

Application of the level set method in three-dimensional simulations of the profile evolution

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ABSTRACT

In this paper, the angular dependence of the etching rate is applied in the three-dimensional simulations of the profile evolution during etching process. Etching rates are determined from the silicon symmetry properties by the interpolation technique using experimentally obtained values. The influence of the KOH concentration on the etch rate is also discussed. As the etchant concentration increases the etching rate decreases, while increasing etching temperature resulted in increased etching rate. Three-dimensional simulation results were obtained using an extension of the sparse field method for solving level set equations that describe the time evolution of the surface during etching process. The obtained simulation results illustrate that relatively simple model with only four parameters describes convex corner undercutting correctly.

Keywords: Chemical etching, silicon, etchants, crystal, solution

1. INTRODUCTION

Etch processes that are widely used in microfabrication are: wet etching where the material is dissolved when immersed in a chemical solution and dry etching where the material is sputtered or dissolved using reactive ions or a vapor phase etchant (see Fig. 1.) [1-5]. Plasma etching is a complex process involving several elementary processes or mechanisms: chemical etching, ion induced or enhanced etching, physical etching, trenching, sidewall passivation and mask erosion. Anisotropic plasma etching has two major components: chemical etching (neutrals and radicals of the plasma) and physical bombardment (ion assisted etching reactions). Wet etching is an etching process that utilizes liquid chemicals or etchants to remove materials from the wafer, usually in specific patterns defined by photoresist masks on the wafer. It is one of the most popular etch process due to some advantages such as low cost, reliability, high throughput and excellent selectivity.

In the isotropic etching, etch rate is the same in all directions, lateral etch rate is about the same as vertical etch rate and etch rate does not depend upon the orientation of the mask edge [6,7]. On the other hand, in the anisotropic etching, etch rate strongly depends on the orientation to crystalline planes and orientation of mask edge and the details of the mask pattern determine the final etched shape.

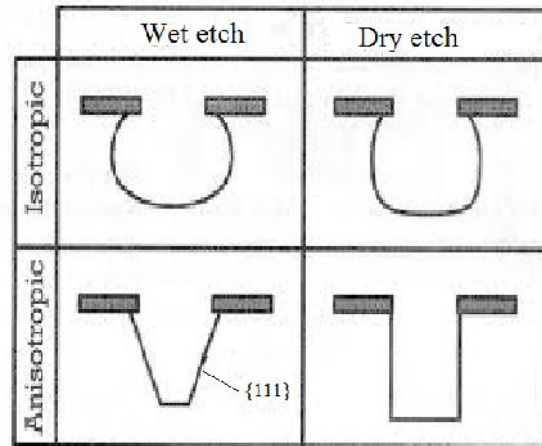


Fig. 1. Etching rate model regions used in our 3D simulations.

The major industrial problems on which modeling may have an impact contain decreasing the time and cost of developing new modelling tools (shortening the time to market), improving the efficiency of optimizing tool performance to meet changing process objectives, and helping to implement real-time process control into operating tools. The potential for using modeling and simulation to benefit industrial users of plasma processes and equipment has never been greater. On the other hand, computational costs continue to decrease steadily, and in the last several years, considerable progress has been achieved in establishing the major modeling strategies that are necessary to achieve practical industrial objectives. Simulation codes, especially for three-dimensional simulation are routinely applied in semiconductor industry for predicting various characteristics such as etch rate [8,9].

In this paper we describe and discuss the application of the experimentally determined etching rates in obtaining three dimensional (3D) etching profile evolution during anisotropic wet etching of silicon with KOH etchant. Simulation results were achieved by using our simulation package (previously well documented in numerous publication [9,10]) based on the level set method for the 3D simulation of the etching profile. Even simple model embedded in our simulation package can be applied for modeling the convex corner undercutting.

2. ANISOTROPIC ETCHING OF SILICON

In semiconductor fabrication, in etching, a high degree of anisotropy is required because it results in adequate copy of the mask pattern, since only the material not directly under the mask are attacked by the etchant. On the other hand, isotropic etchants can etch away even the portion of material that's directly under the mask (usually in the shape of a quarter-circle), since its horizontal etching rate is the same as its vertical rate.

Anisotropic etching involves different etch rates in different directions. One of the example is the $\langle 111 \rangle$ crystal plane sidewalls that appear when etching a hole in $\langle 100 \rangle$ silicon wafer in a chemical such as potassium hydroxide (KOH). Very complicated three-dimensional

structures can be formed by using this technique. In order to perform realistic simulation of the time evolution of three dimensional etching profiles it is crucial to find exact etch rates in all directions. Since the etching rates for only a few principal axes are known, they can be used to determine rate value in an arbitrary direction $\mathbf{N}$ (N_x, N_y, N_z) by an interpolation procedure. We suppose that N_x, N_y and N_z axes are aligned with $\langle 100 \rangle$, $\langle 010 \rangle$ and $\langle 001 \rangle$ crystal directions, respectively. In our calculations we made use of measured etching rates in $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$ crystal directions, for 30% KOH concentration at 70°C taken from ref. [6] ($R_{100} = 0.797 \mu\text{m}/\text{min}$; $R_{110} = 1.455 \mu\text{m}/\text{min}$; $R_{111} = 0.005 \mu\text{m}/\text{min}$).

The point group of silicon's symmetry $m\bar{3}m$ (subgroup of $Fd\bar{3}m$ space group) contains 48 elements. Since it is very difficult or even impossible to assemble angular section using 3 principal directions with which the whole space can be covered by the symmetry operations.

In three-dimensional simulations, three independent vectors are needed to define a basis. In our case, three sections are defined by the principal vectors $A[100, 111, 110]$, $B[100, 111, 101]$ and $C[001, 111, 101]$, as depicted in Fig. 2.

The etching rate R in an arbitrary direction defined by vector $\mathbf{N}$ is given by an interpolation relation (derivation in details can be found in [10]):

$$R(\mathbf{N}) = \begin{cases} \left[R_{100}(N_x - N_y) + R_{110}(N_y - N_z) + R_{111}N_z \right] / N_x; & \mathbf{N} \in A \\ \left[R_{100}(N_x - N_z) + R_{110}(N_z - N_y) + R_{111}N_y \right] / N_x; & \mathbf{N} \in B \\ \left[R_{100}(N_z - N_x) + R_{110}(N_x - N_y) + R_{111}N_y \right] / N_z; & \mathbf{N} \in C \end{cases} \quad (1)$$

Etching rate angular dependence can be obtained by introducing spherical angular coordinates ϕ and θ instead of Cartesian (N_x, N_y, N_z) in accordance with:
 $N_x = \sin \theta \cos \phi$; $N_y = \sin \theta \sin \phi$; $N_z = \cos \theta$

The angular dependence of the etching rate $R(\theta, \phi)$ can be written in the form and shown in Figure 3.:

$$R(\theta, \phi) = \begin{cases} R_{100} - (R_{110} - R_{111}) \cot \theta / \cos \phi + (R_{110} - R_{100}) \tan \phi; & (\theta, \phi) \in A \\ R_{100} + (R_{110} - R_{100}) \cot \theta / \cos \phi + (R_{111} - R_{110}) \tan \phi; & (\theta, \phi) \in B \\ R_{100} + [(R_{110} - R_{100}) \cos \phi + (R_{110} - R_{100}) \sin \phi] \tan \theta; & (\theta, \phi) \in C \end{cases} \quad (2)$$

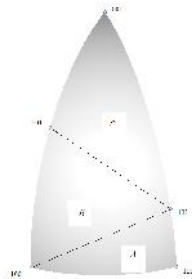


Fig. 2. Model of three interpolation regions used in our 3D simulations.

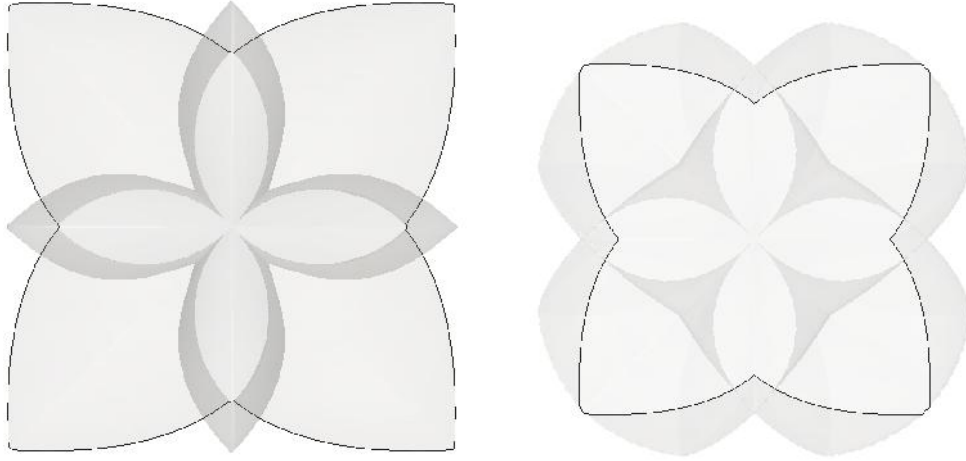


Fig. 3. The angular dependence of the etching rate.

Figure 3 illustrates etching rate in the full angular extent. The presence of cusps in the etching rates reveals the existence of facets in the etching profiles.

3. RESULTS AND DISCUSSION

Figure 4 displays the temperature dependence of the etch rates for various KOH solution concentrations: 20% (open circles), 40% (solid squares), 50% (open triangles) and 60 % (solid circles). It was found that addition of KOH solutions leads to decreasing of the etch rate by approximately 20%. On the other hand, the etch rate increases with increasing the temperature.

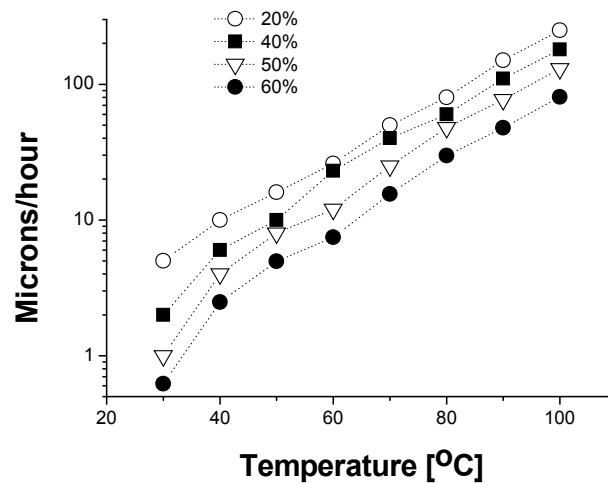


Fig. 4. Dependences of the etch rate on the temperature (expressed in °C) and concentration of the KOH solution.

Values of the etch rates shown in Figures 4 are implemented in simulation package [9, 10] and three-dimensional simulations of the time evolution of the initial square shape object are shown in Figure 5. Initial aperture is aligned to $\langle 110 \rangle$ directions. Convex corner undercutting can be observed. Although, proper modeling of the convex corner undercutting requires inclusion of a great number of high order planes, our results clearly demonstrate that even relatively simple model with only four parameters describes it correctly.

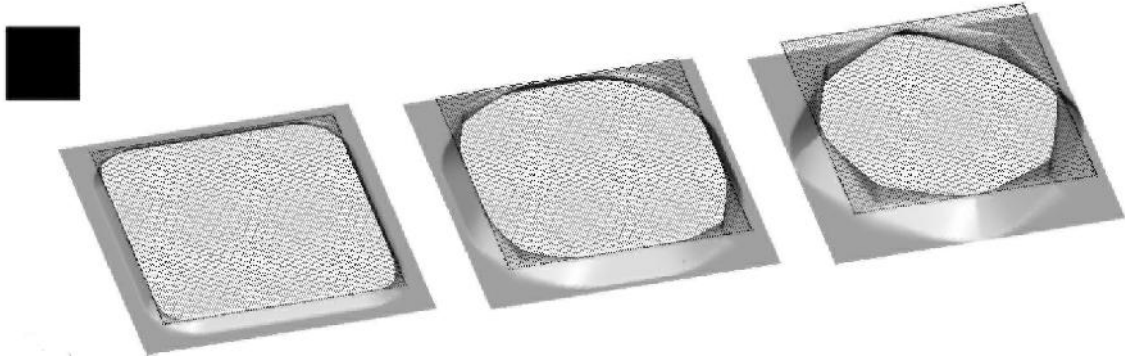


Fig. 5. The time evolution of the simplest square form during equidistant time moments

4. CONCLUSION

In this paper the influence of the temperature as well as concentration of the KOH solution on the etch rates are presented and discussed. Results showed that increasing etchant concentration caused reduction in the etching rate while increasing etching temperature resulted in increased etching rate. The analysis of the obtained results allow us to use them in the three-simulations of the profile time evolution during etching process. Results presented here indicate that the sparse field level set method can be used as an effective tool for wet etching process modeling, and that it is a viable alternative to the cellular automata method, which is today widely used in for that purpose.

"Authors have declared that no competing interests exist."

AUTHORS' CONTRIBUTIONS

M. Radmilović-Radjenović and M. Radjenović performed calculations and the analysis of the results, wrote the protocol and wrote the first draft of the manuscript. All authors read and approved the final manuscript.

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