Control and Improvement of Surface Triangulation for Three-Dimensional Process Simulation

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Abstract

Appropriate meshes are crucial for accurate and efficient 3D process simulation. In this paper, we present a set of tools operating on surface and interface triangulations. These tools allow the improvement of the accuracy of interfaces, the reduction of the number of triangles, and the removal of obtuse not coplanarily compensated triangles. The first tool is used within integrated topography simulation environments based on different data structures, e.g. cell-based and segment-based. The latter two are particularly important for providing appropriate input to mesh generation for 3D process simulation.

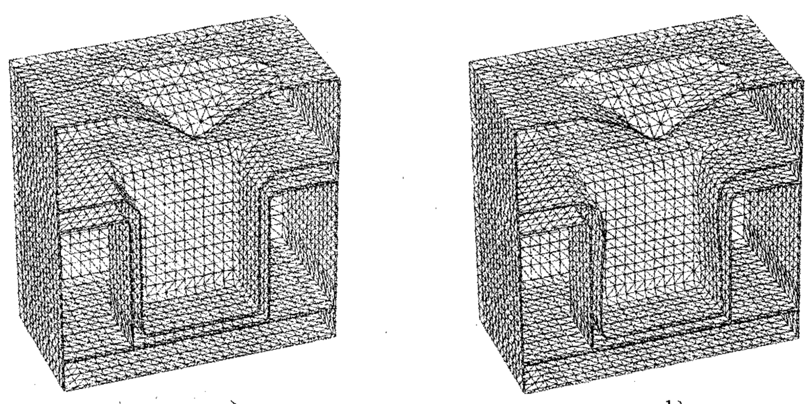
1. Introduction

A key requirement for the application of three-dimensional (3D) process simulation to deep sub-micron device structures is its capability not only to handle arbitrary device geometries but also to do this in a way that both the inevitable discretization errors are controlled and the number of nodes used in the discretization are kept within acceptable limits. Compared with device simulation, in 3D process simulation new challenges arise from the highly nonplanar and time-dependent surfaces and interfaces. In this work three tools have been developed to control and improve surface and interface descriptions resulting from the use of cell-based and triangle-based discretizations, to allow both for accurate topography simulation and for appropriate input to 3D bulk mesh generation.

2. Correction of Surface and Interface Descriptions

Surface descriptions resulting from any numerical algorithm, e.g. cell-based [1] or triangle-based [2] modules for topography simulation, in general lead to discretization errors which may be critical for subsequent process steps. This is especially important in case a process step affects only part of the surface, e.g. for a spacer etching process which physically does not modify the thin oxide below the gate, or if different data structures, like cells and triangles, are used in different process steps. In consequence, the module TRIMERGE (triangulation merger) has been developed to merge that part of the old device geometry which was not physically modified during the process step in question with those parts of the new geometry significantly different from the old one. In this way it is made sure that layers, e.g. thin nonplanar gate oxides, are not modified due to discretization errors or conversion between data formats only. The correction tool TRIMERGE used for the example shown below operates as follows: A triangulated geometry which has been generated from a cell-based one and which therefore is afflicted with inaccuracy is compared to a so-called reference geometry (as obtained directly from an earlier segment-based simulation step) which is exact but which does not necessarily contain all materials of the structure under investigation. Those parts of the inexact geometry which have a distance to the reference geometry smaller than a given threshold value (i.e. which are not affected physically but were modified only due to data conversion) are shifted towards the reference geometry.

In Fig. 1, an example for the application of the TRIMERGE tool is shown. Using the topography simulator SC-TOP [3], a contact hole structure has been created, followed by CVD of a barrier and tungsten to fill the contact. When generating a segment-based description from the cell-based one, the non conformality of the barrier at the sidewall is not resolved (Fig. 1 a). Application of TRIMERGE adjusts the triangles accordingly (Fig. 1 b) so that they fit with the barrier surface as obtained from the segment-based deposition simulator which is part of SC-TOP.



a) b)

Figure 1: Contact hole structure with deposited barrier and tungsten. a): The non-conformality of the barrier at the sidewall ist not resolved; b): application of TRIMERGE leads to the correct barrier profile.

3. Topologically Correct Smoothing

Discretization errors resulting from the numerical simulation of topography steps may lead to an artificial roughness of surfaces which must not be resolved in subsequent process steps and, especially, by a 3D mesh required for bulk process simulation. On the other hand side, even very small surface features, e.g. at the edges of shallow trench isolation (STI) structures, may be technologically relevant and must be resolved. In turn, a topologically correct smoothing algorithm for multilayer structures has been implemented. Starting from a surface or interface triangulation, nodes are identified which must be maintained due to topological considerations, e.g. to avoid a change in the connectivity of layers. All other nodes are checked whether they can be removed without changing any surface or interface, or any polygon where at least two layers meet, by more than given tolerances $d_{min,1}$ and $d_{min,2}$, respectively. As these two parameters can be prescribed based on technological requirements, e.g. the specified target gate oxide thickness, or local thickness data, this allows to automatically select the best compromise between the accuracy of surface description and the desired minimization of the number of discretization elements. Although this is an iterative process, checking one point after the other, the required accuracy of the surface is guaranteed by checking also the distance of points already removed to the surface resulting after removal of the next point.

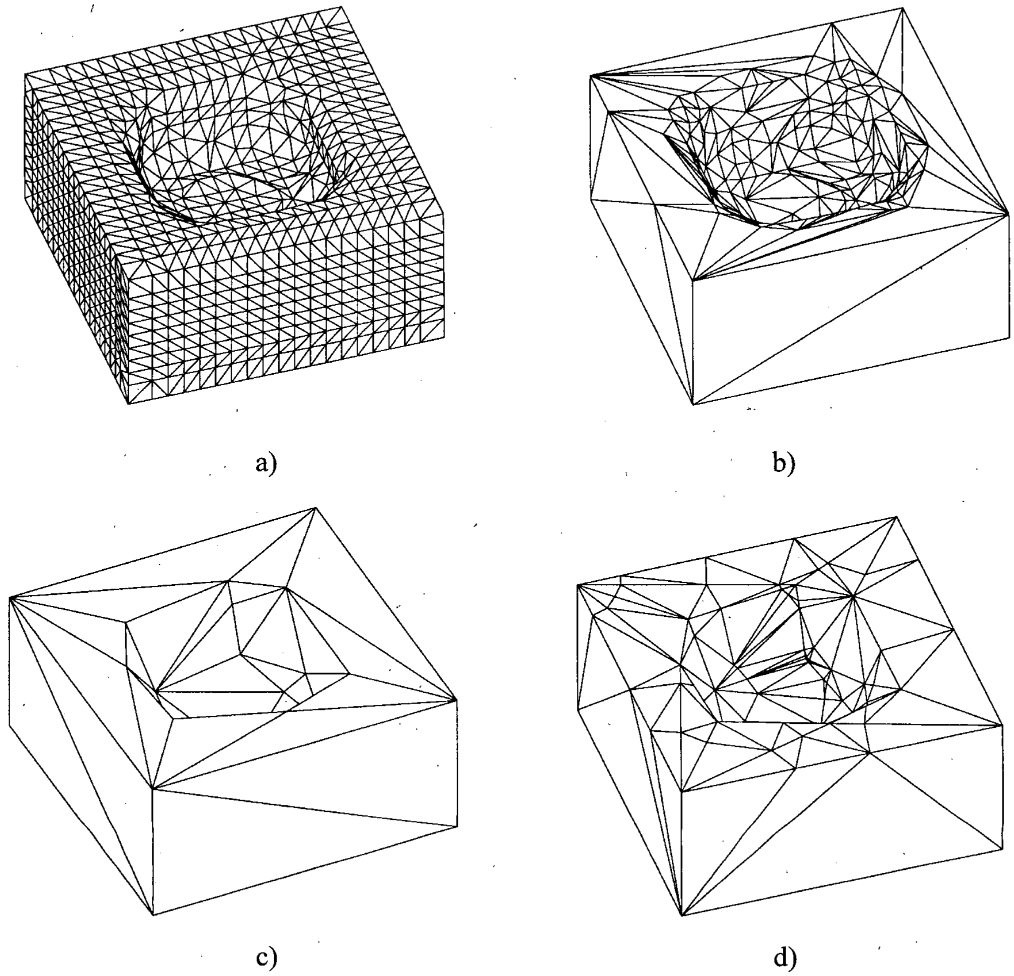


Figure 2: Triangulation (hidden-line plot) of a contact hole in a 2µm · 2µm · 1µm silicon orthogonal parallelepiped: a) initial triangulation after etching, simulated with SC-TOP, consisting of 1472 points, 4410 edges, and 2940 triangles; b) after smoothing with tolerances $d_{min,1}$=0.01µm and $d_{min,2}$=0.01µm, resulting in 197 points, 585 edges, and 390 triangles; c) after smoothing with tolerances $d_{min,1}$=0.05µm and $d_{min,2}$=0.05µm (one step), then $d_{min,1}$=0.1µm and $d_{min,2}$=0.1µm, resulting in 23 points, 63 edges, and 42 triangles; d) after removal of obtuse triangles in triangulation c), resulting in 83 points, 243 edges, and 162 triangles.

Fig. 2 b) and c) show the application of this algorithm for the smoothing of the 3D triangulation of the contact hole shown in Fig. 2 a). That contact hole resulted from the simulation of optical lithography followed by etching, using the 3D topography simulator SC-TOP [3]. Among others, the algorithm developed can be applied to treat multilayer structures, or to remove artificial steps resulting from a cell-based topography simulation by using e.g. half the cell size as smoothing parameter.

4. Removal of Obtuse Triangles

If the nodes of a surface triangulation are requested to be maintained during the generation of a 3D bulk mesh, the properties of the surface triangulation are inherited by the bulk mesh. This means especially that a bulk 3D Delaunay mesh requires the surface triangulation to have the same property when considered as a 2D hypersurface in 3D space. An algorithm has been developed to ensure this Delaunay property of a surface triangulation by successive refinement of not coplanarily compensated obtuse triangles.

Two refinement sequences are started from the obtuse triangle under consideration. They terminate with the insertion of a triangle normal the footpoint of which is within an interval allowing the appropriate refinement of the next earlier triangle in the sequence into two right-angled and one in general non-obtuse triangle. Whereas the first sequence divides the original obtuse angle into two non-obtuse ones, the second one divides the so generated new obtuse triangle into a non-obtuse one and a coplanarily compensated obtuse one. Obtuse triangles which may in exceptional cases be generated during the refinement sequence itself are added to the list of obtuse triangles still to be treated. Furthermore, coplanarity of triangles is used to limit the increase of the number of triangles in case of overlapping refinement sequences to about a factor of 4.

Fig. 2 d) shows the result of the algorithm applied to the smoothed contact hole of Fig. 2 c).

5. Conclusions

Various modules for the control and improvement of surface and interface triangulations have been developed. By their application it can be made sure that discretization errors resulting from topography simulation do not negatively impact on 3D bulk process simulation. Furthermore, by reduction of the number of nodes and improvement of triangle shapes they provide more appropriate surface descriptions for three-dimensional mesh generation and subsequent 3D bulk process simulation.

Acknowledgement

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References

[1] E. Strasser, S. Selberherr, *IEEE Trans. Computer Aided Design* **14**, 1104 (1995).

[2] E. Bär, J. Lorenz, *IEEE Trans. Semicond. Manufacturing* **9**, 67 (1996).

[3] E. Bär, W. Henke, S. List, J. Lorenz, in: *Proc. SISPAD'98* (ed. K. De Meyer, S. Biesemans), Springer-Verlag Wien New York 1998, p. 12.