ANISOTROPIC CRYSTALLINE ETCHING SIMULATION USING A CONTINUOUS CELLULAR AUTOMATA ALGORITHM

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ABSTRACT

We present results on the development of an anisotropic crystalline etching simulation (ACES) program based on a new continuous Cellular Automata (CA) model. The program provides accurate modeling of etching process with high spatial resolution. Implementation of a dynamic CA technique has resulted in increased simulation speed and reduced memory requirements. A first ACES software based on PC platforms has been realized.

Keywords: Etching simulation; Anisotropic etching; Continuous Cellular Automata.

I. INTRODUCTION

Preferential etching of silicon (using EDP, KOH, or TMAH solutions) is a prevalent process step for realizing three-dimensional MEMS structures [1]. Methods for simulating the etching process fall into two categories: Cellular Automata (CA) method and geometric method. In the geometric method, a semiconductor substrate is treated as a continuous entity. In the CA method, on the other hand, a substrate is represented by a large number of cells that reside in a crystalline lattice (e.g. diamond lattice for Si, Fig. 1). A material system is described by discrete spatial, temporal, and cell-state variables. During the etching process, the state of each individual cell, i.e. whether it is removed from or remains within the lattice, will be determined by the strength of chemical bounds and link status of its lattice neighbors. The CA method typically requires more computer memory compared with the geometric method; nonetheless, it exhibits high efficiency and accuracy when handling arbitrarily complex mask shapes and merging of three-dimensional structures.

Conventional CA modeling utilizes discrete cell states; namely, a cell within a lattice can only assert one of two states, “removed” or “not removed”. As a consequence, normalized etch rates along major crystal axes can have two possible values, 1 (indicating finite etch rate) or 0 (indicate zero etch rate). For example, the default ratio of etch rates (for Si) in three major axes, <100>, <110>, and <111>, equals 1:1:0. Obviously, such a model over simplifies the physical etching process. The etch rate of {111} surfaces, though small, is not completely zero; in addition, etch rates for {100} and {110} surfaces are not always identical.

With the advancement of the MEMS CAD [2], more accurate and efficient modeling of the anisotropic etching is required. It is necessary to accommodate various etch rate ratios that are present in different etching systems. In a stochastic CA algorithm [3], the probability of a cell being removed during a particular etch step is not only determined by the neighbor status but also by an assigned random number, Pe. At every etch step and for each cell, Pe will be compared with a prescribed threshold value, Pt, which corresponds to the true etch rate in a particular lattice axis. Specifically, if Pe is greater than Pt, a cell would be removed; if not, it would be retained within the lattice. For example, if the etch rate of {110} planes is 0.5 (normalized against the etch rate of fastest-etching {100} planes), Pt is set to 0.5. As a result, only half of cells on an exposed {110} surface may be removed after each discrete etching step.

The stochastic CA model therefore can handle arbitrary etch-rate ratios. However, it will result in roughened surfaces due to randomized cell removal from a otherwise smooth plane; such surface roughness can be regarded as noise in the simulation results. The stochastic CA model is mathematically convenient but physically incorrect. As the roughness increases, the accuracy of simulation is reduced. In order to achieve a desired spatial resolution of etching results, a much bigger cell set must be used which significantly increases the simulation time.

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II. A CONTINUOUS CA MODEL

We have developed a Continuous CA model to allow arbitrary etch-rate ratios to be incorporated in the etch simulation. A major advantage of the continuous CA model is that it does not generate artificially roughened surfaces and therefore causes no loss of resolution and accuracy. As a fundamental difference between this and other existing CA models (conventional or stochastic), each cell in the system could has non-discrete state variables, with their values ranging continuously between 0 and 1. One convenient non-discrete state of a cell is its thickness (denoted M). A cell can assume arbitrary states between M=0 ("removed") and M=1("un-etched"), corresponding to its extent of removal.

Arbitrary etch rates are incorporated using this new non-discrete state designation. During every etch step (with an associated time T), the dimension of a cell will be reduced by an amount that corresponds to the etch rate of the surface on which the cell resides. As an example, if the etch rate of {110} planes is 0.5 (normalized with respect to the fastest etch rate among all major low-index planes), the mass of cells on these surfaces will decrease by 0.5 in each step (with T being 1). If a cell is previously un-etched (i.e. mass equals 1), the value of its mass would be reduced to 0.5 from 1.0 in one etch step; should the etch continue, the mass would subsequently be reduced to 0 during the next step. In this case, one layer of cells on a {110} surface will be removed in two etch steps. The resultant etch rate is 0.5.

Here, we describe the rules for continuous cell removing in detail. Assuming that the desired etch rate on a particular crystal plane is $E_s \in [0,1]$, and the elapsed time of each etch step is T, then the number of etch steps (NT) that is required to completely remove a cell equals

$$N_T = \left\lceil \frac{M}{E_s T} \right\rceil^{\dagger} \qquad (1)$$

Note that the default value of *T* is 1. To derive the equivalent etch rate, we must consider two cases. If M is a multiple of E_sT, the equivalent etch rate of the surface, $E_s^{'}$, is

$$E_S^{'} = \frac{M}{N_T T} = \frac{M}{(\frac{M}{E_s T})T} = E_S \qquad (2)$$

On the other hand, if *M* is not a multiple of E_sT, then

$$E_S^{'} = \frac{M}{\left\lceil \frac{M}{E_s T} \right\rceil T} \neq E_S \qquad (3)$$

The reason of this mismatch is that when a cell is removed during an etch step *k*, the etching of the next cell will not begin immediately until the next etch step, *k+1* (Fig. 2a). We compensate the mismatch by introducing *time compensation* to the model. The time balance Tb_k of the etch step *k* will be compensated in step *k+1* for the etching of the next cell (Fig. 2b). Thus the time of a specific etch step *k*, T_k, is not always equal to *T*, rather, based on the thickness of the cell in step *k* (M_k), the compensation can be computed by the following formulas.

If $M_k \geq E_S(T + Tb_{k-1})$ then

$$T_k = T + Tb_{k-1} \qquad (4)$$

$$M_{k+1} = M_k - E_S T_k \qquad (5)$$

$$Tb_k = 0 \qquad (6)$$

else

$$T_k = \frac{M_k}{E_S} \qquad (7)$$

$$M_{k+1} = 0 \qquad (8)$$

$$Tb_k = T - T_k \qquad (9)$$

If current cell will be removed in an etch step *k* then formula (9) will be used to compute the time compensation, otherwise, time compensation is zero and formula (5) will be used to set the thickness of the cell for the next etch step. In conclusion, the introduction of time compensation results in $E_S^{'} = \frac{M_k}{T_k} = E_S$ for any etch step *k*.

III. DYNAMIC METHOD

In a static CA method, the program must process a large cubic set of crystal atoms, or cells, in parallel, all of them being evaluated in each simulation step. Even if some cells remains untouched throughout many etch steps (e.g. if the atom reside deep within the substrate bulk), they must nonetheless be considered in each etch step. Such an algorithm obviously wastes computing resources and increases the time of simulation.

To significantly decrease the memory requirement and increase the speed, we have developed a dynamic method. In the dynamic CA method, only atoms that stay at the interface of the silicon and the etchant are processed in relevant etch steps. These atoms exist in memory as a dynamic atom set, or a virtual surface, which contains active atoms and evolves from a masked plane to a final 3D shape. In each simulation step, every active atom will be processed with CA rules based on its neighbor statuses. When an active atom is to be removed from the virtual surface, the neighbors will become new active atoms and be inserted into the virtual surface. In our simulation, we have found that the dynamic method only requires 2MB memory for $200 \times 200 \times 120$ lattice points while static CA methods need 10MB.

The status of an active atom must be determined even though the neighbors of this active atom do not exist within the virtual surface, or have been removed in previous steps (Each atom may have four neighbors and four links to its neighbors.) We save neighbor

† $A = \lceil B \rceil$ means that A is the smallest integer that is not smaller than B.

information to the pre-allocated space for the four links of each atom. The information is not gathered passively by the atom itself, but changed actively by its neighbors. When an active atom is to be removed, it will inform its neighbors for the change of link status.

We have established new rules for predicting the evolvement of virtual surfaces and identifying the position of newly-inserted active atoms. The spatial coordinates of atoms are based on the lattice structure (Fig. 3). From the diamond crystal lattice (Fig. 1), we could obtain relevant properties of the lattice. First, there are two and only two types of atoms with different link-set types. Atoms are marked in black and white colors to identify different link-set types. Second, atoms with different link-set types are interconnected. All the neighbors of an atom with link-set type I are in link-set type II, or vice versa. Third, on a horizontal plane, atoms' link-set types are the same. Based on these properties, rules for the evolvement of virtual surfaces have been developed for a first time. Three rules, E1 through E3, are summarized in the following.

(E1) A virtual surface is started in a horizontal plane. Active atoms' locations and link-set types are set based on the orientation of the lattice.

(E2) When an active atom named A1 is going to be etched away based on CA rules, its neighbors will be added to the virtual surface if they are not in the surface. The neighbors' positions are calculated from A1's position and A1's link-set type.

(E3) In the virtual surface, a newly added active atom's link-set type is the opposite type of their neighbors'.

Rules E1 and E2 are both related to the lattice's orientation, including its top-surface orientation and edge alignment.

IV. PROGRAM IMPLEMENTATION

We have developed a first PC-based 3-D etch simulator named Anisotropic Crystalline Etch Simulation (ACES) using the continuous CA model and dynamic method. The program can simulate silicon etching with different front-surface orientation in various etchants, which exhibit different etch-rate ratios. It can receive 2-D mask designs in common graphics formats (including CIF, GDSII, GIF, and BMP), generate 3D profile in standard solid-modeling formats, and display results in integrated viewers based on OpenGL or VRML.

With the dynamic method, the simulation speed of ACES is very fast. A etch simulation with a 300 by 300 mask could proceed at the speed of one second per simulation step on a Pentium Pro 200 computer.

V. RESULTS AND DISCUSSIONS

5.1 Etch Rate Characteristics

We used two methods to obtain etch-rate diagrams under different etch-rate ratios. One method is to simulate the etching of a spoke pattern, which is a commonly used feature because it allows graphical representation of the etch-rate distribution. Figure 4a is a simulation result of spoke pattern etching. It matches well with the experiment result, shown in Fig. 4b. However, this method does not yield precise etch rates because the resolution of a lattice is limited. High-accuracy modeling require a large lattice.

A second method is much simpler to implement and offers a high precision. We etch a set of rectangular holes with 5 degrees increments in angular positions. The rectangles are 100-*mm* long and 1-*mm* wide. The shape of each hole changes during etching, but the orientation of a rectangular hole's long edges will not change for a long etch-time. So we could get the etch-rate of the orientation by measure undercuts of the long edges. Since a whole lattice is used to achieve a single etch rate, much more simulation steps could be applied to the lattice to get a big undercut and relatively precise etch rates could be obtained compared with the spoke-pattern etching. This method is not used in experiments because it is time consuming to etch and measure all the holes individually. With help of the ACES, these procedures could be finished quickly. Using the second method, etch rate diagrams for {100} silicon orientation (Fig. 5a) and {110} silicon orientation (Fig. 5b) have been obtained. They are matched with experimental diagrams well except high-index planes which are not implemented in this CA model.

5.2 Anisotropic and Isotropic Etching

The ACES program is capable of simulating both anisotropic etching and isotropic etching successfully. Anisotropically etched tips (Fig. 6a) have been obtained by using continuous CA model. It is well matched with the experiment result (Fig. 6b). The etch-ratio used in the simulation is {100}:{110}:{111} = 1:0.13:0. The continuous CA model can accommodate isotropic etchings successfully. In isotropic etching, the etch rate in all directions are identical. Result of an isotropic etching is shown in Fig. 7. Starting with a mask with a small aperture in the middle (Fig. 7a), a perfectly undercut hemisphere could be obtained (Fig. 7b).

5.3 Continuous CA model vs. Stochastic CA model

Etch results obtained using a stochastic CA model and a continuous CA model are presented in Fig. 8 to illustrate the different results. The simulation results of a square hole mask (Fig. 8a) with these two models when a designated etch-rate ratios of {100}:{110}:{111} = 1:0.8:0.05. The resulted {111} planes based on the continuous CA model is much smoother compared with that based on the stochastic CA model.

VI. CONCLUSIONS

A new continuous CA model and a dynamic method are presented. The continuous CA model greatly extended the capability of CA model. Implementation of a dynamic CA technique has resulted in increased simulation speed and reduced memory requirements. Obtaining etch-rate diagrams and doing isotropic etching validated the continuous CA model and the dynamic method for different orientations.

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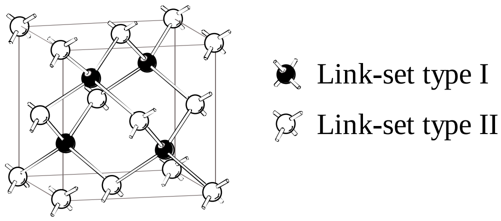


Fig. 1. Schematic diagram of a diamond crystal lattice.

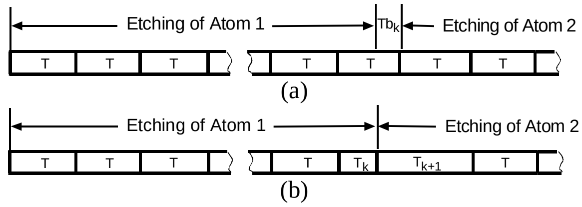


Fig. 2. Simulation process (a) without time compensation; (b) with time compensation

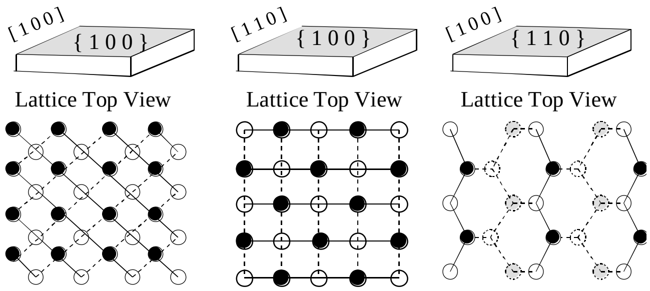
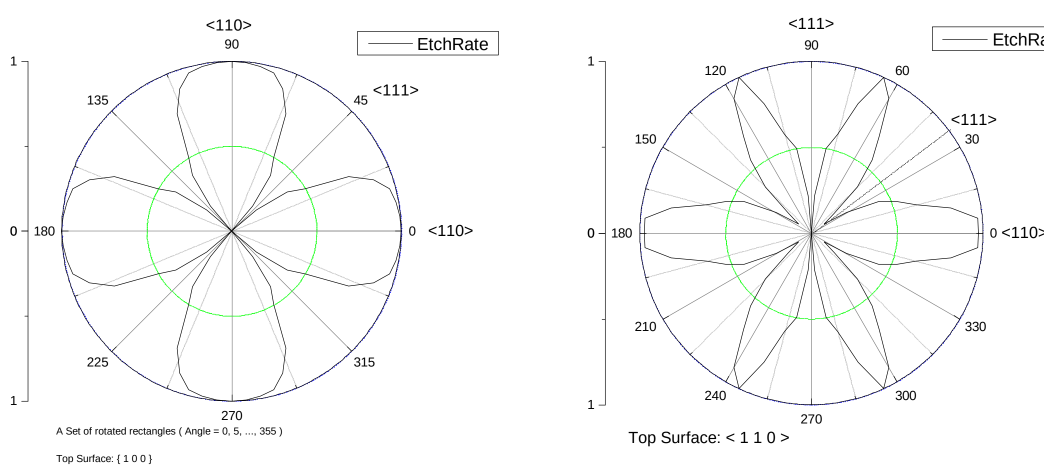


Fig. 3: Top views of models in different orientations. Black spheres and white ones represent atoms with different link-set types.

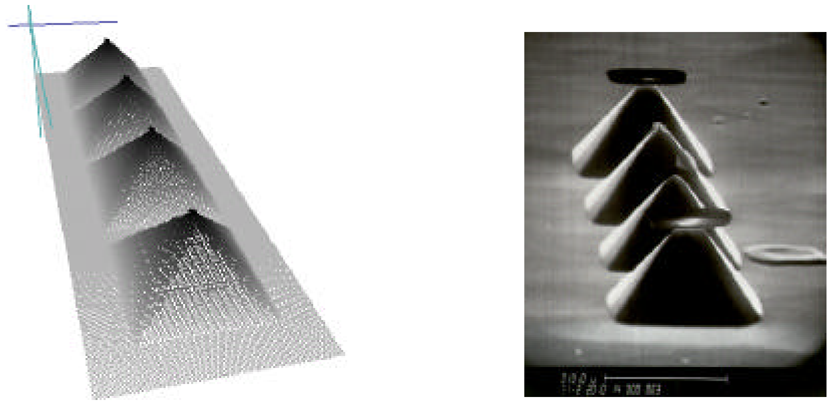
(a) (b)

Fig. 4. Comparison of simulation and etching results using a spoke pattern. (a) simulation; (b) experiments.



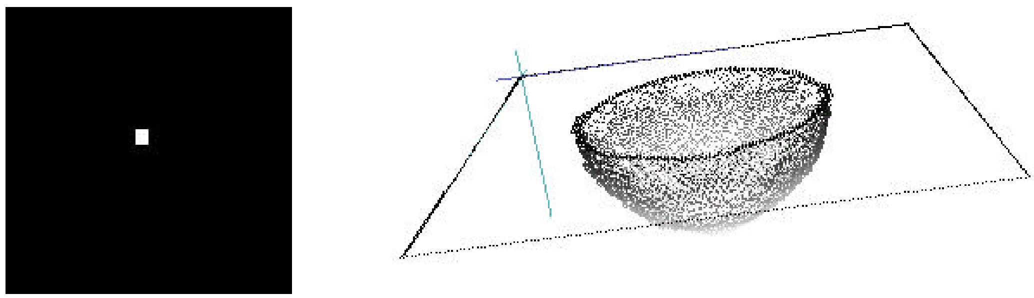
(a) (b)

Fig. 5. Calibrated etch-rate distribution. (a) when the substrate front surface is {1 0 0}; (b) with the substrate front surface being {1 1 0}.



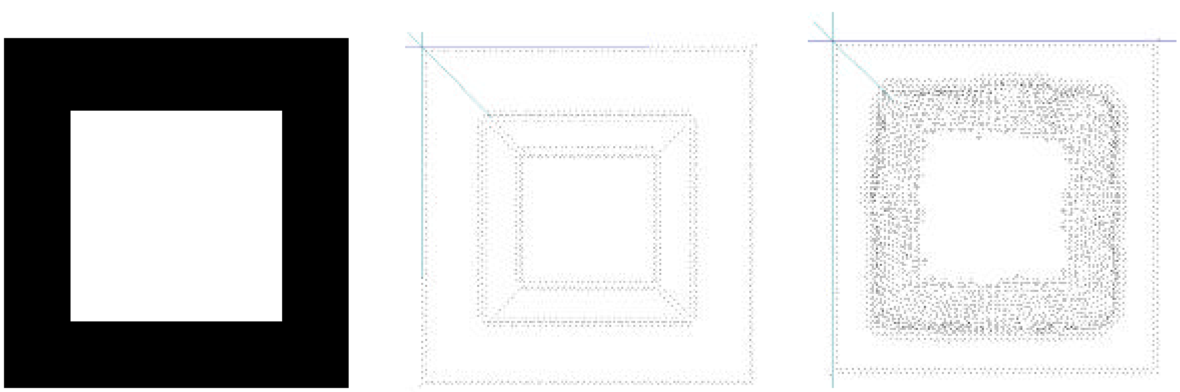
(a) Simulation result (b) Experiment result

Fig. 6. Comparison of simulation and experimental results for an anisotropically etched tip array.



(a) (b)

Fig. 7. Simulation of isotropic etching using the Continuous CA model (etch-rate ratios {100}:{110}:{111} = 1 : 1 : 1). (a) mask shape; (b) etch results.



(a) (b) (c)

Fig. 8. Different simulation results with the continuous CA model and the stochastic CA model. (a) mask; (b) etch results (top view) generated by continuous CA model; (c) results by stochastic CA model. Sidewalls are much more smooth in (b)