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Realistic Step Flow Model for Orientation-Dependent Wet Etching Implemented in a Modular TCAD Environment

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In this paper we present a new simulation tool for orientation-dependent wet etching of silicon which is based on a new model proposed by Schröder.(1) What is essential is the experimentally observed result that the so called "fast etching planes" causing the characteristic shape of underetched convex etchmask corners are not really crystallographic planes. We demonstrate in basic examples that our simulation approach using this "step flow model of three dimensional structuring" can be used to obtain the detailed morphology of the etched structures, and provides the flexibility for embedding the simulator in a modular technology computer aided design (TCAD) platform which comprises all process steps encountered in microtechnology.

1. Introduction

We present a new simulation tool for three-dimensional orientation-dependent wet etching of $Si_{\{100\}}$. The implemented algorithm is based on a model proposed by Schröder,(1) which can explain the convex corner undercutting (Fig. 1) in pure aqueous potassium hydroxide (KOH) solutions. The new aspect incorporated in this model is the experimental observation that the so-called "fast etching planes", which are commonly invoked as the cause of the characteristic shape of underetched convex etchmask corners, are not really crystallographic planes. Instead, these areas (denoted "B" in Fig. 1) are the envelope surfaces of bunched steplines originating from kink sites on the intersecting {111} planes.

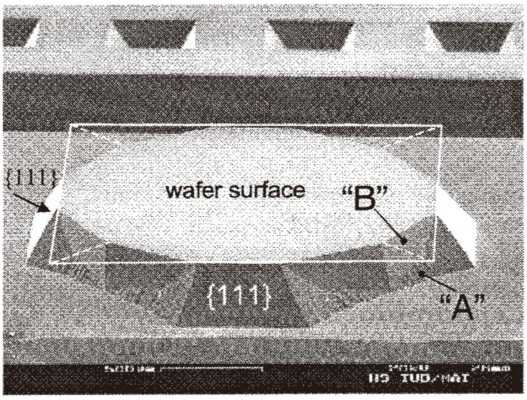

Fig. 1. Micrograph of a mesa structure with square etch mask and four convex corners.

These steplines move in the <112> direction during the etch process, which is conceived as peeling off {111} planes on the surface in the lateral direction. The coarse "A" areas are residues of this process. Further details are given in ref. 2.

2. Numerical Modeling

The mathematical method used in our simulation approach was originally developed for digital image processing and later adapted to the purpose of efficient topographic simulation.(3) The basic concept is to represent the etch body and its exterior as a black and white image (black = material, white = no material) which is altered by the action of a certain set of operations. Each time step of the etching process is modeled as a so-called "erosion operation", where a properly chosen "structuring element" acts on the etch body to mark all material that has to be removed next. The structuring element is a three-dimensional body such as a sphere or an ellipsoid, the shape of which has to be adjusted to the specific etching mechanism under consideration. The geometrical configurations during the etch process are described by a cellular representation in order to ensure an efficient numerical implementation. The simulated region is discretized by a partition of equally shaped volume elements ("cells") which are labeled by a material index indicating their location inside or outside the etch body. The time evolution of the etch front is represented by the temporal change of the material indices of the cells which, in turn, is controlled by the structuring element.

The structuring element is shifted parallel to the current etch front (i.e., the momentary surface cells, cf. Fig. 2). If the center of a cell is touched by the structuring element, this cell is marked for removal. In the following etch step, the set of all marked cells is abraded by turning their material index into the index of the etchant. We adapted this method for the implementation of the step flow model in an existing simulator.(3) A multiple-valued

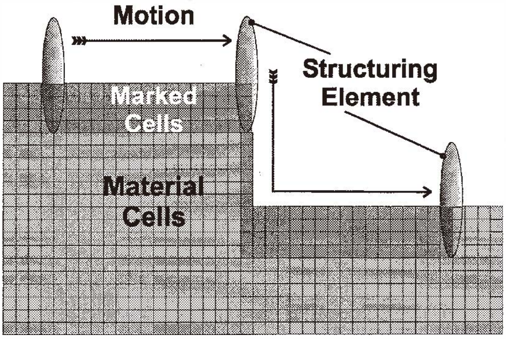

Fig. 2. Schematic of the erosion operation using an ellipsoid as the structuring element. Cells in dark gray are removed in the following etch step.

material index characterizes the specific etching behavior of each cell. In this way the simulation of substrates containing layers of different materials can be efficiently carried out.

The use of a realistic three-dimensional model offers the possibility of simulating the etching of pre-structured wafers, obtained by laser micromachining or other etching processes (reactive iron etching (RIE), plasma etching), as well as double-sided wafer etching. This flexibility is the prerequisite for embedding the etching simulator in a modular TCAD platform which includes all process steps encountered in microtechnology.

Figure 3 illustrates the basic concept of the step flow model applied to a simple cubic grid. The convex corner of the mask is already underetched; the dark gray cells represent the kink site generation points in which the steplines have their origin. The existing steps (drawn in light gray) are moved in the lateral direction, as indicated by the arrows. Proceeding in this way, the progressive erosion of material is described as a layer-by-layer peel-off process. For the implementation of this mechanism in the simulator, we had to extend the original erosion algorithm in such a way that the structuring element is not moved across the entire surface of the simulation area. Instead we have to trace the locations where kink sites are generated as well as the positions of the existing steps. To this end, we have to set up and solve the equations of motion for kinks and steps (Fig. 4) and then apply the next erosion step accordingly.

The orientation and magnitude of the structuring elements at a given cell position on the etch front are derived from the specific properties of the respective cell which, in turn, result from the equations of motion of kinks and steps comprising the crystal surface.

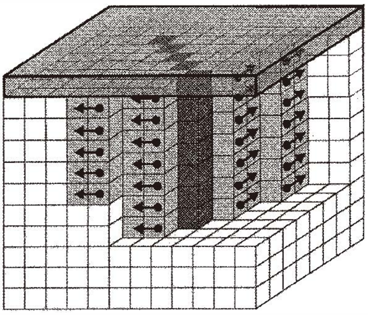

Fig. 3. Basic concept of a step flow model with kink site generation points (dark gray) and steps (gray).

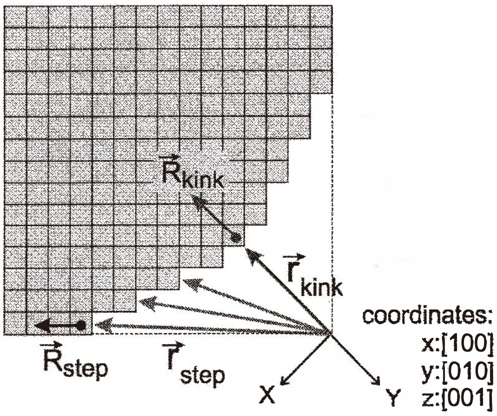

Fig. 4. Top view of the simulation area showing locations and etch rates of kinks and steps.

3. Results

Figure 5 shows the simulation result of an underetched convex corner in {100}-silicon exposed to a KOH/H_2O solution. The typical morphology observed at underetched convex corners is reproduced by our simulation as is demonstrated by comparison with the SEM micrograph in Fig. 1.

The discretization of the simulated region is set to be coarser than the real dimensions of the fine steps in area B in consideration of the limited computational resources available. Furthermore, the material discretization is performed on a simple cubic grid oriented along the [110] direction to ensure compatibility with other simulation tools. Therefore, the real shape and orientation of the fine steps visible in the SEM micrographs is not fully resolved,

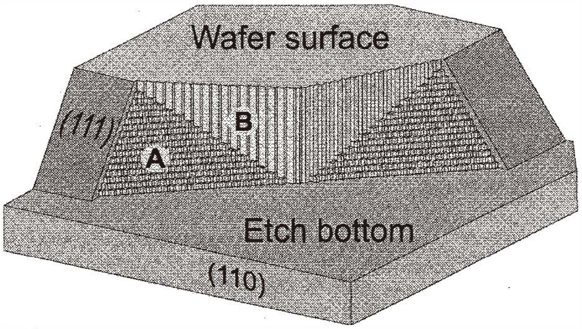

Fig. 5. Simulation of a convex corner etched in pure KOH (33 wt%, 80°C).

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] directions to obtain the correct surface orientation of area B. It is notable that the interaction between two B-type areas originating from different convex corners and contacting each other is accurately described. This is displayed in Figs. 6(a) and 6(b), which show an actual micrograph and the simulation of a beam structure oriented in the <110> direction. The morphology of this structure is the result of the interaction of the two convex corners at the mask edges, which are indicated by the white lines. Note that, in a postprocessing step, the discretization of the structures was smoothed for better visualization. The coarse A-type areas also appear to have a regular shape in the figures, since the statistical mechanisms that cause the irregular morphology are currently not included in our simulation model.

A complex interaction of convex corners appears if an etch mask exhibits edges with arbitrary angles or even curved edges. According to the step flow model, every mask edge which is not aligned in the <110> direction exhibits unstable points where kink sites are induced and the characteristic shape of a convex corner emerges right at the beginning of the etching. Therefore, the 3D structure of the etch body resulting from an arbitrarily oriented mask edge is caused by the interaction of those convex corners. Consequently, in our simulation approach any curved or beveled mask edge can be composed of an array of convex corners in such a way that the edge under consideration is approximated by line segments oriented in the <110> direction. As an example, Fig. 7 shows the approximation of a circle which, in turn, represents the mapping of the circle to the cellular material discretization of the mask geometry. In this way the inherent approximation of a curved line by the material discretization for our simulation approach automatically produces convex corners along the curved mask edge.

For the etch simulation underneath the circular mask in Fig. 7, the material discretization of the mask has to be refined. Therefore, every mask cell is subdivided again into 64 cells. Then all convex corners which have been created by approximating the curved mask are treated like single convex corners (cf. Fig. 4) at the very beginning of the etching. With progressing etch depth, the interaction of kinks and steps which originate from all these

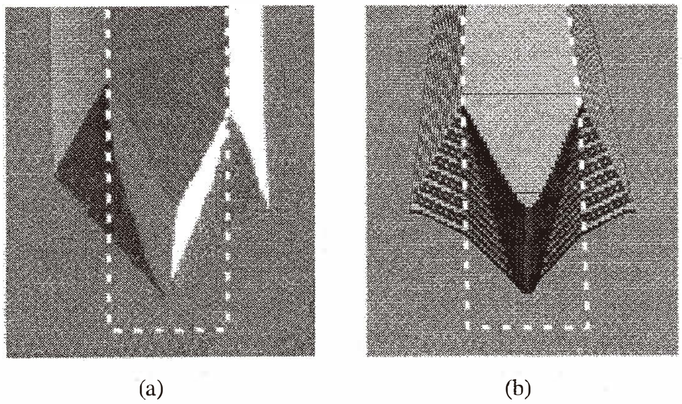
(a) (b)

Fig. 6. Micrograph and simulation of a beam oriented along the <110> direction.

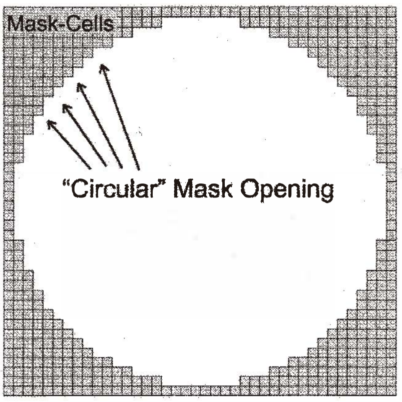

Fig. 7. Top view of a circular mask opening. The curved line of a real circle is approximated by the cellular material representation creating a large number of convex corners.

convex corners determines the further evolution of the etch body. Figure 8 shows a close-up image of a part of the circular etch mask with the refined grid on which the etching simulation is carried out. Figures 9(a) to 9(c) display simulation results obtained with the circular etch mask of Fig. 7 (the mask is not drawn for better visualization).

After a sufficiently long period of etching only the stable {111} planes remain and form a pyramid-shaped hole, as shown in Fig. 9(c).

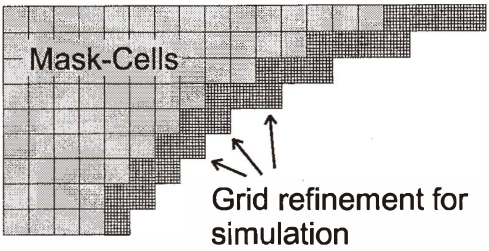

Fig. 8. Curved mask edge with refined grid as required for the evolution of the convex corners at the beginning of the simulation.

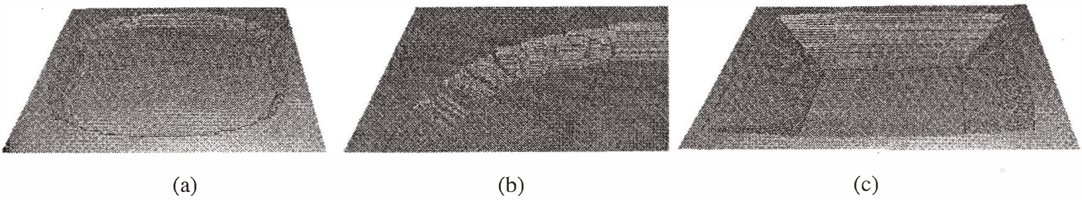

Fig. 9. (a) Etch simulation of a circular mask. (b) Close-up of the upper left corner. (c) Stable {111} planes remain.

4. Conclusions

We conclude that the simulation of orientation-dependent wet etching on the basis of the step flow model as proposed in ref. 1 enables us to correctly reproduce the detailed morphology of the etch front. Thus it provides a solid basis for the predictive simulation of progressively complex micro-electromecahnical systems (MEMS) structures. The compatibility with a professional TCAD environment allows for the efficient design of complicated etch mask compensation structures, potentially in combination with other materials and structuring techniques. Moreover, employing methods adapted from digital image processing, we can keep the simulation times short and the computational effort affordable, even for 3D process simulation.

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