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Accurate Simulation of Pattern Transfer Processes Using Minkowski Operations

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SUMMARY A new method for simulation of etching and deposition processes has been developed. This method is based on fundamental morphological operations derived from image and signal processing. As the material surface during simulation moves in time, the geometry either increases or decreases. If the simulation geometry is considered as a two-valued image (material or vacuum), etching and deposition processes can be simulated by means of the erosion and dilation operation. Together with a cellular material representation this method allows an accurate and stable simulation of three-dimensional arbitrary structures. Simulation results for several etching and deposition problems demonstrate accuracy and generality of our method.

key words: *simulation, etching, deposition, minkowski operations*

1. Introduction

Computer modeling of topography processes such as plasma assisted etching, ion milling, thin film evaporation, and sputtering becomes increasingly important for semiconductor technology development. The numerical algorithms for surface movement play a key role in the development of new simulators and lead to major differences in accuracy, robustness, and efficiency of the simulation tools.

In recent years several surface evolution algorithms have been proposed to build three-dimensional topography simulators. Most of them are extensions of the two-dimensional string [1], cell [2] or ray [3] algorithms introduced in the 1970s. Ray-tracing and volume-removal methods have been successfully used in three-dimensional lithography simulation for photoresist development [4]-[6]. A few methods introduced thus far have been reported for three-dimensional simulation of etching and deposition processes [7], [8]. Surface advancement algorithms offer highly accurate results, though with potential topological instabilities such as erroneous surface loops which result from a growing or etching surface intersecting with itself. Cell-removal algorithms can easily handle arbitrary structures. They do not exhibit the looping problem encountered in surface advancement methods, but they suffer from inherent inaccuracies, because they favor certain etch directions [9].

We developed a new method for simulation of etching and deposition processes. This method is based on fundamental morphological operations used in image and signal processing and allows accurate simulation of arbitrary three-dimensional structures. In Sect. 2 we start with a description of the morphological operations used for surface advancement in our simulator. In Sect. 3 we go into detail about data structure and implementation of the simulation tool. Finally, in Sect. 4 we present several simulation results both in two and three dimensions.

2. The Morphological Approach

Morphology is the name of a general method in image processing used for many purposes, including edge detection and segmentation of images. Several fundamental operations provide a well defined methodology for altering a given image with respect to some predetermined geometric shape [10]. The basic goal of topography simulation is to determine the time-evolving surface of the material. As the surface moves in time, the initial simulation geometry either increases or decreases. If we consider the initial geometry as a black and white image (material or vacuum), morphological operations can be used to simulate the surface movement.

We first consider the *Minkowski addition*. Given two images A and B in the Euclidean plane R^2, we define the Minkowski sum as

$$A \oplus B := \bigcup_{b \in B} A + b. \tag{1}$$

$A \oplus B$ is constructed by translating A by each element of B and then taking the union of all resulting translations.

The *translation* of the image A by b is defined by

$$A + b := \{a + b : a \in A\}. \tag{2}$$

As an example let A be the unit disc centered at (2, 2) and let $B = \{(4, 1), (5, 1), (5, 2)\}$ as shown in Fig. 1. Then the Minkowski addition evaluates to $A \oplus B = [(A + (4, 1)) \cup (A + (5, 1)) \cup (A + (5, 2))]$.

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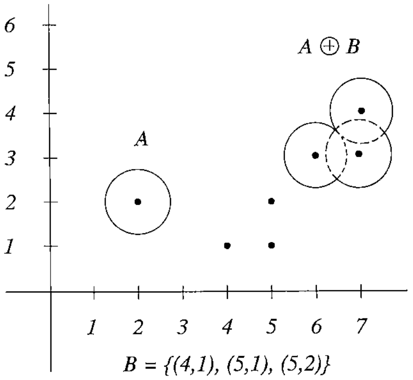


Fig. 1 Minkowski addition.

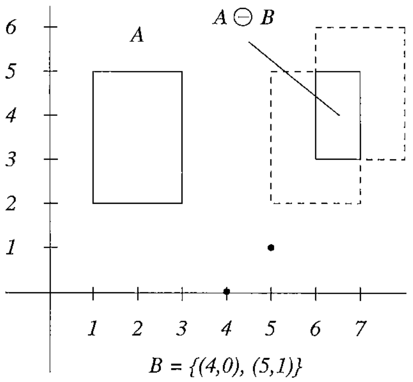


Fig. 2 Minkowski subtraction.

The second fundamental operation is *Minkowski subtraction*. Given two images A and B in R^2, we define the Minkowski difference as

$$A\ominus B := \bigcap_{b\in B} A+b. \tag{3}$$

In this operation, A is translated by every element of B and then the intersection is taken. Considering a rectangle A and let $B=\{(4,0),(5,1)\}$ as shown in Fig. 2. The Minkowski subtraction in this case is $A\ominus B=[(A+(4,0))\cap(A+(5,1))]$.

Applying these operations to a given image provides us with the terms of *erosion* and *dilation*. Let us assume an image A as drawn in Fig. 3. As a result of the Minkowski subtraction $A\ominus B$ (B is the ellipse centered at the origin as shown in Fig. 3) we observe the effect of "shrinking" the image A in a manner determined by B. We define the *erosion* of A by B as

$$\mathscr{E}(A,B):=A\ominus(-B)=A\ominus B, \tag{4}$$

if the image B is symmetric with respect to the origin. When A is eroded by B, the latter is called a *structuring element* or *structuring filter*. Corresponding to the erosion operation is the operation of *dilation* which is defined as

$$\mathscr{D}(A,B):=A\oplus B. \tag{5}$$

Dilation has the effect of "expanding" an image determined by the structuring element B as shown in Fig. 4.

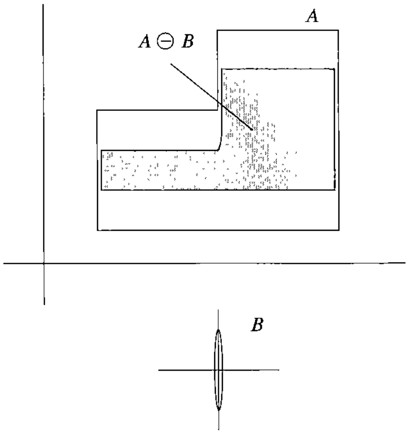


Fig. 3 Erosion as shrinking.

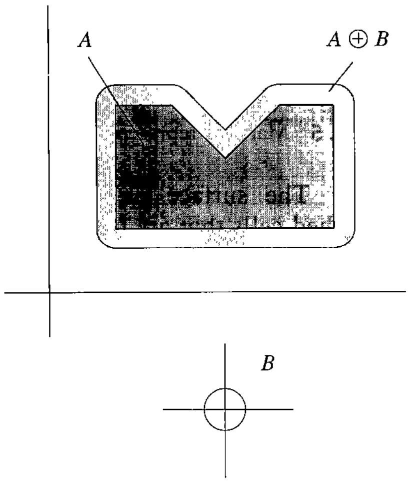
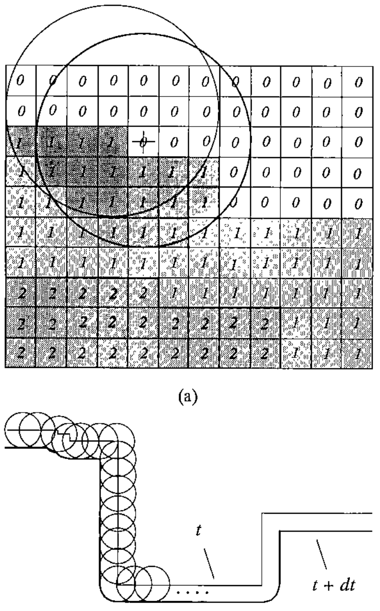


Fig. 4 Dilation as expanding.

Minkowski addition and subtraction are the basic morphological operations. The capability of altering an given image helps us to solve the problem of tracing a time-evolving surface during an etching or deposition process. Etching of a material can be described using the erosion operation, whereas deposition can be simulated by means of the dilation operation. The way how the surface moves at a certain time step is determined by the spatial dimension of the applied filter as shown in Figs. 3 and 4.

3. Data Structure and Implementation

The simulation geometry is basically considered as a two-valued image (material or vacuum). Figure 5(a) illustrates the material representation of the simulation tool. We use an array of square or cubic cells, where each cell is characterized as etched or unetched. Additionally, a material identifier is defined for each cell, therefore material boundaries need not be explicit-

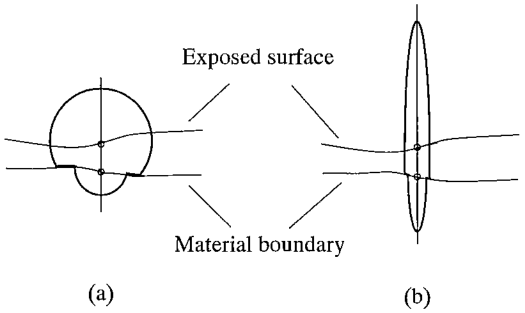


0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
1	1	1	1	0	0	0	0	0	0	0	0
1	1	1	1	1	1	1	0	0	0	0	0
1	1	1	1	1	1	1	0	0	0	0	0
1	1	1	1	1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1	1	1	1	1
2	2	2	2	2	1	1	1	1	1	1	1
2	2	2	2	2	2	2	2	2	1	1	1
2	2	2	2	2	2	2	2	2	1	1	1

(a)

(b)

Fig. 5 Material representation.



(a) (b)

Fig. 6 Composite filters at material boundaries, (a) isotropic and (b) anisotropic movement of surface points.

ly represented. The surface or etching boundary consists of unetched cells that are in contact with fully etched cells. Cells on the surface are exposed to the etching medium or to the deposition source, and etching or deposition proceeds on this surface. A linked surface cell list stores dynamically etch or deposition rates of exposed cells. To advance the etch front spatial filter operations based on the erosion or dilation operation are performed along the surface boundary as shown in Figs. 5(a) and (b). During an etching process, all cells within a filter are etched away, while cells outside stay unchanged. Usually, for anisotropic three-dimensional simulation filters are ellipsoids, for isotropic movement of surface points filters are spheres, although there is no restriction on the filter shape. The spatial dimension of an applied filter determines how far a surface point moves. The main axes of an ellipsoid are given by the local etch or deposition rates multiplied by the time step. After each time step the exposed boundary has to be determined. Therefore all the cells in the material are scanned. Material cells are surface cells if at least one cell side is in contact with an already etched cell. The exposed sides of the detected surface cells describe the etch or deposition front at a certain time step.

When the surface passes from one material to another, filter operations must be performed by using composite filters as shown in Fig. 6. The important question is how the surface evolves at the boundary, since interfaces lead to an abrupt change in etch rates. Therefore, filter operations are performed selectively on a given material. That means, filter operations on cells of a given material will only remove cells of the same material. If a filter extends over a material boundary it will demand an additional filter operation performed selectively to the second material. The etch rate for this second filter operation is calculated regarding the etch rates on both side of the interface and depending on how far the filter reaches into the other material.

Many processes are strongly affected by the shape of the surface. Modeling of realistic etching and deposition processes requires information about shadowing of surface points and local surface orientation. Additionally, some surface regions will have a restricted view of the "sky" above the wafer which for instance determines the amount of incoming flux during a sputter deposition process. To calculate realistic etch or growth rate distributions an efficient shadow test has been implemented in order to determine if a cell on the surface is shadowed through other cells or not. The problem whether a certain part of the sky is visible from a viewing point on the surface can be reduced to a series of shadow tests. The "sky" is divided up in several parts and a shadow test determines if a part is visible from a given surface point or not. All this information is used to calculate the etch or growth rate distribution along the surface boundary starting from a primary given rate. The calculated etch or growth rate distribution and the angular flux distribution of incoming species in turn influences the shape and direction of the applied filters and thereby the evolution of the wafer surface.

4. Simulation Results

The first simulation result presented here (Fig. 7(a)) shows a physical vapor deposition of titanium over a trench structure. Data and experimental results were taken from [11]. The direction and the rate of growth for a point on the surface depend on flux contributions arriving from several directions and on the solid angle visibility. The flux distribution function of the incident particles at the wafer surface is given by $\cos^{1.3}\phi$ (where ϕ means the incident angle with respect to the flat wafer surface normal). The deposition rate at a surface point is obtained by integrating over the visible

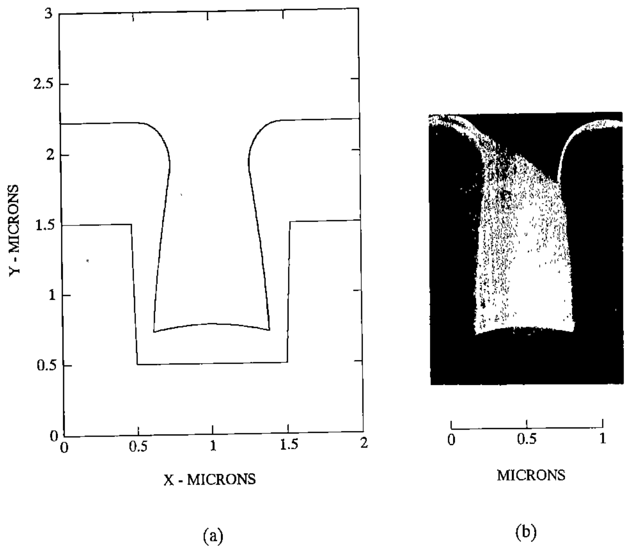


Fig. 7 Simulation of physical vapor deposition, (a) simulation result and (b) experimental result.

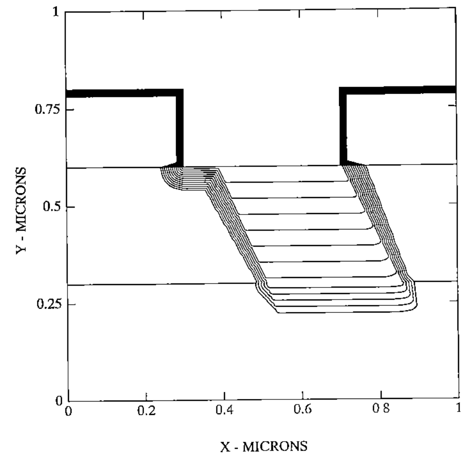


Fig. 8 Simulation of reactive ion etching.

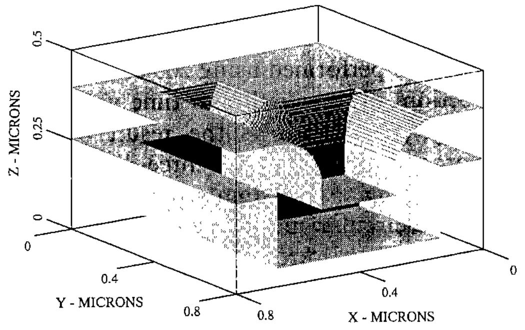


Fig. 9 Simulation of isotropic deposition.

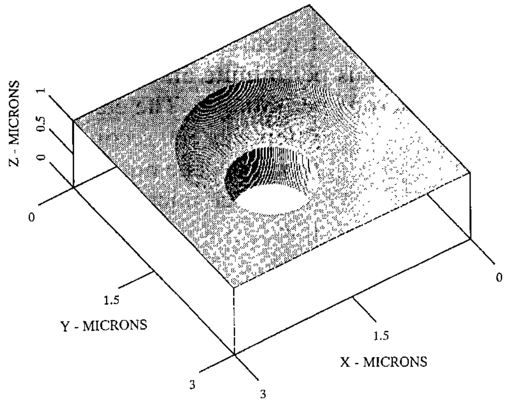


Fig. 10 Simulation of contact hole etching.

part of the vapor stream. Therefore the spatial dimensions of the ellipses varies along the surface as a result of shadowing. The deposition rate on a flat substrat for this example was 0.03 microns per minute. The deposition time was 1400 seconds, the time step was 350 seconds. The simulation was done using 400 cells per micron in each direction. The calculation time for this example was 49 seconds.

Figure 8 shows the simulation of reactive ion etching. The flux arrives with an angle of twenty degrees. This etching process is modeled using a directional and an isotropic etch rate component. The flux can be shadowed and has a local $\cos\phi$ rate dependency (where ϕ denotes the angle between incident flux and local surface normal vector). Therefore at each time step two filter operations along the surface boundary are performed. The spatial filter for the directional component is a very small ellipse applied with a tilt angle of twenty degrees. This filter operation is only performed at unshadowed regions. The directional etch rate component models the ion-enhanced surface etching effects due to ionic species. The spatial filter form for the second (isotropic) etching step is a circle modeling the chemically reactive gas. Figure 8 shows a silicon substrat with a nitride layer above and a resist mask on top. The etch rates (in microns per minute) for the three materials are:

material	directional rate	isotropic rate
resist	0.0000	0.0015
silicon	0.0400	0.0050
nitride	0.0100	0.0070

The etching time was 720 seconds simulated with time steps of 60 seconds. We used 800 cells per micron in each direction. The calculation time for this example was 31 seconds.

Figure 9 shows three-dimensional isotropic deposition of oxide over a silicon substrate to simulate a chemical vapor deposition process. In contrary to surface advancement algorithms there is no need for special treatment of convex or concave corners. Using spherical filter shapes the surface evolves perfectly isotropic. The deposition rate for this example was 0.03 microns per minute. The deposition time was 300 seconds, the time step was 100 seconds. Therefore the radius of the spherical filter is 50 nanometers. The simulation was performed using 200 cells per micron in each direction. The calculation time was 36 minutes.

Finally, Fig. 10 shows the result of sequential etching processes to simulate three-dimensional contact hole etching. The simulation for this example starts with a circular mask opening of 1 micrometer diameter. The first isotropic etching process etches the substrate to a depth of 0.5 microns. The spatial filter for the isotropic etching step is a sphere. The etching rate for this step is 0.03 microns per minute. The etching time was 1000 seconds simulated with time steps of 250 seconds. This isotropic etching process is followed by a directional etching step for 0.5 micrometer additional material removal. The directional etch rate is 0.040 microns per minute and the isotropic etch rate is 0.008 microns per minute. The etching time for the directional etching step was 800 seconds simulated with time steps of 200 seconds. The number of cells for this example was 100 cells per micron in each direction, the calculation time was 43 minutes.

All the simulations were performed on a HP 9000/755.

5. Conclusion

A new method for simulation of etching and deposition processes was presented. Fundamental morphological operations derived from image and signal processing provide the basis for describing the surface movement at a given time step. The precalculated etch or growth rates along the surface and the angular flux distribution of incoming particles influence the shape and direction of the applied filters and therewith the surface evolution. Together with a cellular material representation this method allows an accurate and stable simulation of arbitrary structures.

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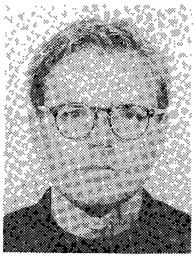

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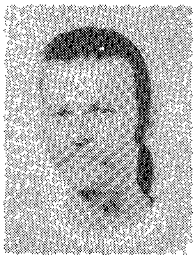

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