

Application of the level set method in three-dimensional simulations of the etching profile evolution for producing nano-scale devices

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Refined control of etched profiles represents one of the most important tasks of manufacturing process. This paper contains the results of the three dimensional (3D) modeling and simulation of the profile evolution during plasma etching as well as anisotropic wet etching of silicon based on the level set method. In the case of isotropic and anisotropic plasma etching, the type of the etch process is defined by the velocity function. For the anisotropic wet etching, however, etching rate function is determined from the silicon symmetry properties, by means of the interpolation technique using experimentally obtained values of the principal [100], [110], [111], and high index [311] directions in KOH solutions. Presented results confirm that the level set method can be used as an effective tool for etching process modeling.

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1. Introduction

In semiconductor technology isotropic etching is non-directional removal of material from a substrate via a chemical process using an etchant substance which may be a corrosive liquid or a chemically active ionized gas, known as a plasma. On the other hand, anisotropic etching can be regarded as a non-isotropic etching. The most important commercial application of anisotropic etching is in semiconductor chip processing, where photolithography is used to print resist lines on silicon wafers [1]-[3].

The potential for using modeling and simulation to benefit industrial users of plasma processes and equipment has never been greater. Plasmas are used in about 30% of all semiconductor manufacturing processing steps, and about the same fraction of processing equipment is plasma-based in a typical microelectronics fabrication facility. Furthermore, 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. Nevertheless, low-temperature plasma processing science is a relatively young field, and has not therefore received the in-depth, sustained attention that is required to have a significant, timely impact in industry. This situation is perhaps most evident in the area of the database for physical and chemical processes in plasma materials processing.

A major complication in this process is the fact that industry uses a large variety of gases and materials in plasma processes and equipment. Since time and resources are always limited, experiments are expensive and time-consuming, and therefore it may be necessary to augment these measurements of fundamental data with theory. Computational techniques are useful, but may require

careful testing since the methodologies are sometimes not fully mature.

Level set method, introduced by Osher and Sethian [4,5], is a highly robust and accurate computational technique for tracking of moving interfaces in etching, deposition and photolithography processes. It originates from the idea to view the moving front as a particular level set of a higher dimensional function, so the topological merging and breaking, sharp gradients and cusps can form naturally, and the effects of curvature can be easily incorporated. The level sets are used in image processing, computer vision, computational fluid dynamics, material science, and many other fields. Detailed exposition of the theoretical and numerical aspects of the method, and applications to different areas can be found in references [4] and [5]. During last several years several variants of level set methods have been developed with application to microelectronic devices fabrication problems. The profile surface evolution in etching, deposition and lithography development is a significant challenge for implementation of numerical methods in front tracking.

In this paper we have demonstrated the application of the level set method in three-dimensional (3D) profile evolution during completely different etching mechanism: plasma etching and wet etching [6, 7]. The obtained simulation results indicate that the level set method can be used for the modelling the morphological evolution of the surface induced both by plasma and wet etch processes.

2. Level set method

The level set method represents a numerical technique for tracking interfaces and shapes representing a surface using an auxiliary function $\varphi(t, \mathbf{x})$ at a certain time t , called the level set function [12, 13]. The initial surface is

represented as the zero level set of the function $\varphi(t, \mathbf{x})$ by $\{\mathbf{x} \mid \varphi(t, \mathbf{x}) = 0\}$ and its time evolution is caused by the surface processes in the case of the etching. If the surface moves in the normal direction with velocity $R(t, \mathbf{x})$, then unknown function $\varphi(t, \mathbf{x})$ can be determined by solving a Hamilton-Jacoby equation [4, 5]:

$$\frac{\partial \varphi}{\partial t} + R(t, \mathbf{x}) |\nabla \varphi| = 0, \quad (1)$$

where Hamiltonian function is given by $H = R(t, \mathbf{x}) |\nabla \varphi(t, \mathbf{x})|$ and where $\varphi(0, \mathbf{x}) = 0$ determines the initial surface. Having solved this equation the zero level set of the solution is the sought surface at all later times. In order to apply the level set method a suitable initial function $\varphi(0, \mathbf{x})$ has to be defined first. The natural choice for the initialization is the signed distance function of a point from the given surface.

The numerical solution of the level set equation (1), however, requires sophisticated techniques. Several approaches for solving level set equations exist which increase accuracy while decreasing computational effort. Simple finite difference methods fail quickly. Upwinding methods, such as the Godunov method, fare better; however the level set method does not guarantee the conservation of the volume and the shape of the level set in an advection field that does conserve the shape and size, for example uniform or rotational velocity field. Instead, the shape of the level set may get severely distorted and the level set may vanish over several time steps. For this reason, high-order finite difference schemes are generally required, such as high-order essentially non-oscillatory (ENO) schemes, and even then, the feasibility of long-time simulations is questionable.

In our calculations the sparse-filed method has been utilized employing an approximation for the distance function that makes it feasible to recompute the neighborhood of the zero level set at each time step. In that way, it takes the narrow band strategy to the extreme. During these processes the etching rate, that defines the surface velocity function $R(t, \mathbf{x})$, depends on the geometric characteristics of the profile surface itself. The type of the etch process in simulation is defined by the velocity function¹¹. In the case of the isotropic etching the dependence of the surface velocity on the incident angle is described by an expression: $R = R_0$ (isotropic in all directions). Although it is the simplest form of angular dependence, it describes the isotropic etching process correctly. The velocity functions $R = R_0 \cos \theta$ corresponds to the anisotropic etching, where θ represents the angle between surface normal and the direction of the incoming particle.

3. Results

Since the velocity during the isotropic etching is equal in all directions, the profile evolution may result in undercutting as depicted in Fig. 1. In most cases, the desired etch profile is square shaped. To obtain this perfect

profile, etch and passivation have to be carefully balanced and if need reajusted as the aspect ratio of the structure increase. etch ratio of the structure increase.

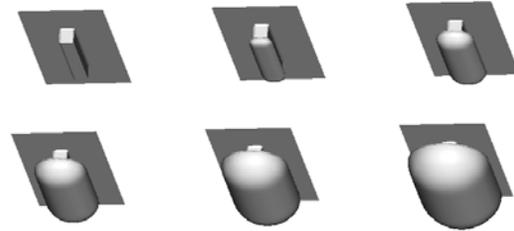


Fig. 1. Isotropic etching – Feature profiles for $R = R_0$ at six equidistant (reduced) etching time moments.



Fig. 2. Anisotropic etching - Feature profiles for $R = R_0 \cos \theta$ at six equidistant (reduced) etching time moments.

The time evolution of the etching profile, when etching rate is proportional to $\cos \theta$ is presented in Fig. 2. This is the simplest form of angular dependence, but it describes the ion enhanced plasma etching process correctly [8]. In this case we expect that the horizontal surfaces move downward, while the vertical ones stay still. This figure shows that it with optimal amount of smoothing gives minimal rounding of sharp corners, while preserving the numerical stability of the calculations. Actually, this is one of the most delicate problems in the etching profile simulations.



Fig. 3. Etching through a square mask in $\{100\}$ plane aligned to $\langle 100 \rangle$ directions. Profiles at six equidistant (reduced) time moments.

In the case of wet etching, potassium hydroxide (KOH) represents the most common and the most important chemical etchant, because of its excellent repeatability and uniformity in fabrication, and its low production cost. In actual calculations we made use of measured [9, 10] etching rates in [100], [110], [111] and [311] crystal directions, for 30% KOH concentration at 70 °C ($R_{111} = 0.005 \mu\text{m}/\text{min}$, $R_{100} = 0.797 \mu\text{m}/\text{min}$, $R_{110} = 1.455 \mu\text{m}/\text{min}$ and $R_{311} = 1.436 \mu\text{m}/\text{min}$).

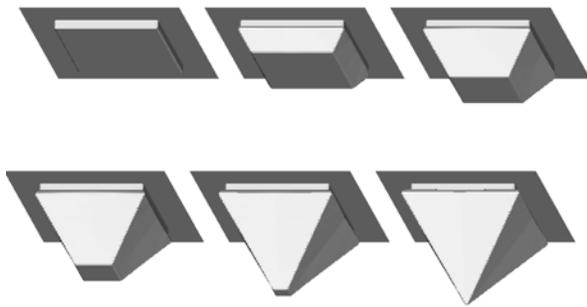


Fig. 4. Etching through a square mask in $\{100\}$ plane aligned to $\langle 110 \rangle$ directions. Profiles at six equidistant (reduced) time moments.

The first example is etching through a square openings in the $\{100\}$ silicon plane with edges aligned to $\langle 100 \rangle$ and $\langle 110 \rangle$ directions. The time evolution of the etched profiles is shown in Fig. 3 and 4, respectively. Formation of the V-shaped cavities consisting of only $\{111\}$ planes is reproduced correctly in accordance with the expectations.

4. Conclusion

In this paper the three dimensional simulations based on the level set method have been performed in order to study the influence of the different etch process on the profile evolution. The obtained simulation results demonstrate profile evolution during completely different process such as plasma etching and wet etching of silicon. Having in mind the the most significant application of chemical etch process, the obtained simulation result for the isotropic etching can be useful in advanced logic device manufacturing is the so called resist trim process.

On the other hand, in the case of wet etching, etching rate angular dependence is calculated on the base of the silicon symmetry properties, by means of the interpolation technique using experimentally obtained values of the principal [100], [110], [111], and high index [311] directions in KOH solutions. The calculations are performed using an extension of the sparse field method for solving three dimensional (3D) level set equations in the case of non-convex Hamiltonians. It is shown that regardless of the initial shape the profile evolution ends with the crystal form composed of the fastest etching planes, $\{110\}$ in our model. The obtained results show that level set method can be used as an effective tool for plasma as well as wet etching process modelling, and that is a viable alternative to the Cellular Automata method which now prevails in the simulations of the wet etching process.

Acknowledgements

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