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Polygonal Geometry Reconstruction after Cellular Etching or Deposition Simulation

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Abstract

This paper provides a new algorithm for the recalculation of a polygonal geometry representation after the computation of etching and deposition simulations based on a cellular geometry representation. The purpose of that algorithm is to avoid totally any discretization errors in those parts of the geometry which were not affected by the surface movements resulting from the simulation.

1. Introduction

In two-dimensional process simulation, etching and deposition simulations are central steps. The thereby required surface advancement algorithms are often performed on a cellular geometry representation, e.g. [1]. During the simulation each of the cells contains one material type. Etching and deposition is modeled by changing the material type of some cells, leaving their geometric extensions unchanged.

Therefore it is necessary for each etching or deposition simulation step during the process simulation, to discretize the original polygonal geometry (OPG), run the simulation and recalculate a final polygonal geometry (FPG) representation. Former algorithms, e.g. [2], use only the final discrete geometry description to compute the FPG. Discretization errors occur all over the geometry, which demand regriding of every geometry conform grid defined on the original geometry. In addition discretization errors of subsequent etching or deposition simulation steps might accumulate and under certain circumstances endanger the accuracy of the whole process simulation.

To minimize these problems a cellular algorithm was developed which generates the FPG by combining informations from the OPG, the original discrete geometry and the final discrete geometry. This algorithm totally avoids any discretization errors in those parts of the geometry which were not affected by the surface movements resulting from the simulation. Therefore the extensions of the cells giving the accuracy of the discretization must only be adjusted to the minimum extensions of the affected parts of the geometry. Structures much smaller than the resolution of the discretization will keep their original shape when they were not affected by the etching or deposition simulation.

2. The Algorithm

The computation of the FPG starts with a copy of the OPG: Firstly, in the main part of the algorithm, a provisional polygonal geometry is assembled by the following three steps which are performed on the cells of the discrete geometry:

1. **Classification:** Every cell of the discrete geometry is classified depending on the original and final materials of the cell itself and all it's neighboring cells. These have to be taken into account because the regions of the OPG usually do not correspond to the borders of the cells. Five different types of cells are distinguished:

   Etched Cells: a cell is classified as etched if the material changed to vacuum due to the simulation, or if it is originally vacuum and one of its neighboring cells changed to vacuum.

   Partially Etched Cells: the original and final material of the cell is not vacuum and at least one of the neighboring cells changed to vacuum in the final discrete geometry. This category is necessary to describe accurately etching at etch stops.

   Deposited Cells: the material changed from vacuum to the deposited material, or the cell was originally containing some material and one of its neighboring cells changed to the deposited material.

   Original Vacuum Cells: the original and final material is vacuum and the cell is not classified as etched, partially etched or deposited before.

   Original Material Cells: the original and final material is not vacuum and the cell is not classified as etched, partially etched or deposited before.

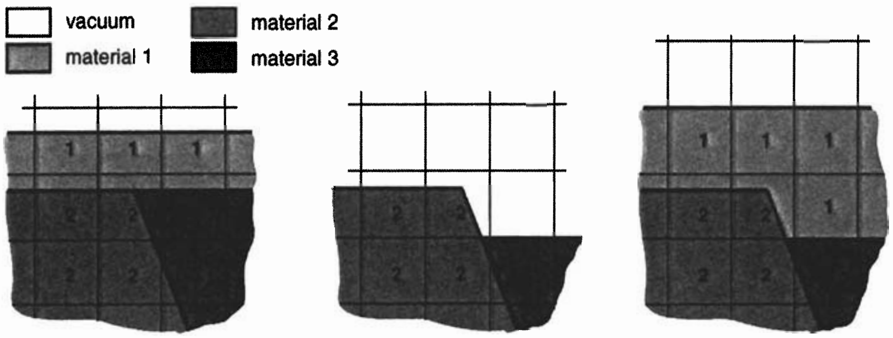
2. **Geometry-Extraction:** For etched, partially etched and deposited cells a polygonal description of the original geometry is computed. This description contains every part of the OPG which is located inside of the cell, informations about the material types inside and outside of the borders of the cell and the classifications of the cell and all its neighboring cells. (Fig. 2 shows an example for this geometry extraction using quadratic cells.)

3. **Geometry-Correction:** the FPG inside of the recent cell is computed by modifying the polygonal description of the cell dependent on the classification of the cell:

   Etched Cells: Any region of the geometry which does not contain vacuum is removed from the provisional polygonal geometry.

   Partially Etched Cells: Every region of such a cell which is not containing the material itself and is bordering to an etched cell is removed from the provisional polygonal geometry. Remaining parts of the borders to neighboring cells which are classified as *Original Material Cell* or *Etched Cell* are added to the provisional polygonal geometry to ensure a consistent description of the geometry.

   Deposited Cells: Regions of the geometry containing vacuum are replaced by regions containing the deposited material and added to the provisional polygonal geometry like newly created borders to cells which were classified as *Original Material Cell* or *Original Vacuum Cell.*

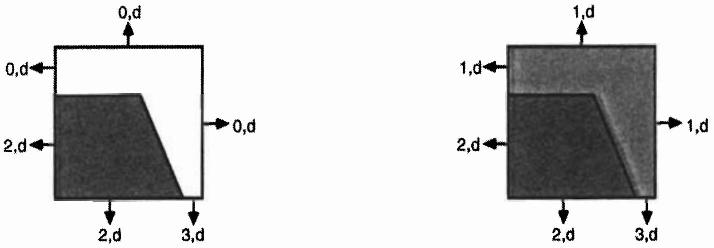


(a) (b) (c)

Figure 1: Discrete and polygonal geometries. (a) original, (b) etched, (c) redeposited

Fig. 1 shows a two-dimensional example for the construction of the FPG after an etching and deposition simulation. In Fig. 1a the discretization of th OPG is demonstrated. In this example the material of a cell is determined by the material type of the OPG at the center of the cell. The resulting discrete and polygonal geometries after removing some cells by an etching simulation are presented in Fig. 1b. Fig. 1c shows the resulting discrete and polygonal geometries after the redeposition of material 1 on top of the geometry of Fig. 1b.

In Fig. 2 the extraction and modification of the polygonal geometry is demonstrated for this simulation step for the cell in the center of Fig. 1b. The cell contains the material type 2 and is classified as a deposited cell. The redeposition of material 1 is simulated by changing the material type of the face in the northeast of the cell, and correcting the material references at the borders of the cell. After that the local geometry is inserted into the provisional polygonal geometry.



(a) (b)

Figure 2: Extraction and modification of the polygonal geometry for the redeposition simulation of the cell in the center of figure 1b and 1c. The vectors at the borders give the material types outside of the cell and the classifications of the neighboring cells. (d. . . deposited)

The structure which is thereby created contains a high number of segments. Therefore in a second step the face structure is simplified and locally smoothed as far as it is not defined by parts of the OPG. The extent of reduction can be controlled, and the number of segments is often drastically reduced. Fig. 3 shows the polygonal geometry

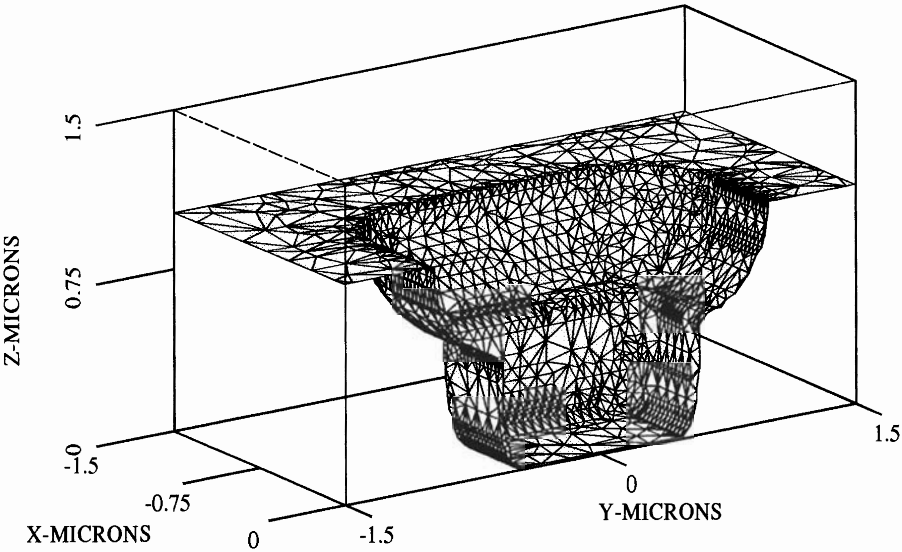


Figure 3: A square contact hole.

which was obtained after the simulation of a complete three-dimensional contact hole etching process.

3. Conclusions

The algorithm is highly independent from the dimension and shape of the discretization cells. Possible restrictions arise only out of numerical and algorithmic problems during the computation of the inner geometry of the cells. Therefore it is applicable to a large group of problems which require temporary conversions from polygonal to discrete geometry representations.

The increased computational effort of this new algorithm can be justified by considerable savings of calculation time in following regriding algorithms, because these have only to be applied in those parts of the geometry which actually changed during the etching or deposition simulation.

Acknowledgements

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