A Multistage Smoothing Algorithm for Coupling Cellular and Polygonal Datastructures

Andreas Hössinger**, J. Cervenka*, and Siegfried Selberherr**
*Christian Doppler Laboratory for TCAD in Microelectronics at the Institute for Microelectronics
**Institute for Microelectronics, TU Vienna, Gusshaustrasse 27-29, Vienna, Austria
Telephone: +43-1-58801/36027, Fax: +43-1-58801/36099, Email: Hoessinger@iue.tuwien.ac.at

Abstract— **When cellular based topography simulation is coupled with polygonal data structures it is necessary to extract a triangular representation of the surface of the simulated structure after a deposition or an etching process from the cellular discretization. In this work an advanced multistage cellular postprocessing algorithm is presented which is capable of generating a smooth triangulated surface with a relatively small number of triangles even for practical applications in semiconductor process simulation. All structural edges are maintained by the smoothing algorithm while almost all artificial edges are removed from the surface discretization.**

I. Introduction

For the simulation of etching and deposition processes cellular algorithms [1] can be the method of choice due to their high robustness. However, they suffer from the fact that the cellular data structure is not directly compatible to polygonal based data structure used for the simulation of other semiconductor process steps like finite element simulators for annealing processes.

In [2] it has been demonstrated that this problem can be overcome by using a combination of polygonal and cellular data structures within the simulator. Roughly speaking the movement of the topography front is simulated using a cellular discretization, while the final simulation result is obtained by intersecting the generated process front with the input structure which is maintained in the polygonal data format.

Even if the method described in [2] seems to be straight forward on first glance, some critical problems have to be solved when using it within a simulation tool. The major problem is the generation of a smooth triangulated representation of the process front from the cellular discretization. According to our recent experience a multistage smoothing and simplification algorithm has turned out to be most successful to satisfy that purpose.

II. Simulation Flow

The algorithm proposed in this paper has been implemented into the three-dimensional etching and deposition simulator **TOPO3D** ([2], [3], [4]). Fig. 1 shows the simulation flow of the simulator. At the beginning the simulation structure is initialized. Than the actual simulation is performed. Therefore **TOPO3D** provides cellular algorithm based as well as polygonal algorithm based models. As a result both types of models generate a triangular discretization of the front of the topography process. The quality of this triangulation

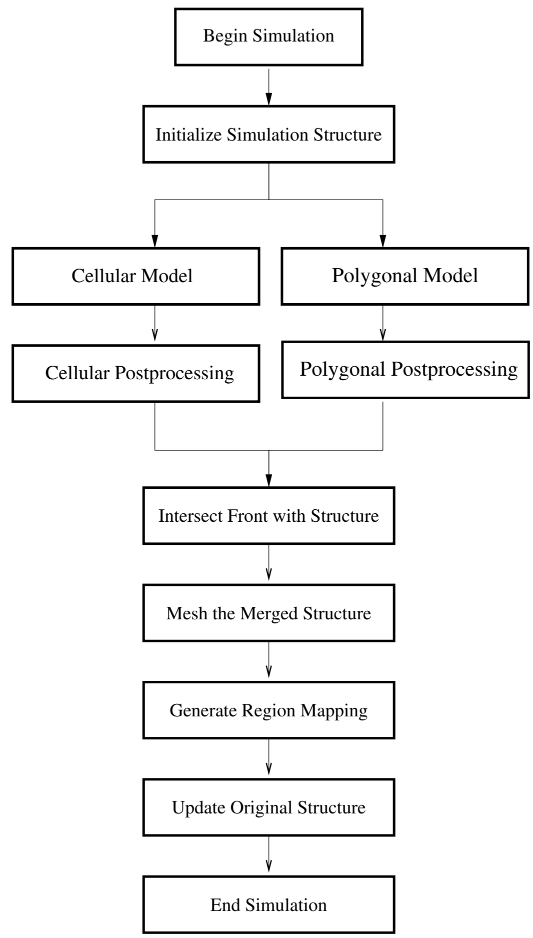

Fig. 1. Simulation flow of **TOPO3D**

is improved by a postprocessing step before the front is intersected with the interfaces of the original structure. Afterwards a tetrahedrized representation of the merged structure is generated and separated into several single-connected regions. The regions are mapped to regions of the original structure and exposed regions are removed. With the mapping information a new consistent structure which maintains all information originally contained in the input file is generated.

In order to perform the cellular postprocessing a multistage smoothing and simplification algorithms has been integrated into **TOPO3D**, since it is very crucial to extract a smooth description of the process front to ensure the convergence

 0-7803-7826-1/03/$17.00

of the succeeding volume meshing step. Furthermore the number of tetrahedral elements contained in the volume mesh is dramatically increased, if many artificial edges are contained in the triangular discretization of the process front.

III. The Cellular Postprocessing Algorithm

The postprocessing algorithm consists of four stages

- Surface extraction
- Smoothing
- Coarsening
- Simplification

A. Triangular Surface Extraction

The first stage of the algorithm is used to extract a triangulated representation of the process front. This is performed by applying a marching cube algorithm [5] to the cellular data. Thereby a set of triangles is extracted for each cell which is surrounded by at least one vacuum cell. The number of triangles and their shapes depend on the location of the neighboring vacuum cells. For a single test cube which is surrounded by eight cells 256 different cases of arrangement have to be distinguished by the marching cube algorithm.

By extracting a set of triangles for each test cube which contains vacuum as well as material cells a contiguous surface is generated. Fig. 2 shows the triangulated topography front extracted by the marching cube algorithm. The edge length of the triangles in the marching cube discretization is of the order of the cell size. This means that the process front is made up of a huge number of triangles. Another problem is that even if the marching cube algorithm does minor smoothing by considering the surrounding of a test cube, the surface discretization still contains a lot of artificial edges. Therefore two additional postprocessing stages are required to get a smooth surface with as few as possible triangles.

Our investigations have raised that applying smoothing before coarsening is the best approach since it is only possible with a huge effort to avoid a degeneration of the surface triangulation if the coarsening stage is applied first.

B. Smoothing Stage

In order to get rid of most of the artificial edges all points connected to artificial edges are moved during the smoothing process. This is performed iteratively by applying small displacements to some point of the surface triangulation, as shown in Fig. 3. In order to decide whether a point should be moved mainly two criteria are checked (Fig. 4).

On the one hand side the curvature is analyzed. If the curvature is small the point is only surrounded by approximately iso-planar triangles and therefore needs not to be smoothed. Furthermore a typical property of a point on an artifical edge is that the curvature of at least one connected point has an opposite sign. This is why a point can be excluded from the smoothing process, if the curvature is smooth in the surrounding of the point. Worth mentioning is that due to performance reasons just an approximated curvature is used in the smoothing stage [6]. The approximate curvature C_{approx} is the average of the projection of all edges connected to a point onto the normal vector of the surface at that point.

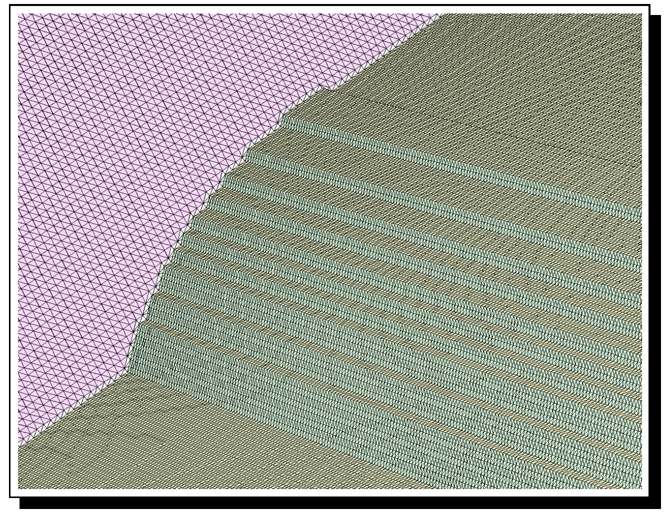

Fig. 2. Process front after marching cube discretization (332718 triangles)

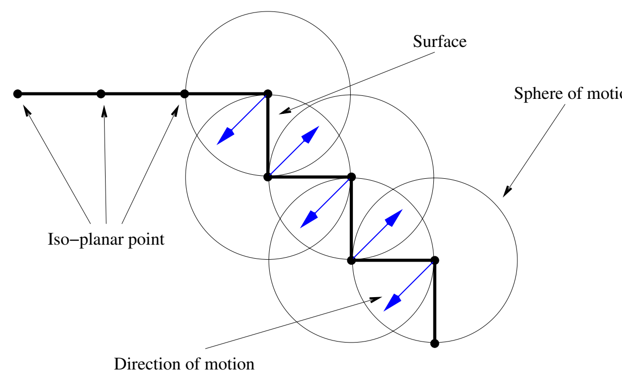

Fig. 3. Illustration of the point offset mechanism in the smoothing stage

$$C_{approx} = \frac{1}{N_{edges}} \cdot \sum_{edges} \vec{e} \cdot \vec{n_s} \qquad (1)$$

$\vec{e}$ is the vector of one edge and $\vec{n_s}$ is the normal vector of the surface at the test point. It is approximately calculated as the sum of the normals of all triangles connected to the test point.

On the other hand side the distance of a point from its original position is analyzed. Since the maximal error of the cellular discretization is less than $\frac{\sqrt{3}}{2} \times$ the cellular resolution, the distance of the real surface from the discretized surface is smaller than the size of the discretization error. This defines a sphere of motion for each point around the original position of the point. If a point would leave its sphere of motion within one smoothing iteration, it is not moved.

Besides the selection of the points which have to moved during the smoothing process their direction of motion is a critical aspect. Within each iteration step the direction of motion of one point is calculated as the sum of the normals of all triangles connected to this point. The distance of motion is set to $\frac{1}{10} \times$ the cellular resolution. If the distance of motion exceeds the length of one edge or the height of one triangle

 0-7803-7826-1/03/$17.00

connected to the point, the motion is damped in order to inhibit a degeneration of the surface triangulation.

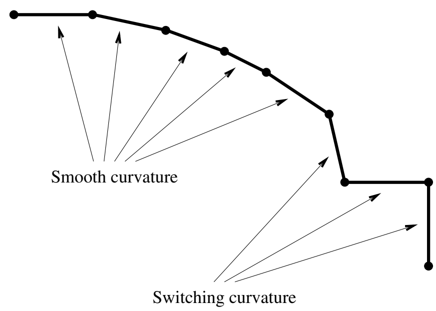

Fig. 4. Illustration of the point selection method in the smoothing stage

The consistency of the surface triangulation is checked after all points have been moved, and point movements which have violated the consistency are reversed in a repairing step. Since the smoothing operation has to preserve the bounding box of the surface discretization, a special treatment is applied to the boundary points (point contained in the rectangular bounding box). Their freedom of motion is restricted to two dimensions or even one dimension, if the point is placed in the corner of the bounding box.

Fig. 5 shows the surface triangulation after applying smoothing steps while the number of points which can be moved decreases.

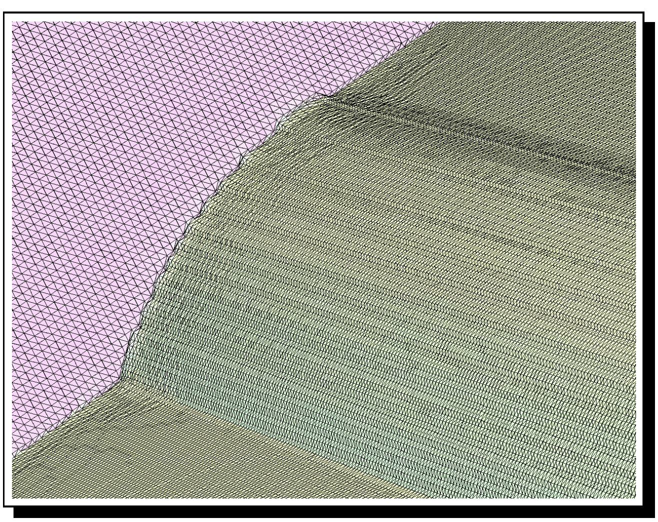

Fig. 5. Process front after applying the smoothing stage (332718 triangles)

At the end of the smoothing stage the number of triangles is still very high. Therefore two stages are applied afterwards to significantly reduce the number of triangles.

C. Coarsening stage

During the coarsening stage triangles are removed by collapsing triangle edges to a single point. Due to performance reasons only two simple criteria are checked in the coarsening stage to determine whether an edge can be collapsed. On the one hand side there are edges which contain at least one iso-planar point and on the other hand side edges which are connected to two iso-linear edges. In the first case the edge is located within a larger plane, while in the second case the edge is part of a larger structural edge (Fig. 6).

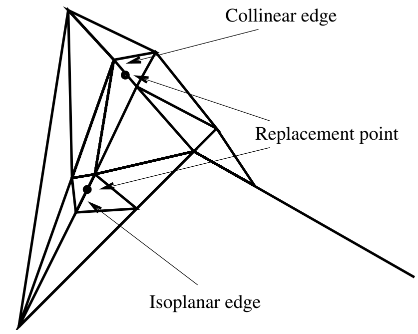

Fig. 6. Illustration of the edge removal algorithm in the coarsening stage

In general, when an edge is collapsed it is replaced by the point in the middle of the edge. But if one point of the collapsed edge is located at a structural edge, this point is chosen as the replacement point. Thereby a modification of the surface topology is avoided.

There are some cases where the collapsing of an edge results in a degeneration of the surface triangulation as shown in Fig. 7. Therefore the consistency of the surface triangulation is checked after each edge collapse operation and the edge collapse is reversed in case of a consistency violation.

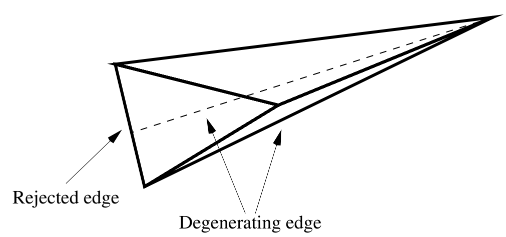

Fig. 7. Example for an edge which degenerates the surface triangulation if it would be removed

Since the vast majority of triangles are located within iso-planar regions after the smoothing stage the coarsening stage is capable to significantly reduce the number of triangles, as shown in Fig. 8. Anyhow, there are still a lot of unnecessary triangles especially within curved regions, which are eliminated by the following simplification stage.

D. Simplification stage

As well as the coarsening stage, the simplification stage uses the edge collapse algorithm to get rid of triangles. The same consistency checks and the same selection criteria for the replacement points are applied, but an alternative more sophisticated edge selection criterion as proposed in [7] is used.

The idea of the edge selection mechanism is to calculate the distance of any replacement point generated during the simplification process and to collapse an edge only if the distance

 0-7803-7826-1/03/$17.00

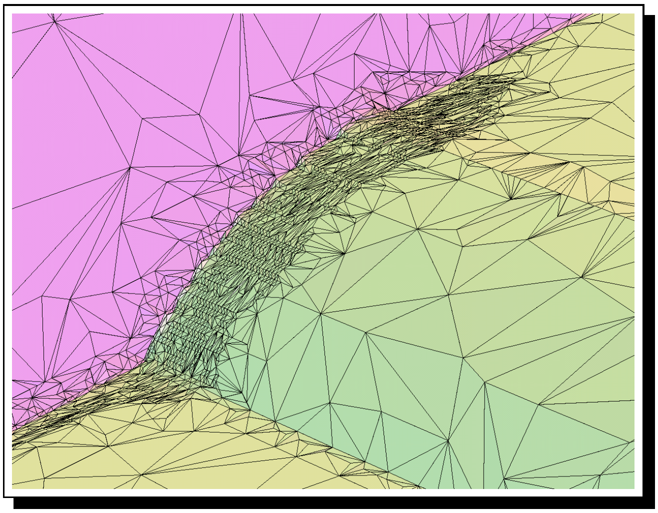

Fig. 8. Process front after applying the coarsening stage (24302 triangles)

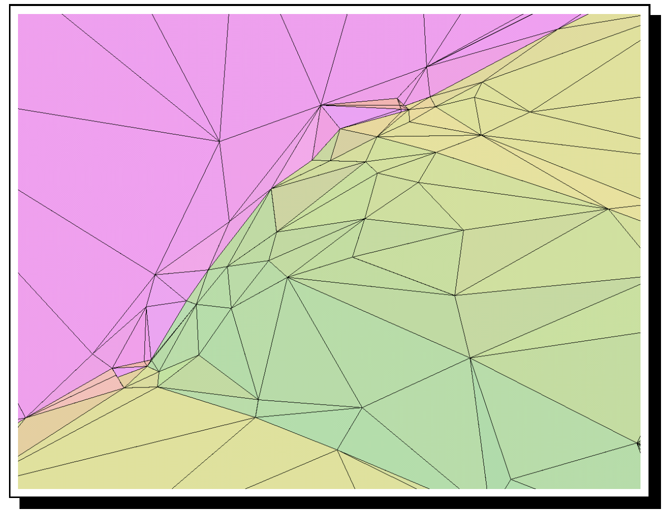

Fig. 9. Process front after applying the simplification stage (710 triangles)

does not exceed a certain limit. Within the simplification stage we again have chosen the cellular resolution as the limit for the selection algorithm since this is the minimal resolvable feature size of the cellular algorithm.

Since the calculation of the distance of a replacement point from the original surface is extremely time consuming and requires to store two representations of the surface (the original surface and the simplified surface), an approximation for the distance is proposed in [7]. Using the 4×4 distance matrix $\mathbf{M}$ derived for each point (2), the distance d of the point from the surface can be calculated by (3).

$$\mathbf{M} = \sum_{triangles} \left(\begin{pmatrix} \vec{n}_{tri} \\ \vec{n}_{tri} \cdot \vec{p} \end{pmatrix} \bigotimes \begin{pmatrix} \vec{n}_{tri} \\ \vec{n}_{tri} \cdot \vec{p} \end{pmatrix} \right) \quad (2)$$

$$d = \begin{pmatrix} \vec{p} \\ 1 \end{pmatrix} \cdot \mathbf{M} \cdot \begin{pmatrix} \vec{p} \\ 1 \end{pmatrix} \quad (3)$$

$\vec{p}$ is the position vector of the point, $\vec{n}_{tri}$ is the normal vector of a connected triangle. When a replacement point is added to the surface a distance matrix $\mathbf{M_R}$ has to be calculated for the new point by summing up the distance matrices $\mathbf{M_{E1}}$ and $\mathbf{M_{E2}}$ of the corner points of the collapsed edge (4).

$$\mathbf{M_R} = \mathbf{M_{E1}} + \mathbf{M_{E2}} \quad (4)$$

While the distance is zero for points contained in the original surface the distance calculated by (3) is greater than zero for a replacement point.

Although the selection mechanism used in the simplification stage would also select edges already eliminated by the coarsening stage, it is preferable to use both stages since the selection mechanism used in the simplification stage is more time and memory consuming. This is more critical as long as there is a large number of points in the surface triangulation. The surface discretization at the end of the simplification stage is shown in Fig. 9.

IV. Conclusion

We present a multistage smoothing and coarsening algorithms for cellular based etching and deposition simulation, which has been implemented into the three-dimensional process simulator **TOPO3D**. It can significantly reduce the number of triangles in the surface triangulation and it removes almost all artificial edges generated by the cellular discretization. Due to the small number of triangles in the surface also the number of the tetrahedral elements generated by the subsequent volume meshing step can be kept small.

V. Acknowledgment

This work has been supported by the Austrian Program for Advanced Research and Technology from the Austrian Academy of Science.

References

[1] W. Pyka, R. Martins, and S. Selberherr, “Efficient algorithms for three-dimensional etching and deposition simulation,” in *Simulation of Semiconductor Processes and Devices*, K. D. Meyer and S. Biesemans, Eds. Leuven, Belgium: Springer, Sept. 1998, pp. 16–19.

[2] A. Hössinger, T. Binder, W. Pyka, and S. Selberherr, “Advanced hybrid cellular based approach for three-dimensional etching and deposition simulation,” in *Simulation of Semiconductor Processes and Devices*, Athens, Greece, Sept. 2001, pp. 424–427.

[3] T. Binder, A. Hoessinger, and S. Selberherr, “Rigorous integration of semiconductor process and device simulators,” *IEEE Trans.Electron Devices*, to be published 2003.

[4] T. Binder and S. Selberherr, “Object-oriented wafer-state services,” in *14th European Simulation Multiconference*, R. V. Landeghem, Ed. Ghent, Belgium: Society for Computer Simulation International, May 2000, pp. 360–364.

[5] W. Lorensen and H. Cline, “Marching cubes: A high resolution 3D surface construction algorithm,” *Computer Graphics*, vol. 21, no. 4, pp. 163–169, 1987.

[6] M. Meyer, M. Desbrun, P. Schröder, and A. H. Barr, “Discrete differential-geometry operators for triangulated 2-manifolds,” in *Visualization and Mathematics III*, H.-C. Hege and K. Polthier, Eds. Heidelberg: Springer-Verlag, 2003, pp. 35–57.

[7] M. Garland and P. Heckbert, “Surface simplification using quadric error metrics,” in *Proceedings of SIGGRAPH 97*, 1997, pp. 209–216.

 0-7803-7826-1/03/$17.00 © 2003 IEEE