Three-dimensional Triangle-based Simulation of Etching Processes

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Abstract **– A software module for the three-dimensional simulation of etching processes has been developed. It works on multilayer structures given as triangulated surface meshes. The mesh is moved nodewise according to rates which in this work have been determined from isotropic and anisotropic components. An important feature of the algorithm is the automatic detection of triple lines along mask edges and the refinement of triangles at these triple lines. This allows for the simulation of underetching. The capabilities of the algorithm are demonstrated by examples such as the simulation of glass etching for the fabrication of a phase shift mask for optical lithography and the etching of an STI trench structure.**

I. INTRODUCTION

Three-dimensional simulation of etching is up to now done to a great part by cell-based methods [1]. However, with shrinking feature sizes as e. g. thinner gate oxides, it becomes more and more difficult to resolve whole transistors by cells with sufficient accuracy. A remedy to this problem could be to triangulate the surface, using an adaptive triangulation which provides the required accuracy and to move the triangles according to the etch rates.

Within this work, a triangle based algorithm has been developed which is capable of simulating etching processes for multilayer structures, using the hierarchical Boundary Format available within the ISE TCAD framework [2].

II. RATE DETERMINATION AND SURFACE MESH MOVEMENT

The etch time and the isotropic and anisotropic component of the etch rate for each material have to be specified. From the isotropic and anisotropic components, the resulting etch rate is determined for each triangle, but could in principle also be calculated externally by a physical model. For the results shown in this paper, the etch rate r is calculated by

$$r = r_{iso} + r_{aniso} \cos\theta$$

where r_{iso} and r_{aniso} denote the isotropic and anisotropic rate, respectively, and θ is the angle between the normal vector of the corresponding triangle and the z-axis of the underlying co-ordinate system.

Special attention must be paid to the detection and treatment of so-called triple lines. Triple lines appear where "internal" triangles (e. g. under masks) and triangles, which are being etched, meet each other. To allow for the realistic simulation of underetching, a strip through the internal triangles parallel to the triple line(s) is calculated, its width being equal to the isotropic component of the etched thickness for the surface update step. At the intersection of the strip with triangle edges, new points are inserted and the structure is retriangulated accordingly. In order to simulate underetching, the triple points are split and copies of them are generated and moved with the calculated shifts. Copies of the triangles forming the strip are connected with the moved copies of the triple points and belong now to the triangles with access to the etch gas. The same algorithm is used for purely anisotropic etching, hereby choosing a very small isotropic component.

The update of the surface is performed nodewise, where the shifts of the nodes depend on the rates and normal directions of the adjacent triangles. In order to allow for mesh repair and prevention of local self intersections of triangles, the surface is shifted in several steps until the desired etch time is reached.

III. EXAMPLES

Using the topology editor of the topography simulator SOLD-CTM [3], the structure shown in figure 1a has been generated. It represents a silicon dioxide mask on a silicon substrate.

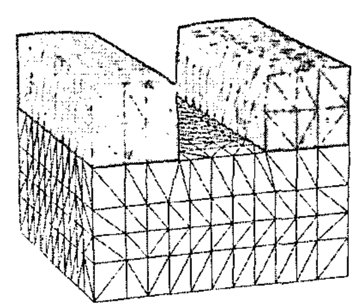

Figure 1a: Silicon dioxide mask on Si substrate. The Si is being etched. Initial structure.

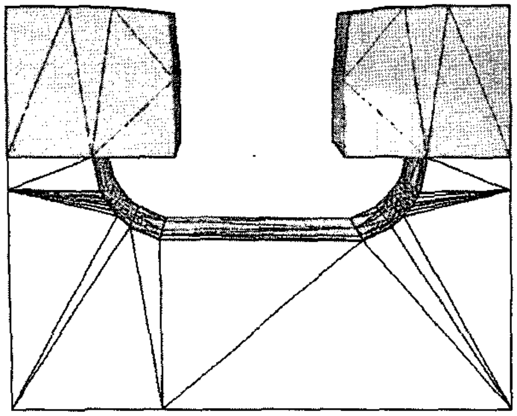

Figure 1b: Simulation of purely isotropic etching with an etch depth of 0.33μm.

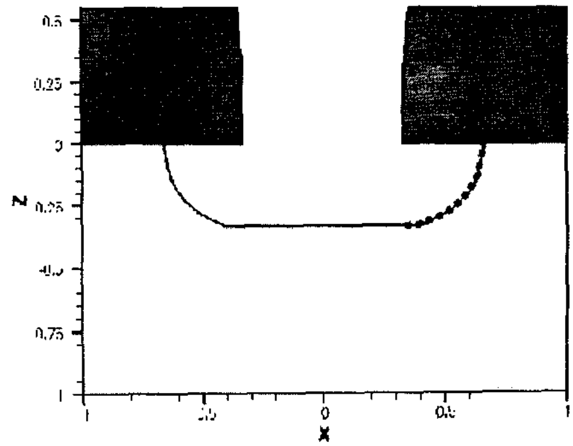

Figure 1c: 2D cut through figure 1b. The points on the right side indicate an exact quarter circle.

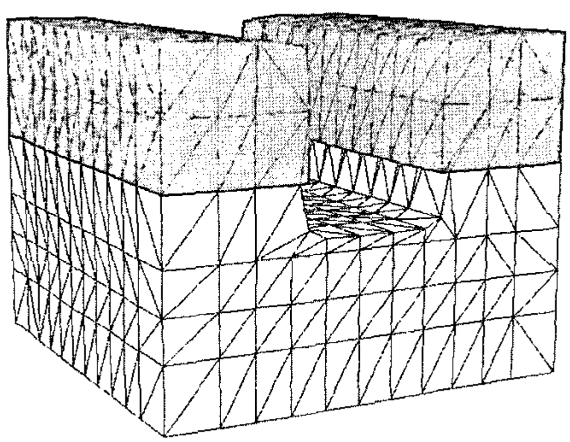

Figure 1d: Simulation with r_{iso} / r_{aniso} = 0.20. Etch depth: 0.24μm.

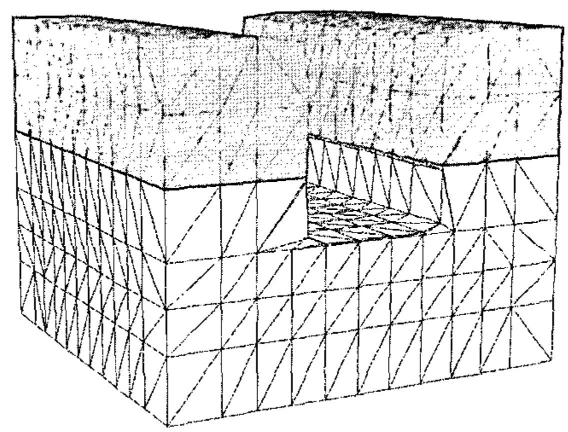

Figure 1e: Simulation with r_{iso} / r_{aniso} = 0.09. Etch depth: 0.29μm.

The simulation of purely isotropic etching has been performed with an etch depth of 0.33μm. To allow remeshing, the surface movement was carried out in 11 steps. Remeshing was performed with YAMS [4] – a tool for coarsening and refining of surface triangulations – to prevent local self intersections. Figure 1b shows the simulation result.

When purely isotropic etching is simulated, a rounding under a mask edge occurs shaped as a quarter circle. Figure 1c shows a two-dimensional cut through the structure given in figure 1b. On the right hand side of the cut, the black points indicate an exact quarter circle which agrees very well with the simulation result.

Figures 1d and 1e show the structure etched with a ratio of the isotropic and the anisotropic component of 0.2:1 (figure 1d) and 0.09:1 (figure 1e). The etch depths are 0.24μm and 0.29μm, respectively. Here, no remeshing with YAMS during the simulation runs has been performed.

The second example demonstrates the simulation of trench etching as part of a process flow for the fabrication of a shallow trench isolated (STI) transistor. The side wall angle was specified to 3°, corresponding to a ratio of isotropic to anisotropic component of 0.05:1. The initial structure shown in figure 2a consists of a silicon substrate with a patterned oxide and nitride layer on top. The silicon is being etched.

A particularly important feature of an STI geometry is the bottom rounding of the etched trench. An at least qualitative reproduction of the rounding is important to allow simulation of effects during subsequent process steps, e.g. the development of stress during liner oxidation. In our approach, besides the rate determination from isotropic and anisotropic components, additional empirically-based shift vector modifications have been implemented to achieve a realistic bottom profile. Prior to the simulation, the surface mesh has been refined at the silicon open to the etch attack using the meshing tools provided within the ISE TCAD framework [2].

Figure 2b shows the result of the simulation of trench etching, figure 2c shows a cross sectional view in which underetching and bottom rounding are visible. For visualisation purposes, the grid resolution for the simulation shown in figure 2b was chosen lower than for the more accurate result represented by the cross section in figure 2c. Figure 2d shows an SEM (scanning electron micrograph) of an STI trench which qualitatively agrees with the simulation.

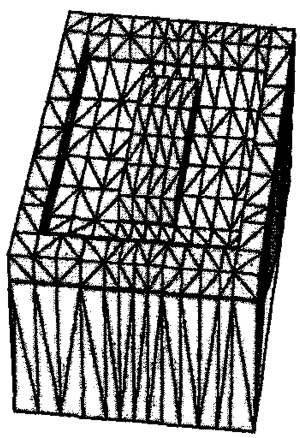

Figure 2a: Initial STI structure.

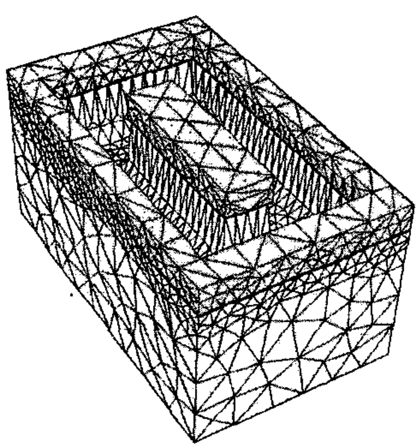

Figure 2b: 3D simulation of trench etching.

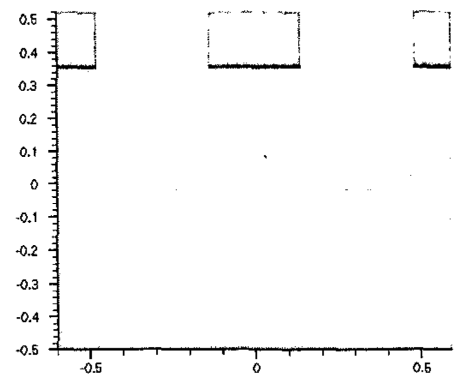

Figure 2c: Cross sectional view of simulation, bottom rounding and underetching are visible.

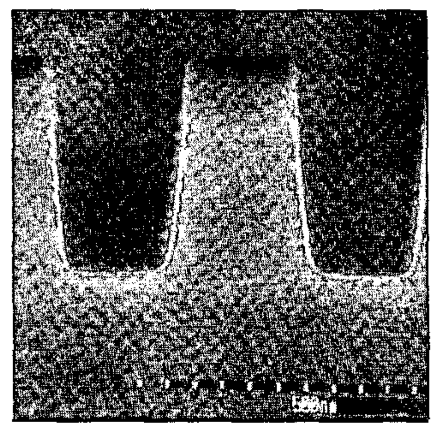

Figure 2d: SEM of an etched STI trench (Hitachi advertisement).

The third example demonstrates the simulation of etching a phase shift mask for isolated and dense lines. The initial structure is shown in figure 3a. The mask consists of chromium, the glass is being etched. Figure 3b shows the phase shift mask after two simulation runs. In the first simulation run, the left side of the structure was covered with an unetchable mask so that only the right side was being etched. In the next step, the right side was masked and the left one was etched. The difference between the depth of the left and the right trench is 248nm, leading to a 180° phase shift when assuming a refraction index of 1.5 for the glass substrate and applying a krypton-fluoride (KrF) laser as a light source for optical lithography. Mask underetching can as well be observed as sloped side walls. Figure 3c shows an SEM of a phase shift mask [5]. The rounding at the bottom visible there cannot yet be simulated because of instabilities during mesh movement with very small triangles.

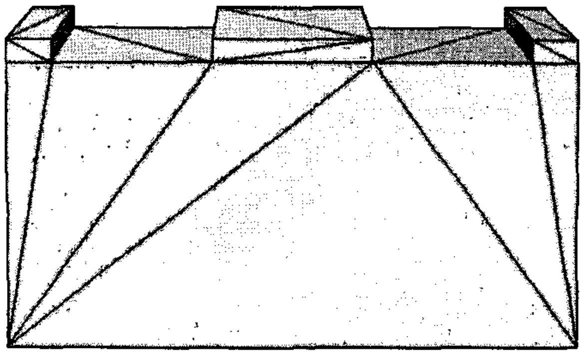

Figure 3a: Phase shift mask for isolated and dense lines before etching. The mask is made of chromium, the substrate is glass.

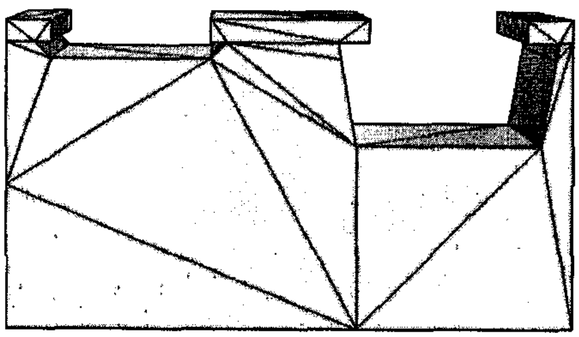

Figure 3b: Etch simulation of a phase shift mask.

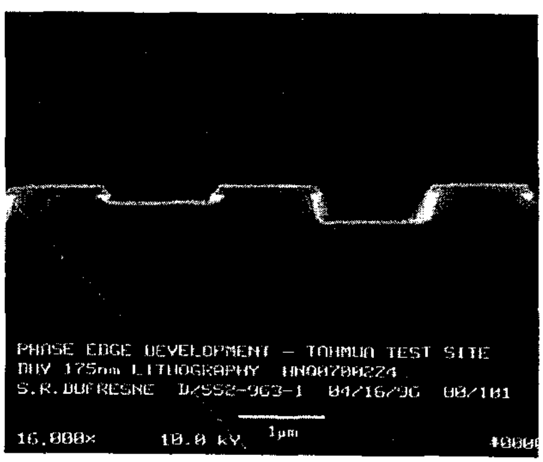

Figure 3c: SEM of a phase shift mask [5].

IV. CONCLUSION

A module for simulating etching processes on a triangulated surface mesh has been developed. The functionality was demonstrated on three examples. In the first one, the influence of different ratios of the isotropic to the anisotropic etch component is examined for a silicon dioxide mask on a silicon substrate. Further more, trench etching for the fabrication of an STI transistor and etching of a phase shift mask have been simulated. For all examples shown, the etch rates have been determined by combining isotropic and anisotropic components. However, due to the concept of the algorithm which separates the calculation of etch rates from the geometrical procedures (e. g. mesh refinement and coarsening) it is possible to couple the simulator also to physical-based models.

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