Three-Dimensional Surface Evolution Using a Level Set Method

A. Sheikholeslami, C. Heitzinger, E. Al-Ani, R. Heinzl, T. Grasser, and S. Selberherr

Abstract— **The application of level set and fast marching methods to the simulation of surface topography in three dimensions for semiconductor processes are presented. Many techniques, including a narrow band level set method, fast marching for the Eikonal equation, extension of the speed function, transport models, visibility determination, and an iterative equation solver are used to obtain a very fast simulator.**

I. Introduction

Three-dimensional topography simulation is still faced with many challenges which limit its general applicability and usefulness. In addition, three-dimensional topography simulation tends to be very CPU and memory intensive to date.

Roughly speaking, various surface representation algorithms for topography simulation in three dimensions fall into three categories [1].

- Segment-based models, such as the facet motion model [2], [3]: In this model a nodal triangularization of the interface is used. The position of the nodes is then updated by determining front information about the normals and curvature of surface facets. Because interstices or duplications between neighboring surface facets occur during their advance along the normal, area-readjustment procedures are needed. However, these procedures induce significant computational error into the simulation result in proportion to the complexity of the process geometry.
- Cell-based models, such as the cellular model [4], [5]: These models can easily handle topological changes and can be extended to three dimensions. However, the determination of geometric quantities such as surface normals and curvature can be inaccurate.
- Level set method-based models [6], [7], [8]: In this method the interface extraction is based on the solution of a hyperbolic partial differential equation. The location of an interface is the zero level set of a higher dimensional function called level set function. This model provides an interesting alternative method for solving the above mentioned problems.

A. Sheikholeslami, C. Heitzinger, E. Al-Ani, and S. Selberherr are with the Institute for Microelectronics, Technical University Vienna, Gußhausstraße 27-29/E360, A-1040 Vienna, Austria, E-mail: sheikholeslami@iue.tuwien.ac.at

R. Heinzl and T. Grasser are with the Christian Doppler Laboratory for TCAD in Microelectronics at the Institute for Microelectronics.

Based on an efficient and precise level set method including narrow banding [9] and extending the speed function [10] in a sophisticated algorithm, we have developed a general three-dimensional topography simulator for the simulation of deposition and etching processes. The simulator works efficiently concerning computational time and memory consumption, and it simultaneously ensures high resolution.

The outline of this paper is as follows. First, we present briefly the level set method. Second, we describe briefly how to extend the speed function combined with narrow banding using a fast marching method. Third, the stability and the complexity of the simulator is discussed. Fourth, we present the transport models. Finally, simulation results are shown.

II. The level set method

The level set method 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 [6]. 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 what is usually determined by physical models and in our case by 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

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

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.

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.

III. Extending the speed function and narrow banding using a fast marching method

In most applications 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 [6] that the signed distance function 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.

Both 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. But calculating the exact distance function from a surface consisting of a large number of small triangles is computationally expensive and can be only justified for the initialization. An approximation to the distance function can be computed by a special fast marching method [6], [10].

IV. Stability and the Courant-Friedrichs-Levy (CFL) Condition

For advancing the level set function we have used a second-order space convex finite difference scheme [11], [12]. Consider Δx, Δy, Δz, and Δt as discretization steps in space and in time, respectively. A necessary condition for the stability of this scheme is the Courant-Friedrichs-Levy (CFL) condition which requires that

$$\Delta t \cdot F_{\max} \leq \min(\Delta x, \Delta y, \Delta z).$$

The CFL condition guarantees that the front can cross no more than one grid cell during each time step. In order to have a stable simulator based on the finite difference method, the CFL condition must be satisfied [12].

However, a fundamental problem stemming from the CFL condition limits the simulator performance. If we increase the spatial resolution by λ, assuming that $F_{\max}$ remains constant, we have to reduce the maximum Δt by the same factor λ, which increases the number of simulation steps by λ for reaching the same thickness. Furthermore, an increase in spatial resolution by λ increases approximately the number of extracted surface elements by λ^2 and then the computational effort of the visibility determination by λ^4. In summary, an increase in spatial resolution by λ leads to an increase in simulation time by a factor λ^5, if one uses the most precise visibility determination.

V. Transport Models

The transport of the particles above the wafer surface specifies the deposition and etch rate. Assume that within a feature the frequency of particle-particle collisions is negligible relative to particle-surface collisions, that is, we are in the molecular or Knudsen regime [13]. In this case the transport of the particles can be simulated using the radiosity model. In the other case the collision of single particles plays a major role and their concentration is determined by the diffusion equation.

A. Particle Distribution for Deposition and Etching

For modeling deposition it is assumed that the distribution of the particles coming from the source obeys

a cosine function around the normal vector of the plane in which the source lies [13], [14]. This implies that the flux at a surface element is proportional to the cosine of the angle between the connecting line between the center of mass of a surface element and the source and the normal vector of the source plane.

A function which has been used for ions in plasma systems for etching processes is the normal distribution $f(\theta) = (2\pi\sigma)^{-1/2} \cdot exp(-\theta^2/2\sigma^2)$ where θ is the angle around the normal vector of the source plane and the angular width of the distribution is specified by σ. For the reflections of particles diffuse and specular reflection are assumed for deposition and etching processes, respectively [13].

B. Visibility Determination

Most of the computation time for simulating the transport of the particles above the wafer by the radiosity model is consumed in determining the visibility between the surface elements. This is an $O(m^2)$ operation, where m is the number of surface elements growing approximately like $O(n^2)$. If the connecting line between the center of mass of two surface elements does not intersect the surface, i.e., the zero level set, those surface elements are visible from each other. In order to decrease the computational effort related to determining the visibility between the surface triangles, we have assumed that two triangles are visible from each other if the center point of the grid cells in which the triangles are located, are visible from each other. Since there are at least two triangles in each grid cell, considerable time is saved.

C. Radiosity Model

The radiosity model assumes that the total flux depends on the flux directly from the source, as well as an additional flux due to the particles which do not stick and are re-emitted. After discretizing the problem the flux vector whose elements are the total flux at different surface elements can be expressed by a matrix equation.

There are two numerical approaches for solving this problem. The first one is to use a direct solver for the matrix equation. Although this is practical in two dimensions [10], it becomes impractical due to the computational effort needed by calculating the inverse matrix for three-dimensional problems. In three dimensions we solve the equation iteratively.

C.1 Iterative Solver

The iterative solution [6] consists of a series expansion in the interaction matrix. Suitably interpreted, it can be viewed as a multi-bounce model, in which the number of terms in the series expansion corresponds to the number of bounces that a particle can undergo before its effects are negligible. This approach allows to check the error remainder term to determine how many terms must be kept. Since most of the particles either stick or leave the domain after a reasonable number of bounces, this is an efficient approach. By constructing the remainder term, we can measure the convergence of the expansion and keep enough terms to bound the error below a user-specified tolerance.

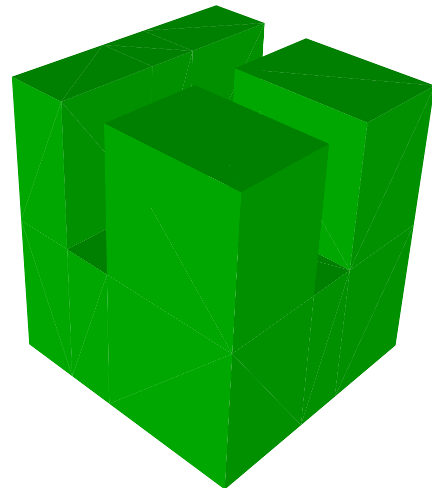

Fig. 1. A T-shape initial boundary for a deposition process.

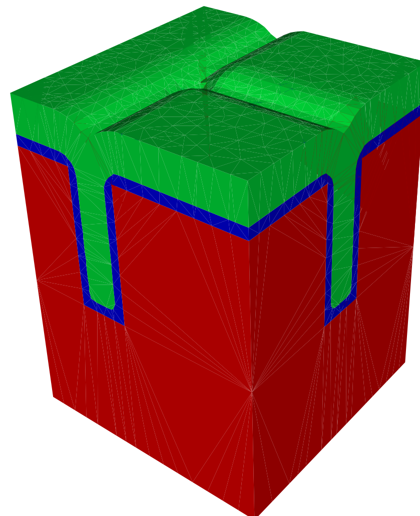

Fig. 2. Simulation result of the deposition of different materials.

VI. Simulation Results

In this section we present some three-dimensional simulation results for deposition and etching processes. We begin with a source deposition into a T-shape initial boundary shown in Fig. 1. Fig. 2 shows the simulation result of a source deposition from a plane located above the trench including visibility and shading effects. The

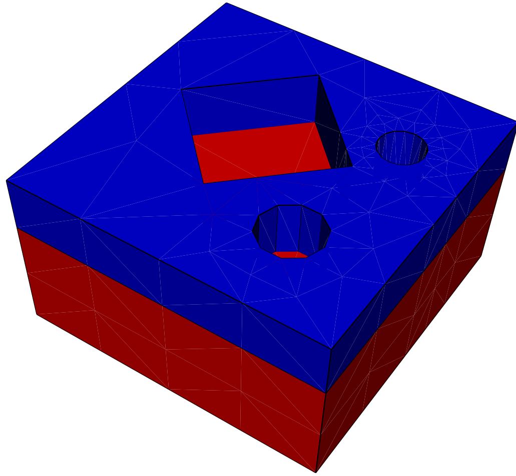

Fig. 3. An initial boundary for an etching process using masking.

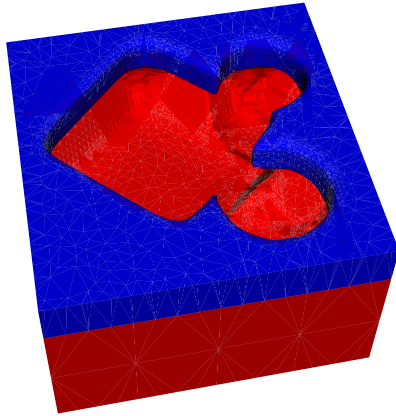

Fig. 4. Simulation result of etching.

deposition simulation have been done for two different materials The particle distribution is a cosine distribution around the normal vector of source plane.

Fig. 4 shows a straightforward simulation of isotropic etching Fig. 3 from which material is being isotropically etched including the masking. As expected, the sides of the trench are cleanly etched away and are rounded.

VII. Conclusion

State of the art algorithms for surface evolution processes like deposition and etching processes in three dimensions have been implemented. A general simulator was developed based on the level set method combining the narrow banding and fast marching method for extending the speed function. The speed of simulation was improved in several steps, e.g., in initialization, visibility determination, and solving the radiosity matrix. Two examples for simulation of etching and deposition processes were presented. The complexity of different parts of the simulator was discussed. Furthermore, the effect of increasing the grid resolution on the simulation time was shown.

Acknowledgment

The authors acknowledge the support of Infineon Technologies, Austria, Cypress Semiconductor Corporation, USA and Toshiba Corporation, Japan for this work.

References

[1] U.H. Kwon and W.J. Lee, 'Three-dimensional Deposition Topography Simulation Based on New Combinations of Flux Distribution and Surface Representation Algorithms,' *Thin Solid Film*, vol. 445, pp. 80–89, 2003

[2] K.K.H. Toh, A.R. Neureuther, and E.W. Scheckler, 'Algorithms for Simulation of Three-Dimensional Etching,' *IEEE Trans. Computer-Aided Design*, vol. 13, pp. 616–624, 1994

[3] E.W. Scheckler and A.R. Neureuther, 'Models and Algorithms for Three-Dimensional Topography Simulation with SAMPLE-3D,' *IEEE Trans. Computer-Aided Design*, vol. 13, pp. 219–229, 1994

[4] W. Pyka, C. Heitzinger, N. Tamaoki, T. Takase, T. Ohmine, and S. Selberherr, 'Monitoring Arsenic In-Situ Doping with Advanced Models for Poly-Silicon CVD,' *Proc. of Simulation of semiconductor Processes and Devices*, Athens, Greece, September 2001, pp. 124–127

[5] W. Pyka, *Feature Scale Modeling for Etching and Deposition Processes in Semiconductor Manufacturing*, Dissertation, Technische Universität Wien, 2000

[6] J. Sethian, *Level Set Methods and Fast Marching Methods*, Cambridge University Press, Cambridge, 1999

[7] A. Sheikholeslami, C. Heitzinger, T. Grasser, and S. Selberherr, 'Three-Dimensional Topography Simulation for Deposition and Etching Processes Using a Level Set Method,' *Proc. of International Conference on Microelectronics (MIEL)*, Nis, Serbia and Montenegro, May 2004, pp. 241-244

[8] C. Heitzinger, J. Fugger, O. Häberlen, and S. Selberherr, 'On Increasing the Accuracy of Simulations of Deposition and Etching Processes Using Radiosity and the Level Set Method,' *Proc. of European Solid-State Device Research Conference*, Florence, Italy, September 2002, pp. 347–350

[9] A. Sheikholeslami, C. Heitzinger, F. Badrieh, H. Puchner, and S. Selberherr, 'Three-Dimensional Topography Simulation Based on a Level Set Method,' *Proc. of Internatonal spring Seminar on Electronics Technolog (ISSE)*, Sofia, Bulgaria, May 2004, pp. 263-265

[10] A. Sheikholeslami, C. Heitzinger, H. Puchner, F. Badrieh, and S. Selberherr, 'Simulation of Void Formation in Interconnect Lines,' *Proc. of SPIE's first International Symposium on Microtechnologies for the New Millennium: VLSI Circuit and Systems*, Gran Canaria, Spain, May 2003, pp. 445-452

[11] C. Heitzinger, *Simulation and Inverse Modeling of Semiconductor Manufacturing Processes*, Dissertation, Technische Universität Wien, 2002

[12] O. Runborg, 'Finite Difference Methods for the Advection Equation,' *Tillam̃pade numeriska methoder II*, May 2003

[13] T.S. Cale, 'Flux Distributions in Low Pressure Deposition and Etch Models,' *J. Vac. Sci. Technol. B*, vol. 9, pp. 2551–2553, 1991

[14] T.S. Cale and G.B. Raupp, 'A Unified Line-of-Sight Model of Deposition in Rectangular Trenches,' *J. Vac. Sci. Technol. B*, vol. 8, pp. 1242–1248, 1990