Three-Dimensional Topography Simulation Based on a Level Set Method

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Abstract

We present a general three-dimensional topography simulator for the simulation of deposition and etching processes. The simulator is called **ELSA** (Enhanced Level Set Applications). **ELSA** is based on a level set method including narrow banding and a fast marching method. Modules for the transport of species, for surface reaction, and for the level set method are its basis.

Introduction

Three-dimensional topography simulation is still faced with many challenges which limits its general capability and usefulness. To date it is very CPU and memory expensive.

Roughly speaking, there are three surface representation methods for developing three-dimensional topography simulators [1]. The first one is the segment-based method, the second one is the cell-based method, and the third one is the level-set method. The segment-based method induces significant computational error into the simulation result, especially in three dimensions, because duplication between the neighboring surface facets occurs during advancing the surface along its normal [2]. Using cell-based method the determination of geometric quantities such as normals and curvature can be inaccurate [3].

The Level set method provides an interesting alternative method for solving the above mentioned problems. The interface is extracted based on the solution of a hyperbolic partial differential equation. The interface is the zero level set of a higher dimensional function which is the so called level set function [4],[5].

The outline of this paper is as follows. First, an optimized method for constructing the initial level set function is presented. Second, we discuss the transport model for species. Third, extending the speed function is briefly described. Fourth, the features of the simulator are sketched. Finally, simulation results are shown.

Initializing

The basic idea of the level set method is viewing the boundary in question at a certain time as the zero level set (with respect to the space variables) of a certain function $u(t,x)$ which is called level set function. Each point on the surface is moved with a certain speed perpendicular to the surface denoted by $F(t,x)$. The surface at a later time t_1 shall also be considered as the zero level set of the function $u(t,x)$, namely $\{\ x \mid u(t_1,x)=0\ \}$. This leads to the level set equation

$$u_t + F(t,\mathbf{x}) \,\|\, \nabla_x u(t,\mathbf{x}) \,\|= 0 \qquad (1)$$

In order to apply the level set method a suitable initial function has to be determined. A good choice is the distance function multiplied by minus or plus one depending on which side of the boundary a point lies. Since we later apply the level set algorithm only in a narrow band, it is sufficient to calculate the signed distance function only in this narrow band. This method reduces the computational effort of initialization in three dimensions from $O(n^3)$ to $O(n^2)$, where n is the grid resolution in each direction.

Transport Models

For modeling deposition it is assumed that the distribution of the species coming from the source obeys a cosine function around the normal vector of the plane in which the source lies [6]. 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 $f(\theta)=(2\pi\sigma)^{-1/2}\exp(-\theta^2/2\sigma^2)$ 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 reflection of the particles diffuse and specular reflection are assumed for deposition and etching processes, respectively [6].

Visibility Test

Most of *the* computation time for simulating the transport of the species above the wafer by the radiosity model is consumed in determining the visibility

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between the surface elements which 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 keep the computational effort at a minimum rate, 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.

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-emmited. 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 using a direct solver for the matrix equation. Whereas this method is very practical in two dimensions, 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.

Iterative Solver

The iterative solution 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 simulation 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.

Extending the speed function

Using the iterative solver we only obtain the speed function on the surface element but not at the grid points. In order to use the level set method the speed function must be suitably extended from the known values. This is carried out iteratively by starting from the grid points nearest to the boundary. Mathematical arguments show that the signed distance function can be maintained from one time step to the next by choosing a suitable extension as follows

$$\nabla F_{ext}(t,\mathbf{x}) \cdot \nabla_x u(t,\mathbf{x}) = 0 \qquad (2)$$

The idea leading to the fast level set algorithm stems from observing that 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 from a boundary 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 [5].

Stability and Complexity

For advancing the level set function we have used a second order space convex finite difference scheme [5]. In each time step the level set function is advanced with this method. A necessary condition for the stability of this scheme is the **CFL** (Courant-Friedrichs-Levy) condition which guarantees the boundary can cross no more than one grid cell during each time step. However, the **CFL** condition limits the simulator performance. If we increase the spatial resolution by a factor λ, the maximum time used in a finite difference method has to be reduced by the same factor leading to an increase of the number of simulation steps by the same factor in order to reach the same thickness. Furthermore, an increase in spatial resolution by λ increases approximately the number of extracted triangles by λ^2 and then the computational effort of the visibility test by λ^4. In summary, an increase in spatial resolution by λ leads approximately to an increase in simulation time by a factor λ^5.

Simulation results

In this section some simulation results obtained by **ELSA** (Enhanced Level Set Application) for deposition and etching processes are shown.

First, we present the result for deposition of a double-T-shape structure given in Figure 1. The species are coming from the X-Y plane above the trench. The point-shape sources of species are assumed to be located symmetrically in this plane and contribute to the direct flux at the surface elements. Figure 2 shows the simulation result including shading effects due to limited visibility between the surface elements and surface element and source points. The grid resolution was 30.30.30 and th simulation time was about 10 minutes on a workstation. The simulator is capable to predict when the void forms. Figure 3 is a cross section of Figure 2 in the X-Y plane.

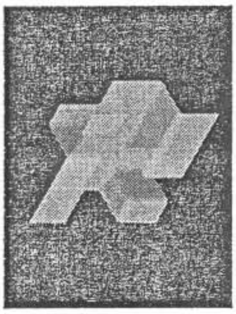

Fig. 1: Initial boundary for a T-shape structure

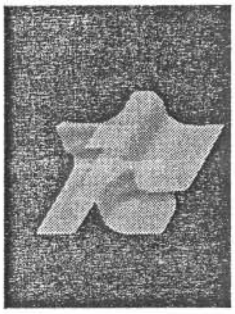

Fig. 2: Final boundary after deposition including shading effects

Figure 4 shows a rectangular trench from which material is being isotropically etched as shown in Figure 5. As expected, the sides of the trench are cleanly etched away and are rounded. Finally, Figure 6 shows directional etching of the same trench which tends to be etched more in vertical direction.

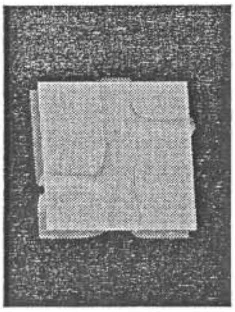

Fig. 3: X-Y cross sectional simulation result of the final boundary

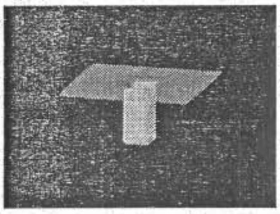

Fig. 4: Initial boundary for a rectangular trench

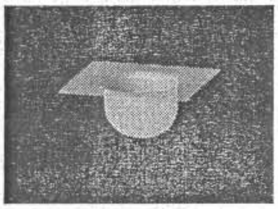

Fig. 5: Simulation result for isotropic etching.

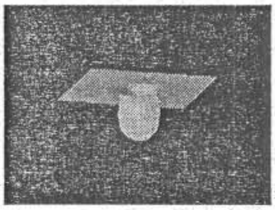

Fig. 6: Simulation result for directional etching

Conclusion

State of the art algorithms for surface evolution processes like deposition and etching processes in three dimensions have been implemented. A general simulator called **ELSA** was developed based on the level set method combining narrow banding and a fast marching method. The speed of the simulator in several steps, e.g., in initialization, visibility test, and solving the radiosity matrix equation has been improved. Therefore, the efficiency of the simulator has been increased compared to conventional level set based simulators.

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