

The role of the etching rates in three-dimensional simulations of the profile evolution

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ABSTRACT

In this paper, angular dependence of the etching rate is calculated on the base of the silicon symmetry properties, by means of the interpolation technique using experimentally obtained values of the principal $\langle 100 \rangle$, $\langle 110 \rangle$, $\langle 111 \rangle$ directions in KOH solutions. The influence of the KOH concentration on the etch rate is also considered. The calculations are performed using an extension of the sparse field method for solving three dimensional (3D) level set equations that describe the time evolution of the surface during etching process. The analysis of the simulation results in the case of the simplest isometric form confirm that regardless of the initial shape the profile evolution ends with the crystal form composed of the fastest etching planes, $\{110\}$ in our model.

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

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1. INTRODUCTION

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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]. 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.

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In etching process etching rates need to be carefully monitored and controlled since an inadequate etch or an excess etch would lead to insufficient removal or the excess removal of a desired layer causing an undesired electrically open or short circuit connections [6,7]. In 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. In contrast to Isotropic etching, in Anisotropic etching, etch rate depends upon orientation to crystalline planes, lateral etch rate can be much larger or smaller than vertical etch rate, depending upon orientation of mask edge to crystalline axes and orientation of mask edge and the details of the mask pattern determine the final etched shape.

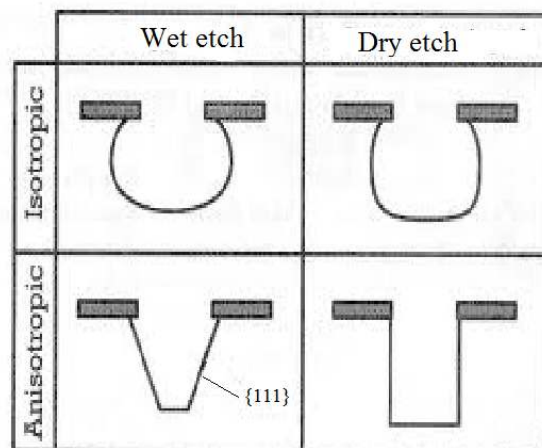


Fig. 1. Etching rate model regions used in our 3D simulations.

In recent days, simulation techniques have blossomed into very effective tools that complement laboratory experiments and analytic models [8, 9]. Simulation codes, especially for three-dimensional simulation are routinely applied in semiconductor industry for predicting various characteristics such as etch rate.

In this paper we discuss the application of the etching rates in obtaining three dimensional (3D) etching profile evolution during anisotropic wet etching of silicon with KOH etchant. Only etching rates along principal directions ($\langle 100 \rangle$, $\langle 110 \rangle$, $\langle 111 \rangle$) of silicon have been considered. Simulation results were achieved by using our simulation package (well documented in previous publication [14]) based on the level set method for the 3D simulation of the etching profile.

2. ANISOTROPIC ETCHING OF SILICON

In semiconductor fabrication, in etching, a high degree of anisotropy is required because it results in a more 'faithful' 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 includes different etch rates in different directions in the material. The classic example of this is the $\langle 111 \rangle$ crystal plane sidewalls that appear when etching a hole in a $\langle 100 \rangle$ silicon wafer in a chemical such as potassium hydroxide (KOH). Very complicated three-dimensional structures can be generated by using this technique. In order to perform realistic simulation of the time evolution of three dimensional etching profiles it is essential 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 actual 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] ($R_{100} = 0.797 \mu\text{m}/\text{min}$; $R_{110} = 1.455 \mu\text{m}/\text{min}$; $R_{111} = 0.005 \mu\text{m}/\text{min}$).

69 The point group of silicon's symmetry $m\bar{3}m$ (subgroup of $Fd\bar{3}m$ space group) contains 48
 70 elements. Since it is very difficult or even impossible to assemble angular section using 3
 71 principal directions with which the whole space can be covered by the symmetry operations,
 72 only 16 out of 48 symmetry elements can be used, i.e. it is necessary to observe only at
 73 1/16th of the full angular extent, that is actually the union of three sections defined by the
 74 principal vectors $A[100, 111, 110]$, $B[100, 111, 101]$ and $C[001, 111, 101]$, as depicted in Fig.
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 77 The etching rate R in an arbitrary direction defined by vector $\mathbf{N}$ is given by an interpolation relation
 78 (derivation in details can be found in [10]):
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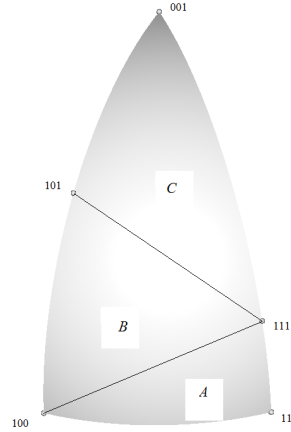
$$80 \quad R(\mathbf{N}) = \begin{cases} \left[R_{100}(N_x - N_y) + R_{110}(N_y - N_z) + R_{111}N_z \right] / N_x; & \mathbf{N} \in A \\ \left[R_{100}(N_x - N_z) + R_{110}(N_z - N_y) + R_{111}N_y \right] / N_x; & \mathbf{N} \in B. \\ \left[R_{100}(N_z - N_x) + R_{110}(N_x - N_y) + R_{111}N_y \right] / N_z; & \mathbf{N} \in C \end{cases} \quad (1)$$

81
 82 Etching rate angular dependence can be obtained by introducing spherical angular coordinates ϕ and
 83 θ instead of Cartesian (N_x, N_y, N_z) in accordance with:
 84 $N_x = \sin \theta \cos \phi$; $N_y = \sin \theta \sin \phi$; $N_z = \cos \theta$

85 The angular dependence of the etching rate $R(\theta, \phi)$ can be written in the form and shown
 86 in Fig. 3.:
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$$88 \quad R(\theta, \phi) = \begin{cases} R_{100} - (R_{110} - R_{111}) \cot \theta / \cos \phi + (R_{110} - R_{100}) \tan \phi; & (\theta, \phi) \in A \\ R_{100} + (R_{110} - R_{100}) \cot \theta / \cos \phi + (R_{111} - R_{110}) \tan \phi; & (\theta, \phi) \in B, \\ R_{100} + [(R_{110} - R_{100}) \cos \phi + (R_{110} - R_{100}) \sin \phi] \tan \theta; & (\theta, \phi) \in C \end{cases} \quad (2)$$

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91 **Fig. 2. Etching rate model regions used in our 3D simulations.**

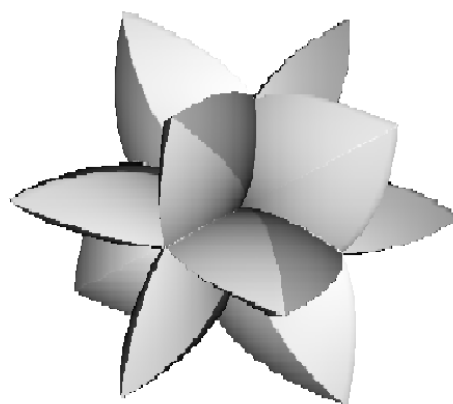


Fig. 3. The angular dependence of the etching rate.

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%.

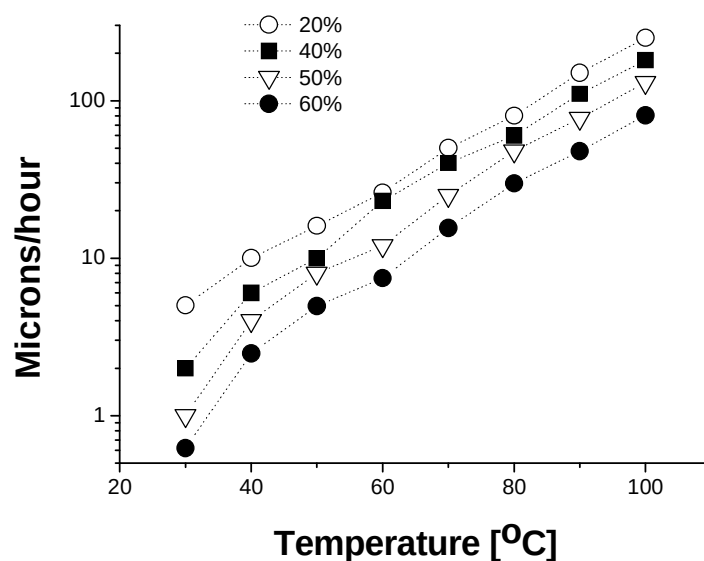


Fig. 4. Dependences of the etch rate on the temperature (expressed in °C) and concentration of the KOH solution.

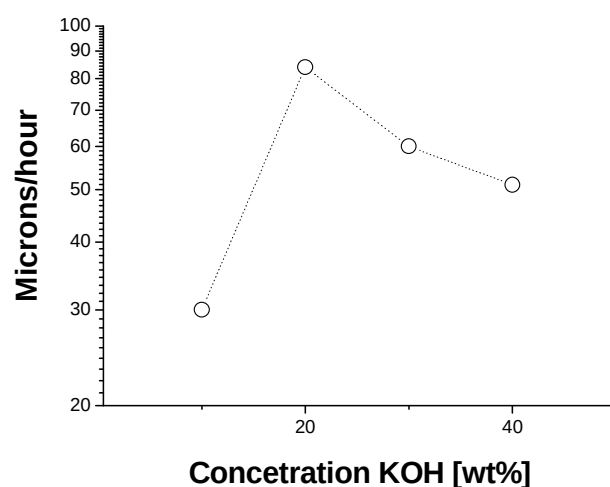


Fig.5. The etch rate versus the KOH concentration at 80°C.

The variation of the etch rate with KOH concentration at the temperature of 80°C are given in Figure 5. Values of the etch rates shown in Figures 4 and 5 are implemented in simulation package [9, 10] and three-dimensional simulations of the time evolution of the initial cube shape made of {100} planes are performed and shown in Figure 6. As can be observed, the initial cube shape gradually transforms to the final (rhombic) dodecahedron made of the fastest etching {110} principal planes, through the combinations of these shapes.

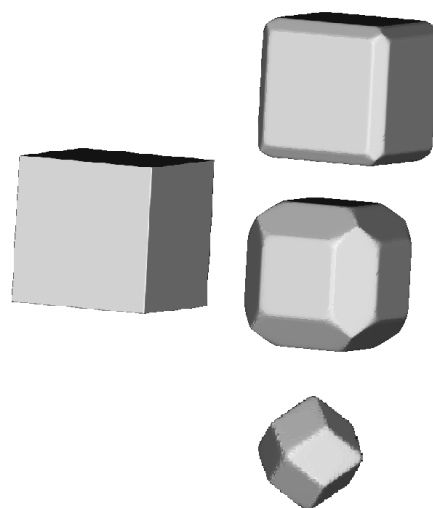


Fig. 6. Changes of the simplest isometric form i.e. cube form are shown for equidistant time moments

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. The analysis of the obtained results allow us to use them in the three-simulations of the time evolution of the cube as a simplest isometric form. It was found that that regardless of the initial shape the profile evolution ends with the crystal form composed of the fastest etching planes, {110} in our model. 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.

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