THE STUDY OF SELF-LIMITED STATE PROFILE AND LEVEL SET SIMULATION OF ANISOTROPIC WET ETCHING ON QUARTZ

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ABSTRACT

This paper reports that the stable self-limited profile can be characterized by the inflection points on etch rate curve of crystal orientation zone from the etched hemisphere experiment, which is different from the method based on searching local minimal and maximal etch rates on cross section plane in previous study. A recognition process is developed to obtain inflection points from the hemisphere experiment, combining with the 3D level set model, the approach allows a quickly locating all the possible self-limited etch planes, arriving at a close approximation to the desired structures, for instance the high aspect ratio and vertical side wall micro structures. Comparing with experiments, it successfully predicts complex facets on micro needle array and other micro structures etched on quartz wafers with good calculation accuracy.

INTRODUCTION

As a trigonal crystal system, a large proportion of quartz orientations have very slow etch rates in anisotropic wet etching. Different angle alignment of mask pattern creates different self-limited state profile. So that there are much more choices of stable structure planes for quartz than silicon in wet etching process. Understanding the principles of self-limited state profiles will help to design high density mask patterns, desired inclination of trench side walls and better mask alignment for double side etching [1, 2]. In practice, silicon crystal only have few stable planes with very low etch rate such as {111} orientation, and in general an arbitrary shaped mask opening on Si{100} wafer will lead to a square or rectangular V-groove comprising of {111} planes. But for quartz etching there are far more stable structure plane choices than silicon. The wide distribution of low etch rate orientations brings difficulty to predict the etching result in current simulator. As figure1 shows, both side walls and the bottom of the simulation results deviate from the experiment.

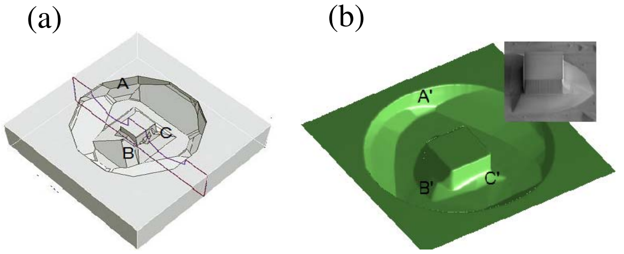

Figure 1: (a) the simulation result of a circular shape with mesa inside by Wulff-Jaccodine method [4]; area A, B and C have deviation from the experiment (b) and the proposed level set model in this paper;

On the other hand, since the etch rate of ICP in quartz etching is much lower than rate of silicon, especially in double side etching with a thickness dimension over hundreds microns, wet etching is still an efficient process. For the trigonal crystal system, an efficient and accurate 3D simulation model will benefit the mask design, optimize process parameters and understand the anisotropy of complex crystal system in wet etching [3, 4]. Understanding the principles of stable transitional and self-limited profiles during quartz etching can help to arrive at a better starting point for mask design.

EXPERIMENT

A single-crystal quartz hemisphere with the diameter of 42mm, as shown in Figure 2(b), is fixed on a special fixture for wet etching. After etching the spherical specimen of alpha-quartz, the surface profile is probed every 2° in angle. The distribution of etch rates shows the trigonal symmetry of the quartz crystal, with maximum values at the center and the corners of the highlighted triangle. Then we select a 4" wafer. After Cr/Au film is deposited etching is carried out in NH4HF2 saturated solution. Complex mesas, cavities and micro needles structures are fabricated on Z cut quartz wafer. A set of groove structures with mask alignment angle θ (0° to 60° with an interval of 5°) in figure 2(a) is etched to identify stable etching profiles. The etch rate of the crystal zone for each alignment angle on the hemisphere experiment data shown in figure 2(b).

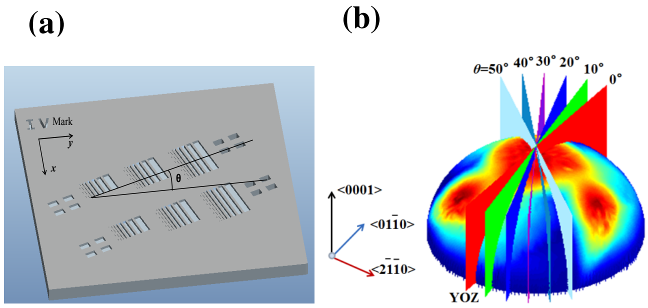

Figure.2 (a) mask with different width for trench structures and definition of the mask pattern alignment angle θ on basis of Y axis; (b) Contour map of etch rate of crystal graphic orientation with etch rate curve planes for mask pattern alignment angle θ;

As figure 3 shows, there are usually 6 typical stable structure planes appearing on the side walls of trench structures etched on Z-cut quartz wafer. Since the crystal plane along the equator of hemisphere has very low etch rate, the etched trench always get vertical *p1* and *p1'* plane. From figure 3, in case that θ is 10 degree the inflection points on etch rate curve is 85.1, 33.5, 89, and 31.6 respectively, which is identical to the inclination angle of structure planes from the experimental result. The measurement of structural planes for all the mask edge alignment from 0 to 60° agrees well with angle values of inflection points. It is observed that usually etch rate and inclination angle of *p2* and *p2'* control the final profile in etching z cut quartz crystal. Different angle of the mask alignment get different stable transitional profiles. Our research shows that the experiment results of trench etching with all θ rotations exhibits that inflection points of etch rate curve lead to the structural planes. By exploring the etch rate curve for mask alignment angle θ in 10°,20°,40°,50° in figure 3, orientations as the inflection points on etch rate curve with high etch rates create stable transitional profile, while inflection points on etch rate curve with low etch rate build self-limited profile. We can draw the conclusion that instead of searching the minimum value of undercutting rate by Wulff-Jaccodine construction method to determine surfaces on micro structures during etching in simulation, the detection of inflection points is an alternatively efficient and rapid way to estimate the stable transitional profiles.

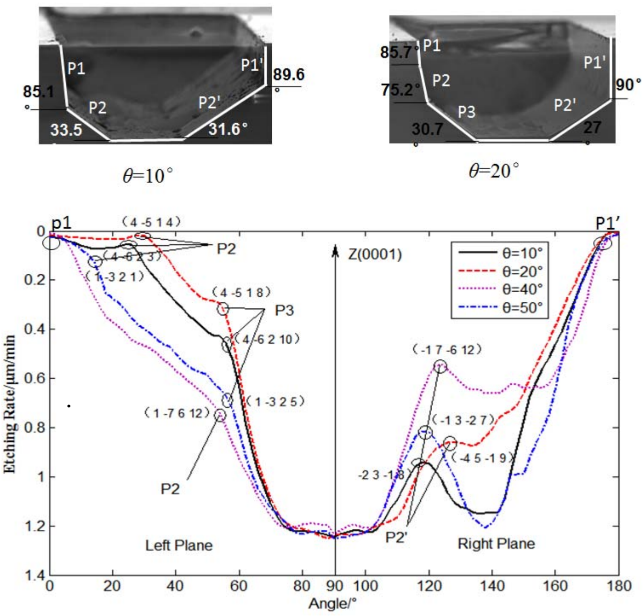

Figure 3: inflection points from etch rate curve of crystal orientation zone with θ in 10°, 20°, 40°, 50° degrees from hemisphere experiment and etch profiles (p1-p3, p1'-p3') from the cross sections of etched trench structures;

INFLECTION POINTS RECOGNITION

Considering the fact that the inflection points on etch rate curve of crystal orientation zone can characterize the structures in quartz etching, The method to recognize all the inflection points from hemi sphere experiment data is developed. Firstly in order to avoid the fluctuation between adjacent points, a smooth optimization process of moving average filter is applied to remove the data noise. Figure 4 shows the comparison of original experimental date of 10 degree rotations crystal orientation zone and the smoothed etch rate curve. By second order difference method processing as equation 1 to the smoothed data, the turning abrupt change of etch rate curve can be clearly identified.

$$\frac{\Delta^2 R}{\Delta^2 x} = \frac{R(i+1)+R(i-1)-2R(i)}{h^2} \quad (1)$$

Where R is the etch rate, x is the angle of crystal zone orientation to XOY plane, h is the step size, h=5; i is the index of the experimental data.

Next, the second order differential curve is fitted and expressed by a polynomial function according to equation 2. As figure 4 shows, the inflection points of crystal orientation zone with angle θ in 10° appear at the maximum value in the plot of polynomial function *R(x).*

$$R(x) = p_1 x^n + p_2 x^{n-1} + \cdots p_n x + p_{n+1} \quad (2)$$

p_i is the parameter of polynomial function, here n is 10.

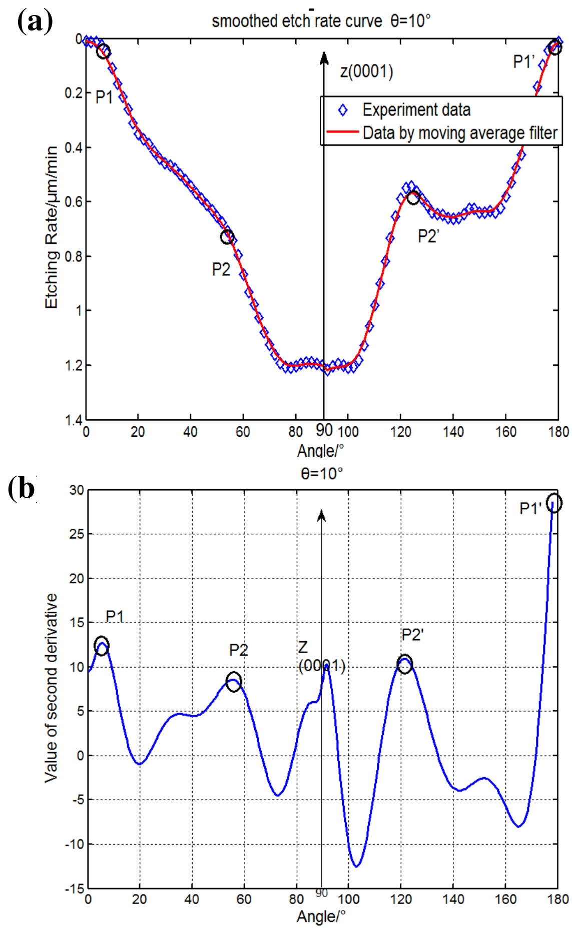

Figure 4: the recognition of inflections points on etch rate curve of crystal orientation zone. (a) etch rate after process of moving average filter; (b) the second order differential curve to locate the infection points;

By using the inflection point recognition method, the comprehensive analysis of possible stable transitional and self-limited profiles is obtained by processing the whole hemisphere experiment. As a stable transitional orientation, *p3* has relatively high etch rate. *p2* plane that lactates on the low etch rate area will develop to self-limited profile during etching.

PROFILE SIMULATIONS

Instead of multiple corrections to achieve a desired structure, Level set simulation can be used to arrive at a much better starting point for mask design [5,6]. Based on surface evolution module, the wet etch is described as a set of moving facets. Level set method can simulate complex topology and undergo orders of magnitude changes in speed. The physics and chemistry processes are contained in one parameter-normal component of the surface velocity. The evolution of the profile can be described by the following Hamilton-Jacobi type equation:

$$\frac{\partial \phi}{\partial t}+V_N|\nabla \phi|=0 \qquad (3)$$

where : $|\nabla \phi|=\sqrt{(\partial\phi/\partial x)^2+(\partial\phi/\partial y)^2+(\partial\phi/\partial z)^2}$, V_N is the normal etch rate (which is a function of the crystallographic orientation of the surface) and the function ϕ describes surface position at all times through the algebraic equation as the following:

$$\phi(x,y,z,t)=0 \qquad (4)$$

For anisotropic etch, equation 3 is the non-convex Hamiltonian. In this study, Lax-Friedrichs is applied to solve the function. The substrate surface in contact with etchant solution is the three-dimensional surface embedded inside the model as zero level set defined in equation 4, and it is evolved according to experimental etch rates. Comparing Figure 1(a) with (b), the simulation result based on level set method is smoother than the simulation result by WJ, but level set model agrees well with the experimental result and shows better accuracy.

PROFILE OPTIMIZATION

Trenches with high aspect ratio is mostly used in fabrication of MEMS structures. By using the level set and inflection point distribution in quartz etching, an optimization process for mask design can be developed for the engineering requirement such as for high aspect ratio and vertical side wall. The computer program for mask design optimization process follows the conditions that:

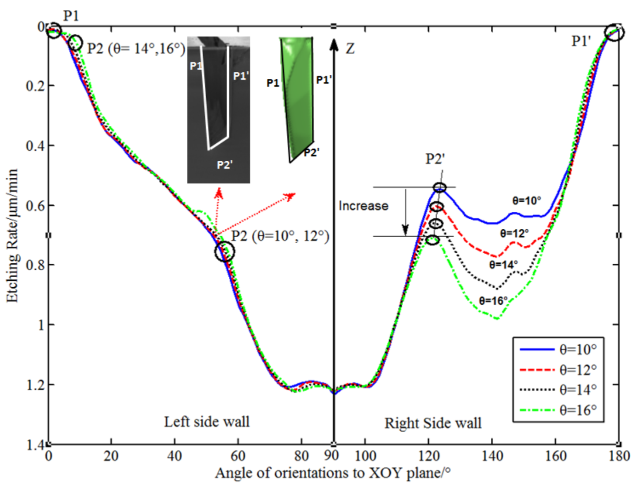

Figure 5: inflection points decision process to calculate the mask alignment for desired vertical side walls, level set simulation of the optimization mask pattern and verification from the experiment.

(1) On the etch rate curve of the crystallographic zone for certain mask edge alignment, there are no low etch rate value as a inflection point whose crystal plane has a small angle to Z cut plane. It means that the inclined angles of *p2* and *p2'* plane should close to vertical direction as much as possible;

(2) If inflection points for *p2* or *p2'* plane whose crystal plane have a large inclination angle to Z cut plane, *p2* or *p2'* planes should have high etch rate values. It means that a fast etching *p2* or *p2'* will help the vertical *p1* or *p1'* develop easily.

(3) Because the undercutting rates of *p3* and *p3'* are higher that *p2* and *p2'*, after long time etching *p3* and *p3'* will vanish during etching. In the end the side wall is formed by *p1, p1', p2, p2',* and their inclination angle to Z cut plane are highly depend on alignment of mask edge.

Figure 5 demonstrates the searching case when θ is in between the crystallographic zone from 10°to 16°. On the right side the etch rate curve, *p2'* increases as angle θ increases. *p2'* gets the maxima value when θ is 16°. A higher etch rate of *p2'* will lead to expose the vertical *p1'* plane faster, which is better to fabricate higher aspect ratio trench structure within the same etching time. On the left side, in condition that θ is 14° or 16°, an inflection point can be found with quite low etch rate. This low etch rate position will finally form an additional inclined self-limited structure plane on the left side.

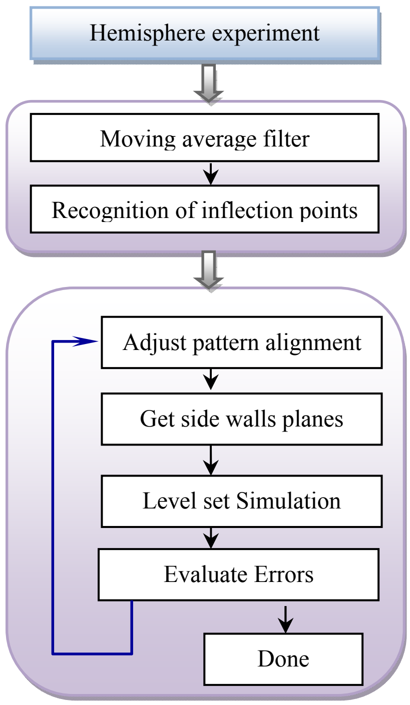

Figure 6: Simulation of quartz etching by coupling level set method and inflection point decision process

In case of 12°, in spite of a large inclination angle of *p2* on the left side plane, *p2* has much higher etch rate. On the right side the etch rate of *p2'* is located at the high etch rate region. We can draw the conclusion that 12° mask edge alignment is the optimum angle of θ to fabricate micro channels with the consideration of perpendicularity and aspect ratio of side walls. The whole optimization process in the simulation program is demonstrated in figure 6.

RESULT AND DISCUSSION

To investigate more complex facets by the proposed method, circular mask was employed to expose a round mesa with a pyramidal base structure. The morphologies of the base of mesa were schematically illustrated in Figure 7. Circular mask pattern on Z-cut wafer creates pyramidal base on the bottom, pillar in the middle surrounded by structure planes and triangular planes formed on top part. As figure 7 shows, pyramidal base consists of three kinds of facets, which were denoted as A, B and C. Because of the circular mask shape, Plane A, B and C belongs to the collection of all inflection points representing *p3* and *p3'*, which can be clearly calculated by level set method.

For etching the micro needle array on quartz wafer, the level set simulation model successfully verifies the orientations of complex facets of micro needle in figure 7. This study shows that the inflection points on etch rate curve by hemisphere experiment plays an important role in understanding the complex facets appeared in quartz etching. The algorithm embedded with level set method improves the simulation accuracy and adaptability comparing with the previous study.

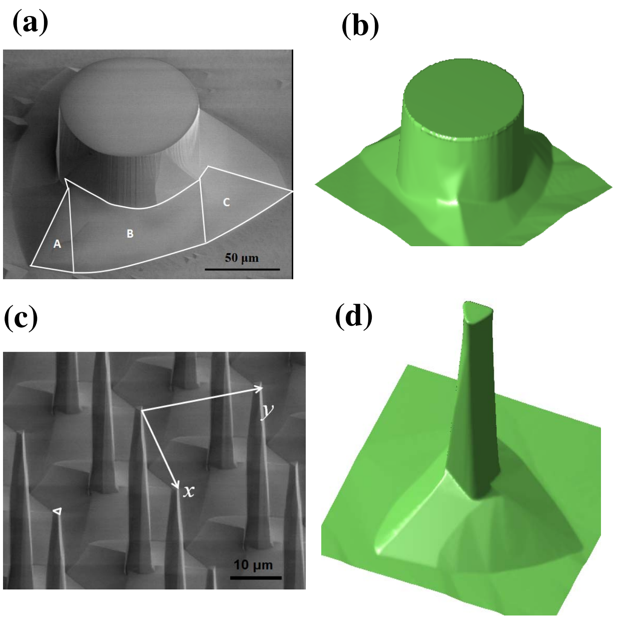

Figure 7: structure planes of micro needle array etched on quartz z-cut wafer in (a), and (c); (b) and (d) are simulation result by the new level set method.

CONCLUSION

By exploring the etch rate curve of the crystallographic zone for the mask edge alignment angle θ from hemisphere experiment data, the orientations as the inflection points on the curve lead to the structure plane in etching process. An analytical method is proposed with moving average filter and second order differences algorithm to retrieve inflection points from hemisphere experimental data. Based on experimental work, orientations as the inflection points with higher etch rate creates stable transitional profile, while inflection points with low etch rate build self-limited profile.

And the simulation program based on level set method is developed to optimize mask pattern design. The evolution of micro needle structure has been simulated and the complex facets in the simulation result follow orientations from the experimental data. The practical application program can be used to determinate process parameters, such as etching time, mask pattern dimension and alignment for the desired microstructures. The proposed level set model allows a rapid and accurate way to predict wet etching of quartz. Furthermore it can be expanded to an efficient method for the simulations of other crystal materials based on etch rates of whole crystallographic orientations from hemisphere experiment.

ACKNOWLEDGEMENTS

We acknowledge financial support by the National Natural Science Foundation of China No.51375093, Prospective research project of Jiangsu Province No. BY2015070-06.

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