Convex Corner Undercutting of \{100\} Silicon in Anisotropic KOH Etching: The New Step-Flow Model of 3-D Structuring and First Simulation Results

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Abstract—In this paper, the mechanism of convex corner (CC) undercutting of Si\{100\} in pure aqueous KOH solutions is revisited by proposing the step-flow model of 3-D structuring as a proper description of the observed phenomena. The basic idea is to conceive the Si\{100\} anisotropic etching process, on the atomic scale, as a “peeling” process of terraced \{111\} planes at \{110\} oriented steps to understand also the arising shape in Si\{100\} etching. On the basis of our new model, we are able to predict the microscopic three-dimensional (3-D) structure of the characteristic CC undercutting without any compensation etchmask structures. Furthermore, the theoretical description has been implemented in a new 3-D simulation tool. Its ability to calculate the shape of simple beam structures of different orientation is experimentally shown.

Index Terms—Anisotropic wet etching, KOH, silicon, simulation.

I. INTRODUCTION

ONE OF THE basic technologies in silicon bulk micromachining is the anisotropic etching in aqueous KOH solutions. In spite of many investigations, the mechanism remains quite unclear, and the apparent shape of the etched structures cannot be satisfactorily explained on the basis of the present models [1]–[6]. This is the main reason for the difficulties in the simulation of anisotropically wet-etched device structures in micromechanics. Particularly in the case of Si\{100\}, there are unsolved problems to understand the convex corner (CC) undercutting (Fig. 1) and to design useful compensation etchmask structures [7]–[11].

Some of the present physical models are based on the assumption that anisotropic etching of silicon in aqueous KOH can be regarded as the reversal of crystal growth in saturated solutions in the state of thermodynamic equilibrium [12], [13]. On this premise, Wulff’s law [14] could be applied. In order to avoid the obvious problem of the missing values for the surface energies, the so-called Wulff–Jaccodine method [15], [16] was derived, which needs the full set of orientation depending etch rate vectors $R_{\{111\}}$ instead of the surface energies. Using that method, several geometric simulation approaches have been done [12], [17]–[20]. Furthermore, the attempts to determine the Miller indexes and the etch rates of all of the conjectural “crystallographic planes” [17], [21]–[24], as well as to explain the experimental results in terms of atomic conditions of the planes (binding energies), are plausible from this point of view. However, particularly for the so-called high index fast etching facets at a CC, there is a wide spread of measured Miller indexes in the literature [7]–[10], [25], [26], and the etch rates of this surfaces cannot be explained by the binding energies of the Si atoms [27]. We also doubt this idea since the chemical and electrochemical reactions take place far from the global thermodynamic equilibrium. The assumption of local states of equilibrium [28] also seems to be improbable since an anisotropic etch process is kinetically controlled [29], [30]. Consequently, the so-called atomistic simulation models [31], [32] do not satisfy the demands on a physics-based simulation tool that could be used for industrial applications.

However, it was revealed by the in situ scanning tunneling microscope (STM) and electrochemical investigations of Allongue et al. [33], [34] that the anisotropic etching can be understood as a step-flow process. That means that the relatively
stable \{111\} planes are attacked at steps and become successively removed in lateral direction. Double back bonded kink sites have increased chemical activity. They are attacked by water molecules from the solution in an anisotropic chemical pathway [35]. We agree with this point of view. Moreover, Van Enckevort [36] showed that the step-flow directions in wet silicon etching within the \{111\} planes are generally \langle11\rangle \text{ and } \langle1\rangle, \text{ respectively. That means that the fine steps are } \langle110\rangle \text{ oriented. Because of energetic reasons, the steps of the } \langle11\rangle \text{ group (in Fig. 2) are more stable, and so the etching into the } \langle11\rangle \text{ directions is kinetically favored. Thus, two groups of possible steps with different etching directions in each case can be distinguished by their step etch rates (Fig. 2).}

Furthermore, it can be speculated that such trains of etching step lines may meet in macroscopic bunches of steps like in gas phase silicon etching [37] and in NH\textsubscript{4}F wet chemical etching [38]. The movement of such steps can be phenomenologically described by kinematic wave theory [39], [40].

The objective of the next sections is to apply the ideas mentioned above directly to Si to order to explain particularly the three-dimensional (3-D) shape of an underetched CC at \langle110\rangle-oriented etch mask edges. This to this end, the new step-flow model of 3-D structuring and the experimental confirmation is summarized [41] and further extended. After that, the theoretical description is implemented in a new 3-D simulation tool, which is able to calculate the shape of CC undercutting accurately. The algorithm applied was originally developed for digital image processing. Finally, the simulation results at beam structures of different geometrical shape, size, and orientation are compared with results that were obtained from etching experiments using the appropriate etch masks.

II. Step Flow Model of 3-D Structuring

To simplify the following derivation, we restrict our considerations to one side of the modeled CC. To this end, the theoretical description is implemented in a new 3-D simulation tool, which is able to calculate the shape of CC undercutting accurately. The algorithm applied was originally developed for digital image processing. Finally, the simulation results at beam structures of different geometrical shape, size, and orientation are compared with results that were obtained from etching experiments using the appropriate etch masks.

The space direction of each step line is designated by the vector \(\mathbf{s}_1\) [Figs. 2 and 3(b) and (c)]. According to Fig. 2, this vector \(\mathbf{s}_1\) on the left side is defined by the intersection line of \{111\} and \{11\} planes. That means that the width of each step is determined by the step etch rate \(R_{121}\) and the specific kinetic etching/bunching conditions. However, the space direction of each step line \(\mathbf{s}_1\) is always constant. Assuming the nature of the area \(B\) to be in the described manner, the mechanism of 3-D structuring at CC can be imagined as follows: along precise \langle110\rangle-aligned etch mask edges, there are normally no mask induced kink sites to generate steps and to “peel” the \{111\} planes. That is the case at very precise aligned V-grooves.

But a rectangular convex etch mask corner can be regarded as a “point of instability,” where kink sites can be generated (origin of the coordinate system in Fig. 3). The actual instability has geometric reasons, but it can be enhanced by the mechanical stresses, which are induced into the silicon substrate by the possibly stressed etch mask materials [42]. This is the starting point of the “peeling” of the first (111) plane at the beginning of the etch attack. Simultaneously, more and more “underlying” (111) plane kink sites become exposed with deeper etching in
the [001] direction, and the lateral etching of these “deeper” (111) planes is started with the step etch rate $R_{[22]}$ in each case. The other already existing steps are further eroded into the lateral [1$\overline{2}$1] direction. In this way, the enfolded area B is formed (Fig. 4). The position of the last attacked kink sites is marked by point $S_u$. This point is called the “step generation point,” i.e., the initial point of instability, which is moved along the trajectory indicated by vector $\mathbf{S}_u$ [Fig. 3(c)]. On the other hand, that means that the position of the first attacked step was moved along the trajectory indicated by the vector $\mathbf{P}_2$ (point P2). This first attacked step was etched the longest time and is the widest removed one. Thus the measured distance $a = |\mathbf{P}_2|$ in Figs. 5 and 6 represents the step etch rate $R_{[22]}$ with etch time $t$ and $\alpha = 60^\circ$ (see Fig. 4).

$$R_{[1\overline{2}2]} = \frac{a}{t \cdot \sin \alpha}.$$  

The distance $b$ is a measure for the “step generation rate” at the point $S_u$, and therewith for the tilt of area B and for the angle $\gamma$ (Fig. 5).

The rough side surfaces of each etched CC [area A, Figs. 4 and Fig. 7(a)] are inevitable residues of this process due to the relative stability of the vertical edge $P_2Q_2$ of the near-{111} side. The orientation of the coarse rips of area A [$\alpha = 120^\circ$ in Fig. 7(b)] reveals that they are also composed of steps of the {111} planes, which are intersected by planes of the {11$\overline{2}$}-group (in Fig. 2) and are etched into the (1$\overline{1}$2)-directions. However, still unclear kinetic/bunching conditions cause the very rough surface and a higher uncertainty of the coordinates of point $Q_2$.

To sum up the explanations above, it can be said that the space coordinates of the enfolding area B (the former so-called high index fast etching facet) are fully determined by the points $S_o$ and $P_2$ and by the vector $\mathbf{S}_u$, which determines the tilt and thereby the third point $S_u = (x_{S_u}, y_{S_u}, z_{S_u})$ on the etch bottom (step generation point). The rough area A is determined by the point $Q_2$. The measurable distances $z, z_{S_u}$ and $\alpha, b$ (Figs. 5 and 6) are determined by the specific etching conditions and are used as the experimental parameters for the modeling. $z$ represents the etch rate in $\langle 100 \rangle$ direction (depth) at the free bottom and $z_{S_u}$ at the step generation point. It has to be measured very close to $S_u$, since $z_{S_u} \neq z$ (the etch bottom in the initially masked area is expected to rise up to the point $S_u$).

It has to be pointed out that all of the still undetermined coordinates of $S_u$ and $Q_2$ can be derived from the proposed model.
In the stipulated specific coordinate system, the \(y\)-axis lies parallel to the vector \(\mathbf{S}_0\) [Fig. 3(c)]. Hence, the three points on the wafer surface can be calculated easily as follows:

\[
P_1 = \frac{\sqrt{2}}{2}(-a,-a,0) \\
P_2 = \frac{\sqrt{2}}{2}(a,-a,0) \\
S_0 = (x_{So}, y_{So}, z_{So}) = (0, \sqrt{2}(b - a), 0).
\]  

Using the step-flow model of 3-D structuring [41], the components of the bottom point \(S_u\) can be calculated as follows:

\[
x_{Su} = 0, \quad y_{Su} = z_{Su} \left(1 - \frac{2b}{a}\right) + y_{So}, \quad z_{Su} = z_u.
\]  

The absolute value of the first term of \(y_{Su}\) is equal to the measurable distance \(q\), which designates the projection of the inclined symmetry edge \(\mathbf{S}_u - \mathbf{S}_0\) onto the vector \(\mathbf{S}_0\) [Figs. 3(c) and 5]

\[
q = |z_{Su} \left(1 - \frac{2b}{a}\right)|.
\]  

The coordinates of Point \(Q_2 = (x_{Q2}, y_{Q2}, z_{Q2})\) can be derived as follows. According to the assumption above, the vector \(\mathbf{S}_2\) (indicating the direction of the coarse step lines) can be given by the vector product of the normal vectors of the \(\{111\}\) plane and the respective plane of the \(\{1\bar{1}2\}\)-group (Fig. 2), i.e., the \(\{211\}\)-plane

\[
\mathbf{S}_2 = \mathbf{n}_{(111)} \times \mathbf{n}_{(211)} = (x_{2}, y_{2}, z_{2}).
\]  

In vector components, this can be written as

\[
\mathbf{S}_2 = \begin{bmatrix} \vec{e}_x \\ \vec{e}_y \\ \vec{e}_z \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} = (0, -1, 1).
\]  

The coordinates of point \(Q_2\) can be obtained by means of the relation [43]

\[
\begin{bmatrix} x_{Q2} - x_{So} \\ y_{Q2} - y_{So} \\ z_{Q2} - z_{So} \end{bmatrix} = 0.
\]  

The combination of (2), (6), (7), and \(x_{Q2} = x_{P2} = a(\sqrt{2}/2)\) yields

\[
\begin{bmatrix} x_{Q2} \\ y_{Q2} - \sqrt{2}(b - a) \\ z_{Q2} \end{bmatrix} = 0.
\]  

Finally, the last still undetermined component \(y_{Q2}\) can be calculated from (8). Herewith the coordinates of \(Q_2\) are given as follows:

\[
x_{Q2} = a \frac{\sqrt{2}}{2}, \quad y_{Q2} = -a \frac{\sqrt{2}}{2} - z_{Q2}, \quad z_{Q2} = z.
\]  

Looking perpendicular onto the wafer, the convex etchmask corners (without compensation structures) become underetched in the characteristic manner shown in Fig. 6. (Both areas \(B\) are indicated.) After measuring the depicted distances, the shape of the CC undercutting can be calculated with the corresponding equations. The measurement of \(q\) (Fig. 6) was used as a proof of the derivation above [41].

Further SEM investigations of etched CC in three defined views were performed in order to proof the \((110)\) space direction of the fine step lines on area \(B\).
Looking parallel to the (110) crystal direction [parallel to the 
\{100\} wafer surface, Fig. 7(a)] on a CC, these step lines were 
found to be parallel to the cross-section line of the adjoining free 
etched \{111\} surface [downward side of the angle \(\beta = 54.7^\circ\) 
in Fig. 7(a)]. This observation confirms that the step lines are 
lying within the (111)-plane.

Looking parallel to the (111) crystal direction [Fig. 7(b)], the 
normal direction of these step lines always encloses the indi-
cated angle of \(\alpha = 60^\circ\). This observation confirms the assump-
tion that the step lines within the (T2T)-plane (Fig. 2).

Looking parallel to the (100) crystal direction and parallel to the 
\{100\} wafer surface directly on the CC [symmetric view, 
Fig. 7(c)], the step lines always enclose an angle of 45° with the 
\{100\} wafer surface. This is the final confirmation that the 
step lines are defined by the intersection lines of the (111)- and 
(T2T)-planes (Fig. 2).

The three different views in Fig. 7 give an experimental con-
firmation that the inclination of the vector \(\mathbf{s}_4\) is \{110\} oriented 
indeed. The quantitative predictions of the proposed step-flow 
model are also confirmed by the experimental results shown in 
[41]. The space position of the coarse step lines (\(\mathbf{s}_2\)) can be seen 
also in Fig. 7 and is found to roughly match the predictions of the 
model.

III. NUMERICAL MODELLING

With a view to future predictive simulation, we implemented 
the above-described step-flow model of 3-D structuring in a 
general simulation tool for 3-D anisotropic etching.

The mathematical method employed in our simulation ap-
proach was originally developed for digital image processing 
and adapted by Strasser [44], [45] for the purpose of efficient 
topography simulation.

The simulation area is discretized by equally shaped volume 
elements, so-called cells, on which mathematical operations are 
carried out to describe the time evolution of the etch front. To 
each cell a list of attributes is assigned such as material prop-
erties and additional crystallographic information concerning the 
location of the cell in the crystal structure. A material 
index characterizes the etching behavior of each cell. All 
computational algorithms are strictly cell-based, and therefore 
it is straightforward to simulate the etching of multilayered 
substrates, which could contain, for example, buried etch stop 
layers of doped silicon or even layers exhibiting completely 
different material properties as for example silicon oxide, 
polysilicon, or metal films. The influence of the isotropic 
etching properties of mask materials can also be treated within 
this simulation concept much more easily than in commonly 
used differential-geometrical methods.

Three-dimensional modeling also offers the possibility to 
simulate the etching of wafers that were prestructured, e.g., by 
laser micromachining or other etching processes (reactive ion 
etching, plasma etching), as well as double-sided wafer etching.

The mathematical operation to model an etching process is 
termed erosion and carried out by using a so-called structuring 
element. This is a three-dimensional body such as, for example, 
a ball or an ellipsoid with variable size and orientation. The 
structuring elements are moved along the surface cells of the 
current geometry. If the center of a cell is touched by the struc-
turing element, this cell is marked for removal. In the following 
etch step, the set of all marked cells is abraded by turning its 
material index into the etchant’s index. In this way, a new etch 
front is obtained after each etch step.

Fig. 8 illustrates the basic idea by a two-dimensional 
schematic example. The center of the structuring element, an 
elipsoid, is placed closely above each material cell (precisely 
speaking, the center of the structuring element is placed at the 
centers of the adjacent nonmaterial cells of each surface cell). 
Each material cell is marked if its center lies in the interior of 
the structuring element. The marked cells are drawn in 
dark gray in Fig. 8, the structuring element is shown at four 
interesting positions of the structure, and the arrows indicate 
the “motion” of the structuring element along the surface. 
The elliptic shape produces an anisotropic etch rate, which 
is smaller in horizontal direction than in vertical direction. 
The structuring elements can change directions of motion and 
move along an arbitrary track on the surface of the simulation 
area to satisfy special requirements for the simulation of more 
complex processes.

This general method has been adapted to the step-flow model 
of 3-D structuring as a special case of an orientation-dependent 
etching process. The procedure works as follows.

The structuring element is locally defined by a step etch rate 
vector \(\mathbf{v}\), which is evaluated for each surface cell. The orienta-
tion and the magnitude of each element is derived from the char-
acteristic properties of the cell under consideration. In Fig. 9, 
a typical set of structuring elements for a step-flow motion is 
shown. After the front sides of the steps are localized, the struc-
turing elements are attached with a precalculated orientation and 
length. In this way, a number of material cells is marked (the 
light gray ones in Fig. 9) that have to be etched away subse-
quently. Please note that every cell may exhibit different etching 
behavior.

A. Description of the Algorithm

Fig. 10(a) illustrates the simulation of the left side of a CC 
etched in KOH/H\(_2\)O solution. The coordinate system and the 
characteristic points and distances are inserted in accordance 
with the schematic drawing in Fig. 3.
Fig. 9. Step etching with structuring elements. The underetched mask cells (dark gray) were partially removed to get a better view of the steps.

Fig. 10. (a) Simulation of the “left” side of a CC with coordinate system and characteristic points (mask is removed). (b) Detailed view of the area at point P_2 showing the step dimensions c and d of the finely stepped area B and the step etch v_{110} rate in [110] direction.

The discretization of the simulated region is chosen coarser than the dimensions of the fine steps of area B subject to the computational resources available. Furthermore, the material discretization is performed on a simple cubic grid oriented along [110] direction to ensure compatibility with an alternative simulation tool. Therefore, the real shape and orientation of the fine steps visible in the SEM micrographs is not resolved, but the enfolding envelope area is calculated accurately. The etch rate vector of the real steps is decomposed into components along the [110] and [100] direction to obtain the correct surface orientation of area B. It is notable that the interaction between two areas B coming from different CCs and contacting each other is accurately described.

Equation (10) gives the correlation between the etch rate of the {121} group and a step etch rate $\bar{v}_{110}$, which is used in the simulation

$$|\bar{v}_{110}| = \frac{|R_{121}|}{\sqrt{2}} \cdot \frac{2b}{\sqrt{(a-b)^2 + b^2}}.$$  (10)

The simulation starts with detecting unstable points of the etch front. In the case of a masked planar wafer as initial condition, these crucial points are induced by mask edges. The volume cell beneath a mask edge is recognized as a kink site, which determines the etching behavior of this cell.

The cells containing kink sites are etched first and their adjacent cells in [110] direction are identified as belonging to a fine step of an area B. Consequently, these cells are etched with a step etch rate $\bar{v}_{110}$ in [110] direction. Proceeding this way, the existing steps are etched and, simultaneously, new kink sites are created at the intersection of underlying (111) planes. In the same way, the etching of the [100]-oriented bottom causes the appearance of new kink site cells at the point S_{11} [see Fig. 10(a)].

Fig. 11. Schematic drawing of the used etch mask structures: (a) {110}-oriented beams and (b) {100}-oriented beam with regular CC at the apex.

Fig. 10(b) shows a detailed zoom-in view of the area around point P_2.

The relation of the step dimensions is given by (11)

$$c = \frac{a-b}{b} - 1.$$  (11)

The step dimensions and step etch rates $\bar{v}_{110}$ can be derived from the measured characteristic distances “a” and “b” introduced in Figs. 5 and 6.

IV. EXPERIMENTAL

Fig. 10(a) shows the simulation of an underetched convex corner in Si_{100} etched in a 0.33 gL^{-1} KOH/H_2O solution at a temperature of 80 °C. We can identify the (100) wafer surface (the mask is already removed), the (100) bottom, and the stable (111) planes. The regular finely stepped areas B are correctly reproduced by the simulation as well as area A, which is formed by stepped residues. They connect the bottom of the structure with the areas B and the (111) side walls. Area A also shows a regular shape, since kinetic effects such as step-bunching are not included in our model. In a postprocessing step, the discretization of the (111) planes and in the [100] direction of the finely stepped area B was smoothed for the sake of better visualization. The typical morphology occurring at underetched convex corners is retrieved by our simulation approach and can be verified by comparison with the SEM micrographs in Fig. 7. The challenge is to apply the developed simulation tool on etch masks of any geometrical shape and to compare the simulated results with the etching results. In a first approach, we used simple beam structures of different geometrical shape, size, and orientation (Fig. 11). Since these structures represent the basic parts of CC compensation structures, they can be recognized as test structures for device simulation.

For the etching experiments we used a double wall etch vessel and additional components (thermometer, stirrer, N_2-bubbling supply, chip holder, reflux condenser) made of high-purity fused silica. The vessel and the mentioned components were cleaned first in H_2SO_4/H_2O_2 and afterwards in HCl. The etching temperature of the system was held constant within (80 ± 0.01) °C. The samples used in this study were from n(P) {100} CZ grown high-quality wafers (1–10 Ωcm). We used 0.33 gL^{-1} KOH/H_2O from Merck (“Selectipur”).

For the visualization of the simulation results, a ray-tracing tool (Povray) was employed.
Fig. 12. Comparison of the rendered simulation results with SEM micrographs of etched \langle110\rangle-oriented etch mask structures [Fig. 11(a)] in 0.33 g/cm$^3$ KOH/H$_2$O at 80°C. (a) and (b) after 30 min, (c) and (d) after 60 min, and (e) and (f) after 167 min.

Please note that the simulations were carried out on a simple cubic grid. Hence, the steps in the simulated pictures are due to the material discretization and not corresponding to the step lines visible in the SEM micrographs and referred to above. However, these pictures generated by ray tracing should provide a three-dimensional impression of the simulated structures. Angles and distances cannot be extracted from these pictures due to the perspective view. For this purpose, the simulation tool can provide user-specified cross-sections of the simulated structures.

In Fig. 12, the simulation and experimental results at two \langle110\rangle-oriented beam structures of the same length but of different width are compared [Fig. 11(a)]. At the wider one of the beams, it can be seen that at the beginning, two of the typical CC undercutting shapes have arisen [Fig. 12(a) and (b)]. After some time, both convex corners are eroded further and have started to overlap [Fig. 12(c) and (d)]. After further etching, the shape has completely changed and is now composed of only the two intersecting outer parts of the (former) convex corner undercutting shapes [Fig. 12(e) and (f)]. Between the beams, nearly complete V-grooves are formed. At the narrower one, this situation is already reached at the first of the three shown time steps because of the smaller geometrical dimensions. With this structure, the expected further time evolution of the wider beam can be studied.

In Fig. 13, the simulation and experimental results at a \langle100\rangle-oriented beam structure [Fig. 11(b)] are compared. Besides the overlapping of neighboring CC, also the vertical (100) surfaces can be seen in the simulation results as well as in the SEM micrographs.

These results show that the developed simulation tool is able to predict the arising etching shape at convex corners and etch-mask structures that are composed of them. It can be assumed that it also works at any etchmask structure.

V. CONCLUSION

We conclude that the shape and morphology of anisotropically etched structures observed in experiments agree with the
Fig. 13. Comparison of the rendered simulation results with SEM micrographs of etched (100)-oriented etch mask structures [Fig. 11(b)] in 0.33 g cm$^{-1}$ KOH/H$_2$O at 80 $^\circ$C. (a) and (b) after 60 min, (c) and (d) after 167 min, (e) and (f) after 258 min, and (g) and (h) after 352 min.

predictions of the new step-flow model of 3-D structuring. According to this model, which was derived for Si$_{[100]}$ from recent STM observations on Si$_{[111]}$ and theoretical considerations on an atomic scale, the flat surfaces B (Fig. 7) at undercutted CC in pure KOH solutions are actually not “high index and fast etching crystallographic planes.” Instead, they should be considered as envelope surfaces from (110)-ori-
tented step lines. They are continuously sidewise enlarged, bunched, and etched in their lateral (112) “peeling” direction. Indeed, to our knowledge this proposal of an anisotropic etch model is the first that provides a consistent description of CC undercutting in KOH etching, which is able to explain and to calculate the shape of both types (A and B in Fig. 7) of the occurring surfaces.
In addition, we have developed a new simulation tool for orientation-dependent etching of silicon in alkaline solutions. The underlying model relies on the assumption that the etching mechanism is properly described by the proposed step-flow model of 3-D structuring. Our three-dimensional simulation tool reproduces the details of the observed morphology like terraces and steps. The results at more complicated etchmask structures are fitted very well by the experimental results. Multilayer materials and multistep structuring processes can easily be incorporated. Using methods of digital image processing, we could achieve acceptable simulation times and comparably low computational expense for three-dimensional process simulations. Furthermore, our model approach is capable of combining the flexibility and precision of atomistic approaches with the reduced requirements on computational resources known from differential-geometrical models. It can be expected that this physics-based simulation tool is able to predict the arising etching shape of any etchmask geometry. Additionally, it is confirmed that the understanding of the step-flow mechanism at convex corners has to be regarded as the key problem. For further developments, it seems attractive to material discretization, which is adapted to the silicon crystal to reproduce the occurring step orientations.

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