnect lines is important for improving capacitance and timing in current memory cells. The cells considered are used in wireless applications such as cell phones, pagers, radios, handheld games, and GPS systems. In backend processes for memory cells, ILD (interlayer dielectric) materials and processes result in void formation during gap fill. This approach lowers the overall k-value of a given metal layer and is economically advantageous. The effect of the voids on the overall capacitive load is tremendous. In order to simulate the shape and positions of the voids and thus the overall capacitance, the topography simulator ELSA (Enhanced Level Set Applications) has been developed which consists of three modules, a level set module, a radiosity module, and a surface reaction module. The deposition process considered is deposition of silicon nitride. Test structures of interconnect lines of memory cells were fabricated and several SEM images thereof were used to validate the corresponding simulations.

Keywords: interconnect lines, deposition, void formation, level set method.

1. INTRODUCTION

Deposition and etching of silicon trenches are crucial processes in semiconductor manufacturing, e.g., for state of the art memory cells. Simulating of these processes enables to predict resulting profiles and eventually voids, and thus optimizing the process parameters depending on electrical characteristics of the devices. In backend processes for memory cells ILD materials and processes result in void formation during gap fill which lowers the k-value of a given metal layer and thereby optimizes the time delay by lowering the intermetal capacitance.

For simulating the above processes in particular, and deposition and etching of silicon trenches in general, one always needs to describe accurately a moving boundary besides the proper treatment of the chemical and physical processes. The moving boundary is usually the surface of the wafer. One approach is to use a cellular format, where the simulation domain is divided into cubic or cuboid cells, and each cell either belongs to the exterior vacuum above the wafer or to interior material.[1] The main advantage of this approach is its robustness and good handeling of critical structures such as high aspect ratio trenches.[2] But one disadvantage of this method is that calculating the required surface normals leads to accuracy problems. Surface normals are very important for computing the fluxes to the surface for simulating the transport phenomena.

The level set method[3, 4] provides an interesting alternative method for solving the above mentioned problems. Furthermore, this approach provides higher spatial resolution on grids of the same size compared to cellular format but in expense of involving more complicated algorithms. Additionally, applying a coarsening algorithm reduces significantly the computational efforts of the simulation and allows to achieve the high resolution which is necessary for accurate simulation of the surface evolution at the trench opening, the trench bottom, and during void formation. Based on the level set method which combines narrow banding and extending the speed function, we have developed the ELSA simulator which consists of three modules. The first module is the level set module, the second module is responsible for the chemical surface reactions at the wafer surface, and the third module simulates the transport of species above the wafer by radiosity.

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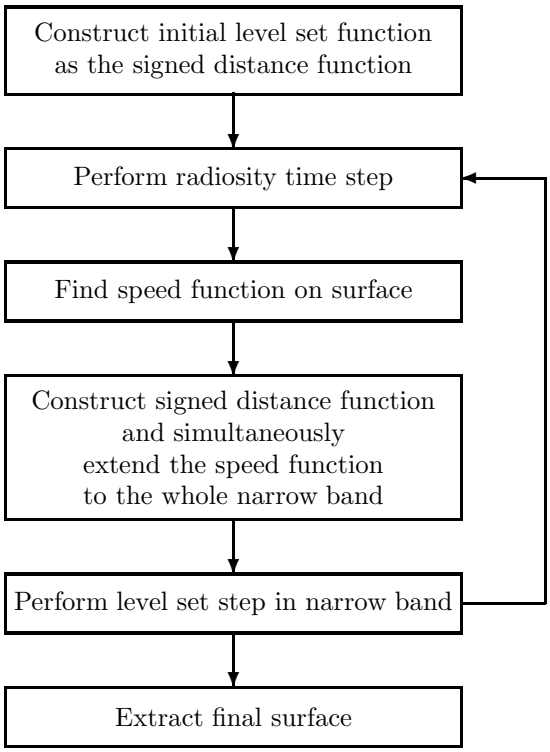


Figure 1. Overview of simulation flow as combination of a physical transport model and surface evolution using the level set method.

The outline of this paper is as follows. Firstly, the simulation flow of ELSA with the basic idea of the level set method and combining the speed function and narrow bandig using a fast marching method are presented. Then a surface coarsening algorithm is presented. Secondly, the different particle transport models and the radiosity model are discussed. Finally, the test structures and simulation results are presented which reproduce the shapes of the trenches very well and good quantitative agreement was achieved as well.

2. THE ELSA SIMULATOR

The feature scale simulation is devided into three steps. The first one is the simulation of the transport of particles in the boundary layer above the wafer by radiosity. The second one is determining the chemical reactions taking place at the wafer surface through the fluxes of particles found in the first step. The last step changes the surface according to the previous steps. This tracking is performed using the level set method. Fig. 1 shows a typical topography simulation flow.

ELSA consists of three modules, namely a level set module, a surface reaction module, and module for particle transport by radiosity. It can be used for simulating all common deposition and etching processes. Its main advantages are an efficient and precise level set algorithm including narrow banding and extending the speed function and a surface coarsening algorithm for significantly reducing the computational demands while ensuring high resolution in critical areas. The initial surface is given by an arbitrary number of points, and a coarsening algorithm can be applied recursively.

2.1. The Level Set Method

The level set method[3] provides means for describing 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 $u(t, \mathbf{x})$, the so called level set function. Thus the initial surface is the set $\{\mathbf{x} \mid u(0, \mathbf{x}) = 0\}$.

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 it is usually determined by physical models and in our case by the etching and deposition processes, or more precisely by the fluxes of certain gas species and subsequent surface reactions. The speed function $F(t, \mathbf{x})$ generally depends on the time and space variables and we assume for now that it is defined on the whole simulation domain and for the time interval considered.

The surface at a later time t_1 shall also be considered as the zero level set of the function $u(t, \mathbf{x})$, namely $\{\mathbf{x} \mid u(t_1, \mathbf{x}) = 0\}$. This leads to the level set equation

$$u_t + F(t, \mathbf{x}) \|\nabla_{\mathbf{x}} u\| = 0, \qquad u(0, \mathbf{x}) \quad \text{given}, \tag{1}$$

in the unknown variable u, where $u(0, \mathbf{x})$ determines the initial surface. Having solved this equation the zero level set of the solution is the sought curve or surface at all later times.

Although in the numerical application the level set function is eventually calculated on a grid, the resolution achieved is in fact much higher than the resolution of the grid, and hence higher than the resolution achieved using a cellular format on a grid of the same size. This is because in the last step, the surface extraction step, where the curve or surface is reconstructed from the function values on the grid, the zero level set is approximated by lines or triangles using linear interpolation. Here it is of course assumed that the level set function essentially remains the signed distance function which is locally a linear function near the zero level set. This is the case with the implementation developed.

Now in order to apply the level set method a suitable initial function $u(0, \mathbf{x})$ has to be determined first. There are two requirements: first it goes without saying that its zero level set has to be the surface given by the application, and second it should essentially be a linear function so that in the final surface extraction step linear interpolation can be applied. A beneficial choice is the signed distance function of a point from the given surface. This function is the common distance function multiplied by minus or plus one depending on which side of the surface the point lies in. The common distance function of a point x from a set M is then defined by $d(x, M) := \inf_{y \in M} d(x, y)$, where d is metric, usually the Euclidean distance. Fig. 2 shows the signed distance function corresponding to the upper SEM shown in Fig. 3.

In summary, first the initial level set grid is calculated as the signed distance function from a given initial surface. Then the speed function values on the whole grid are used to update the level set grid 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 suitably from the values provided on the boundary, i.e., the zero level set. This will be discussed in the next section.

2.2. Extending the Speed Function and Narrow Banding Using a Fast Marching Method

In applications linking to physical models the speed function is not known on the whole simulation domain, but only at the surface. In order to use the level set method it has to be suitably extended from the known values to the whole simulation domain. This can be carried out iteratively by starting from the points nearest to the surface. Mathematical arguments show that the signed distance functions can be maintained from one time step to the next by choosing a suitable extension.

The idea leading to fast level set algorithms stems from observing that only the values of the level set function near its zero level set are essential, and thus only the values at the grid points in a narrow band around the zero level set have to be calculated. As the zero level set moves, the signed distance function in the narrow band has to be maintained.

Both extending the speed function and narrow banding require constructing the distance function from the zero level set in the order of increasing distance. But calculating the exact distance function from a curve or surface consisting of a large number of small line segments or triangles is computationally expensive and can only be justified for the initialization. An approximation to the distance function can be computed by a special fast marching method.[3]

The fast marching method works as follows. First, tag points the boundary value points as *Known*. Then tag as *Trial* all points that are one grid point away. Finally tag as *Far* all other grid points. Then the loop is as follows.

- Begin loop: select the *Trial* point with the smallest absolute value of distance to the boundary.
- Remove this point from *Trial* and add it to *Known*.
- Tag as *Trial* all neighbors of this point that are not *Known*. If the neighbor is in *Far*, remove and add it to Trial.
- Compute the signed distance values of all *Trial* neighbors.
- Return to top of loop till the end of the narrow banding width.

Once we have calculated the signed distance function at all grid points inside of the narrow banding, the extending the speed function can be performed. The speed function values like the signed distance function values are initially known on the boundary, because they can be computed in the physical simulation step by radiosity model and translated at the grid points. Applying the following equation[3] enables extending the speed function at all grid points of the narrow banding.

$$\nabla F_{ext} \cdot \nabla \Phi = 0 \tag{2}$$

where Φ is the constructed signed distace function calculated by the fast marching method.

By intertwining both, extending the speed function and narrow banding, expensive calculations are kept to a minimum. Although the level set method is a seemingly computationally expensive method, since it requires solving a partial differential equation for describing surface evolutions, the computation time consumed for the surface evolution by narrow banding is negligible compared to that required for the physical models, e.g., radiosity, even after applying a surface coarsening algorithm which is presented in the following.

2.3. Surface Coarsening

The most part of the computation time for simulating the transport of particles above the wafer by radiosity model is consumed in determining the visibility between the surface elements which is an $O(n^2)$ operation and solving a certain system of linear equation leading to calculating the inverse of matrix with n^2 elements which is $O(n^3)$ operation, where n is the number of surface elements extracted from the level set grid.

The surface coarsening algorithm walks down the list of surface elements extracted as the zero level set and calculates the angle between two neighboring surface elements. If this angle is below a certain threshold value of a few degrees, the neighboring elements are coalesced into one. After k coarsenig 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 coarsenend elements to the original ones. Note that, although this algorithm can significantly reduce the computation time needed by the visibility test, the visibility test time is still much larger than the computation time needed by the surface evolution step of the level set algorithm using narrow banding.

3. TRANSPORT OF PARTICLES

The transport of particles above the wafer surface specifies the etch and deposition rates. They can be divided broadly in two classes according to the mean freed path length, although this distinction is a very rough classification and the suitable model in each case depends on other considerations as well:

- If the mean free path length is much larger than the simulation domain, the collision of single particles can be neglected and the transport can be simulated using the radiosity model.
- If the mean free path length is much smaller than the simulation domain, the collision between single particles play a major role and their concentration is determined by the diffusion equation.

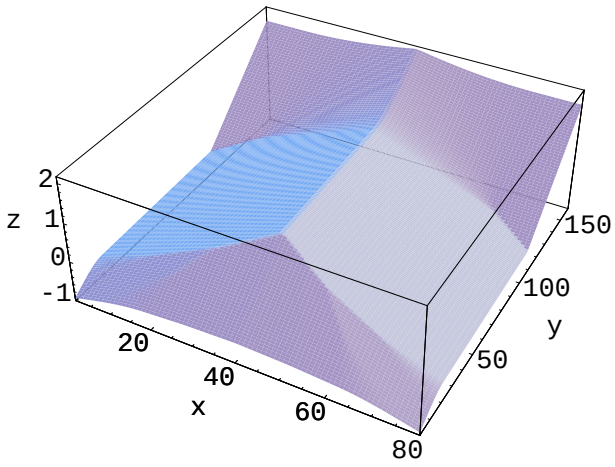


Figure 2. The signed distance function is used as the initial level set function which corresponds to the initialization of the upper SEM shown in Fig. 3.

3.1. The Radiosity Model

The radiosity model assumes that the total deposition flux depends on deposition directly from the source, as well as additional deposition due to particles which do not stick and are re-emitted. The expression for the flux is a matrix relation after discretizing the problem. There are two numerical approaches for solving this equation. The first one is to use a direct solver for the matrix equation. In two dimensions, this is practical; for large three-dimensional problem this becomes impractical due to the computational effort. The second approach is to construct an iterative solution to the matrix equation based on a series expansion of the interaction matrix. Based on our simulations in two dimensions the difference between these two methods according to computational time is negligible and thus we have used the first model because it is preciser than the second one.

A formulation of the radiosity method is given as follows.[3] The flux coming to the surface elements can be written as,

$$\text{Flux} = \beta_0 I_s + \beta \Psi L I_R. \tag{3}$$

Here I_s is the vector of fluxes coming from the source to the surface elements, I_R is the vector of fluxes that arrive because of reflections, β_0 is the sticking coefficient for particles coming directly from the source, β is the one for secondary bounces, L is the diagonal matrix containing the length of the surface elements and

$$\Psi_{ij} = \frac{n_i \cdot (t_j - t_i) \cdot (t_i - t_j)}{\pi |t_j - t_i|^3} [i \text{ visible } j], \tag{4}$$

where t_i are the centroids of the surface elements, n_i their unit normal vectors, and $[i$ visible $j]$ is 1 or 0 if the surface element j is visible from i or not. After some straightforward algebraic manipulations the following relationship

$$\text{Flux} = \frac{\beta - \beta_0}{1 - \beta} I_s + \frac{\beta(1 - \beta_0)}{1 - \beta} \underbrace{L^{-1}(L^{-1} - (1 - \beta)\Psi)^{-1}}_{T:=} I_s \tag{5}$$

is obtained. 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 does not have to be repeated for each species.

Figure 3. SEM image of a test structure with trenches of different widths. Metal layers M2 and M3 of the interconnect structure of a memory cell are shown. In the upper row (M3 layer) the trenches are about 0.45 μm wide and a nitride film was deposited. In the lower row (M2 layer) silicon dioxide was deposited from TEOS.

4. SIMULATION RESULTS

Test structures of interconnect lines of memory cells were fabricated and several SEM images thereof were used to validate the corresponding simulations. For metal line M3 the deposition of silicon nitride was simulated. The detail in Fig. 3 shows the metal layers M2 and M3.

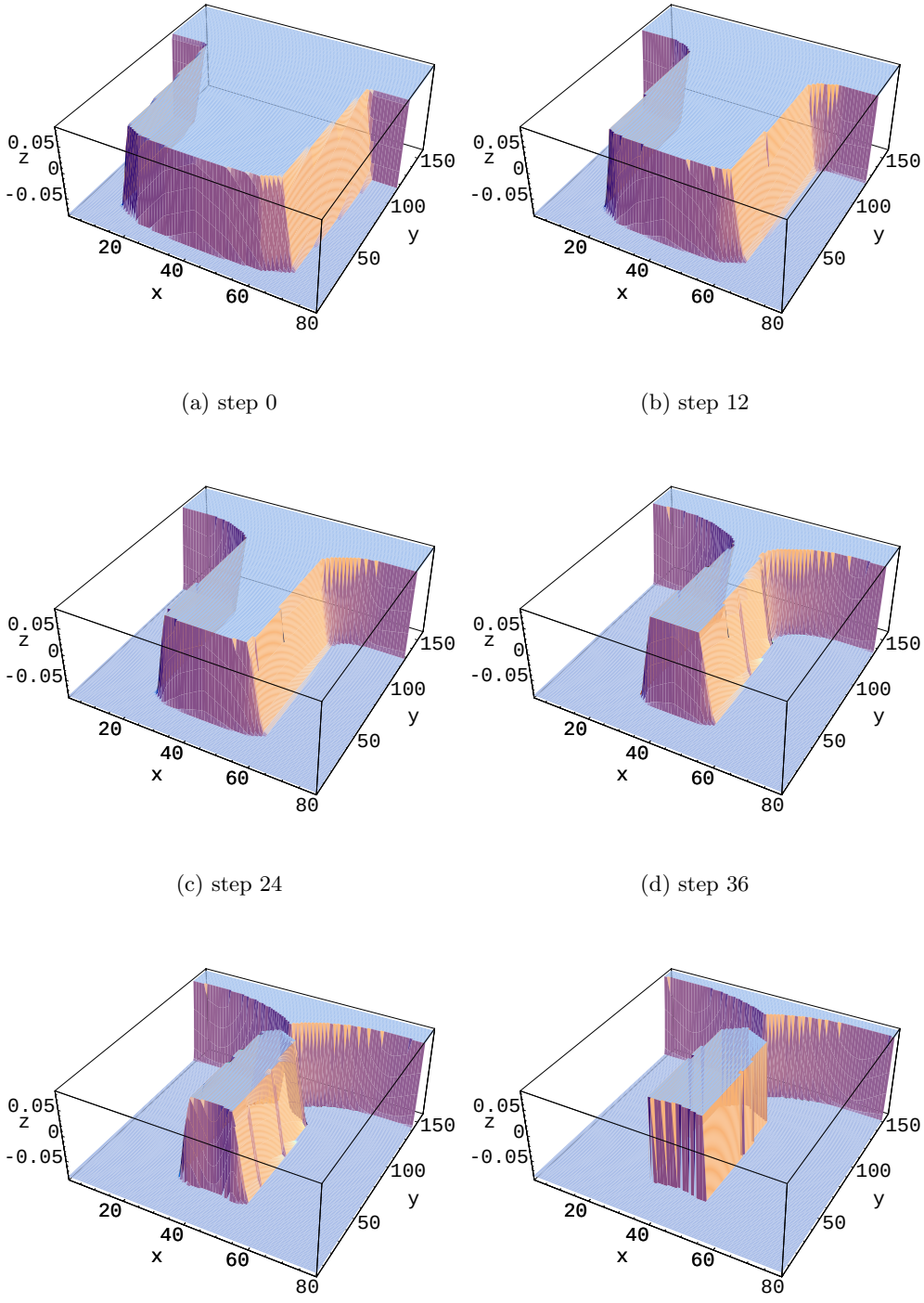
The path of the species above the wafer surface is tracked in radiosity simulations where reflection happens in a luminescent manner. The computational effort of the level set algorithm with narrow banding is negligible compared to the evaluation time of the physical models.

An example of void formation after silicon nitride deposition is given in Fig. 5. Fig. 4 shows the corresponding level set functions of the upper SEM shown in Fig. 3 in different time steps. Shape and position of the void are reproduced correctly in simulation.

5. CONCLUSION

State of the art algorithms for surface evolution processes like deposition and etching processes have been implemented. A general simulator called ELSA was developed based on the above mentioned algorithms which can be used for simulating all common deposition and etching processes. The speed of radiosity simulation was improved by two methods. The first one is an algorithm which performs three level set computations in parallel; calculating the signed distance function by a fast marching algorithm, extending the speed function, and dynamically moving the narrow band according to the new zero level set. The second method is a coarsening algorithm which guarantees fine resolution of the surface in parts of the boundary with relatively high curvature, i.e., where it is needed most. This parts are typically the opening of the trench and its bottom. At the same time the resolution is lowered where possible which reduces the demands on computational resources significantly.

The shape and position of voids in nitride films occuring in backend manufacturing processes were simulated accurately. The voids determine the capacitance of the interconnect lines, which is crucial for the performance of the final memory cell.



(a) step 0

(b) step 12

(c) step 24

(d) step 36

(e) step 48

(f) step 60

Figure 4. The intermediate level set grids at step 0, 12, 24, 36, 48, and 60 during the simulation in Fig. 5. Inside the narrow band the signed distance function is retained until the end of simulation, whereas the signed distance values of the other points have been substituted with the width of the narrow band multiplied by 1 or -1 depending on their position.

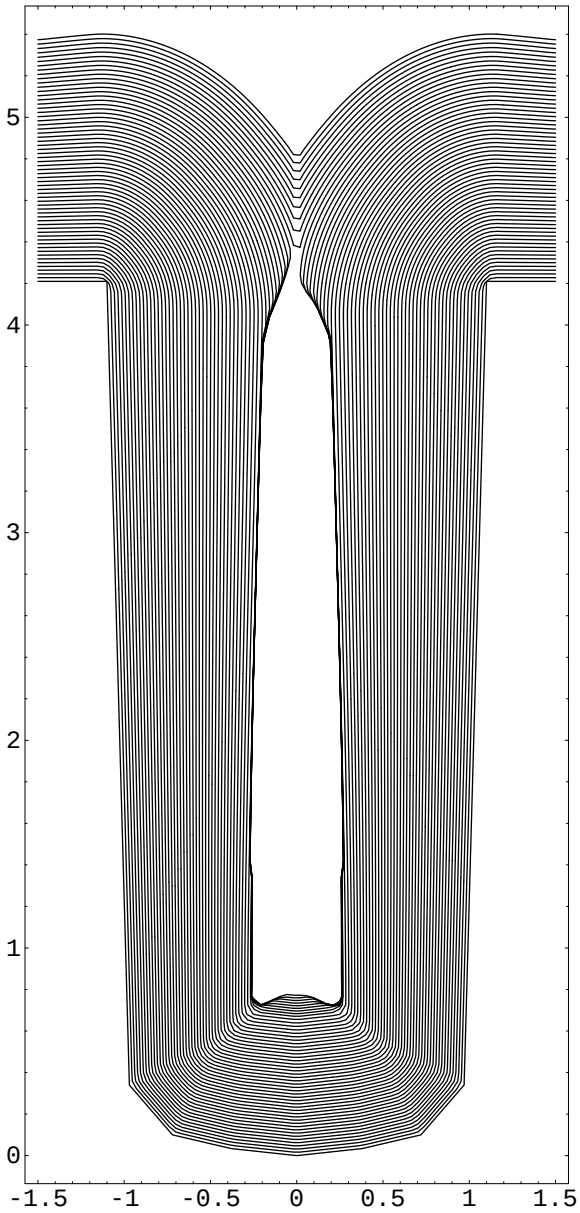


Figure 5. Simulation of void formation corresponding to Fig. 3. A level set grid of $80 \cdot 160$ points was used.

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