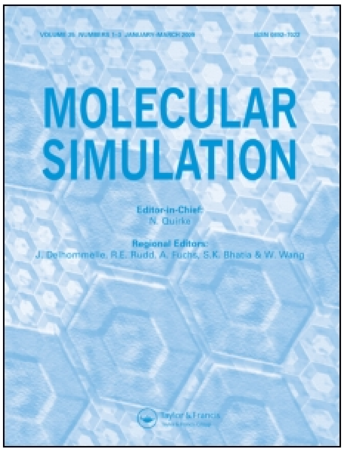

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Three-dimensional numerical simulation for anisotropic wet chemical etching process

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Three-dimensional numerical simulation for anisotropic wet chemical etching process

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In this paper, we present result on the development of a simulation tool for the three-dimensional anisotropic wet chemical etching for bulk micromaching. Our developed simulator comprises step of calculation the movement of the surface. It is based upon the data structure with movement of the surface cell list which has list and list 2, respectively. The surface cell has the topography evolution information which has etch properties according to crystallographic position of surface cell and cell volume value. The topography evolution information evolves movement of the surface. The performance of our developed simulator was investigated with our three-dimensional simulation results. Several simulation results demonstrate our simulation tool which is quite efficient for the design and development of MEMS device structure. The developed simulator demonstrates the applicability of complex three-dimensional MEMS device structure. We demonstrate the simulation of the anisotropic wet chemical etching process of basic exemplary structures featuring the virtual fabrication of an MEMS structure manufactured by means of bulk micromachining.

Keywords: Anisotropic etch simulator; Wet etching; Three-dimensional simulation; Bulk micromaching

1. Introduction

Anisotropic wet chemical etching is still one of the fundamental techniques employed in silicon bulk micromaching technology [1]. The recent growth in the number of microelectromechanical system (MEMS) devices that are being fabricated using bulk silicon micromaching technology has necessitated efficient design and development [2]. The bulk micromachining technology removes selectively significant amounts of silicon from a substrate. It constructs undercut structure that is required to form membranes on one side of wafer or to make a variety of trenches, holes. In the anisotropic wet chemical etching process, the etching procedure for bulk micromaching technology is commonly realized by using wet chemical etchants in order to obtain a significant underetching structure. The underetching structure is separated isotropic and anisotropic. These properties of etched geometries are the main responsible for the reactants and including the shapes of the masks used to define the etched regions. Although isotropic etching etchants is used to such bulk micromaching technology, usually anisotropic wet chemical etchants such as potassium hydroxide (KOH), ethylene-diamine pycocatechol (EDP) and tetramethyl-ammonium hydroxide (TMAH) are used reasonable in MEMS single-crystal silicon-based process [3].

In the case of semiconductor process, exact understanding of topographical evolution is important for optimizing the front-end semiconductor process such deposition and etching. To predict geometry of etched structure must consider information of surface reactions [4–5]. Like semiconductor process, the exact understanding of etched result in MEMS device has reduced wasted time and the number of micro-fabrication test iterations. But, it is often difficult to predict the result of etching single-crystal silicon with typical wet etchants such as KOH, TMAH and EDP due to the anisotropic nature of the etching that is taking place. Despite many research efforts have been made on the development of novel schemes which allows the designer to figure out the topographical evolution of the surface during fabrication process of the MEMS devices such as bulk silicon micromaching technology. And most of the available simulation software is specialized stand-alone programs, featuring no embedding in general-purpose topography simulation tools [6–10]. But the fabrication of progressively complex MEMS structures often requires

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additional processes for the three-dimensional structuring of bulk silicon.

In this paper, we present a simulation tool for the three-dimensional anisotropic wet etching of single-crystal silicon. Our simulation method allows for an efficient three-dimensional simulation. Also, our simulation tool can easily be extended to corporate different materials with various etching properties.

2. Simulation method

Our simulation method simulates movement of the surface through a list structure, so called the surface cell.

The simulation region is divided into units of hexahedron-shaped cells. The material index information is assigned at each cell to be divided. Also, the location information is assigned by a location index indication which express location of inside or outside the etch body. The topography evolution information is assigned only at surface cells. The topography evolution information has etch properties according to its crystallographic position and cell volume value that evolves movement of the surface. The surface cells are constituted the list for the efficiency of the memory and computation. Figure 1 is a schematic diagram illustration the surface cell list composition for a surface topography expression of the case of anisotropic wet chemical etching.

In the anisotropic wet chemical etching process, anisotropic etchants etch attack certain crystal planes much faster in one direction than in another direction. For the case of silicon, ⟨100⟩ and ⟨110⟩ planes etch at much higher rate than ⟨111⟩ planes. This etch rate selectivity is used to create various cavity and groove structures. Etching at concave corners on (100) silicon stops at (111) intersections. But convex corners are undercut, allowing cantilevers rapidly undercut and released. This mechanism is explained as removing {111} planes on the surface in lateral direction [11]. For the purposed of efficient topography simulation, our simulation method adapt to the surface cell list which is composed two lists.

The surface cell list is composed the surface cells to be removing ⟨110⟩ planes and ⟨111⟩ planes (list 1). The surface cell list is composed the surface cells to be removing ⟨100⟩ planes (list 2). The data structure to perform the above surface cell list is shown figure 2.

Referring to figure 1, surface cell list has list 1 and list 2, respectively. Our developed simulator has five major data structures consisting of "PhList", "PgList", "ph", "pg" and a linked list of pointers to the surface cells. The "PhList" express surface cell of list 1. The "PgList" express surface cell list of list 2. The "ph" and "pg" points to topography evolution information. The surface cell lists are kept in two separate arrays so that they may have different information depending on etch properties. The surface cell list is consisted of linked list. A linked list is created containing the array address of several surface cells. The "NoList" express an end of surface cell list.

As above mentioned, the composed surface cell list is used to do the simulation for the movement of the surface. The surface cell list is composed two lists according to normal vector of crystallographic planes. We perform the list construction such as following steps: (a) extract normal vector formed by crystallographic plane with surface cell, which the material index of cells is same. (b) Separate lists with each crystallographic plane into surface cell list. The exposed direction of surface cell is same, or the angle between normal vectors of each surface cell is within critical angle. (c) Find common list with crystallographic plane. Finally, (d) couple list with same crystallographic plane.

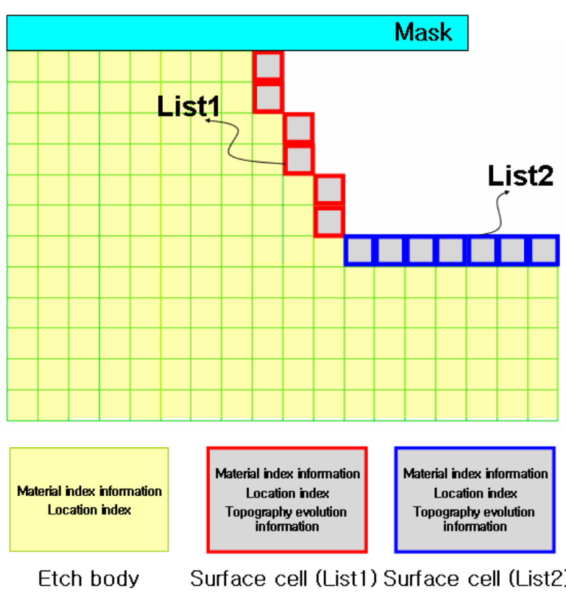

Figure 1. The cell list composition for a surface topography expression of the case of anisotropic wet chemical etching.

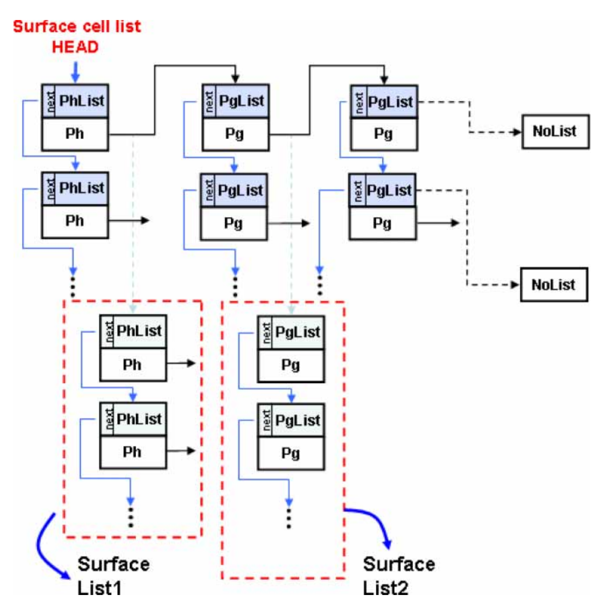

Figure 2. The data structure of surface cell list.

Each surface cells are moved according to the etch properties. The etch properties is different according to its crystallographic direction. Our simulation tool uses etch properties to determine displacement direction of surface cells through the normal vector of crystallographic planes. Figure 3 is a schematic view illustrating the method defining displacement direction according to a normal vector of surface cells with crystallographic plane. The displacement direction is calculated by summing up the normal vectors of surface cells.

Our simulation tool uses the mathematical method. During the time evolution of the etch front, which is represented by the change of the material index information of each cell. The topography evolution information are assigned to surface cells to determine the etch properties according to its crystallographic position.

During the simulation, an equation (1) is used to express movement of the surface cells.

$$\vec{P}_i(t + \Delta t) = [\vec{P}_i(t) + e_i \cdot \Delta t \cdot \vec{c}_i] \cdot g_i \tag{1}$$

The plane displacement direction $\vec{c}_i$ is determined by the crystallographic properties of the surface cell. The g_i is used to determine whether cell has been etched away, the position vector $\vec{P}_i$ from t to $t + \Delta t$ is calculated. The position of new surface cells that exposed by the proceeding of the etch front. The etch rate e_i is determined from experimental data.

Etch rates for a given temperature and concentration of the etchant is not the same for the different silicon crystal planes. Figure 4 shows a graphical representation of the silicon etches rate dependence on the crystalline plane, etchant temperature, and etchant concentration.

The surface cell is removed according to the following procedure as the simulation method illustrated in figure 5. At single time step, the list of surface cell is searched. The surface cell list is composed two lists according to normal vector of crystallographic planes. The movement of surface cell is determined displacement direction according to a normal vector of surface cells with crystallographic plane. During the next time step, the surface cells moves

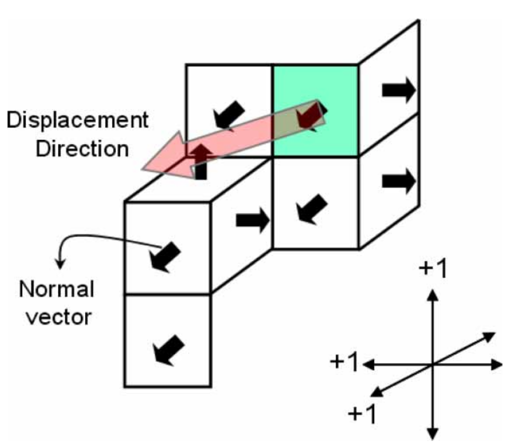

Figure 3. A normal vector of surface cell with crystallographic plane.

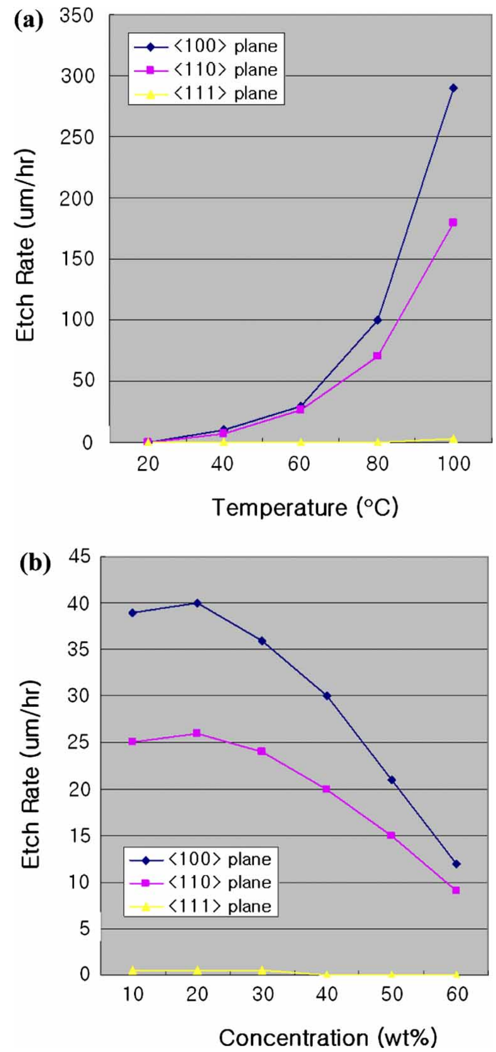

Figure 4. (a) Etch rate of single-crystal silicon according to a temperature at fixed concentration of 35 wt%, (b) etch rate of single-crystal silicon according to a concentration at fixed temperature of 60°C.

position exposed by the proceeding of the etch front along the vector of displacement direction. The information of the surface cells of initial position were transferred to the new surface cells exposed by the proceeding of the etch front. The time step is updated. Finally, newly exposed cell is added surface cell list, before the next time step may begin. The surface cells are removed until time T is reached. Time (T) is defined according to the user's selection. The final etched shape is obtained, as shown in figure 5(b).

3. Result and discussions

In this section, we show a series of results using the above simulation method. Our simulation method was applied to the cases anisotropic wet chemical etching process such as the construction of comb driver resonator and spring-mass system. Also, our simulation method is applied to predict etched shape for isotropic wet chemical etching process.

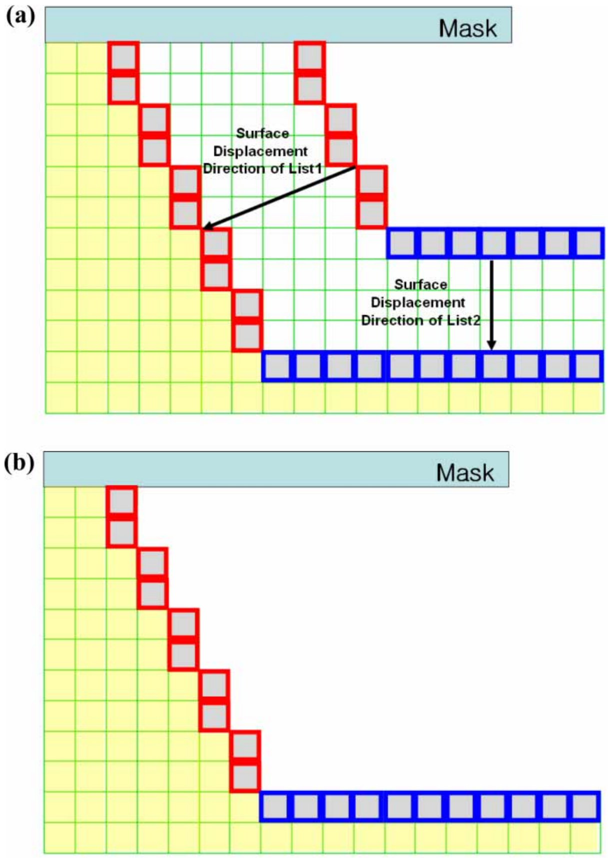

Figure 5. (a) Motion of surface cells along displacement direction and generation of new etch front during the time step, (b) the final etched shape after removing the etched cells.

Several simulation results demonstrate our simulation tool which is quite efficient for the design and development of MEMS device structure.

3.1 Isotropic wet chemical etching

Figure 6 shows result of wet etching a simulation which predicts the etched shape for isotropic etchants.

According to our simulation method, simulation region is divided into units of hexahedron-shaped cells. The simulation region is used the size 200 μm × 150 μm × 30 μm. This structure has total 900,000 (200 × 150 × 30) cells. This resulting is a final profile structure on the wafer after simulation in accordance with the user-defined layout and the processing of isotropic wet chemical etching procedure. The generated structure shows that, by means of our simulation method, fully isotropic topographical shape.

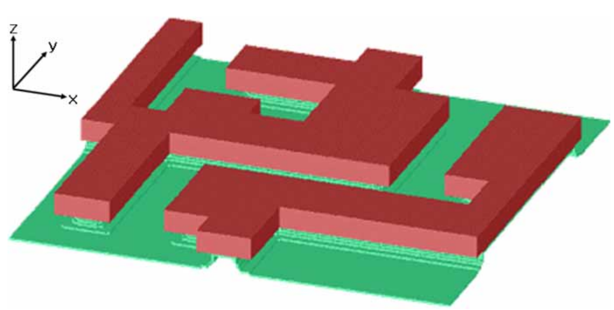

Figure 6. A schematic diagrams illustrating the result of wet etching a simulation which predicts the etched shape for isotropic etchants.

3.2 Comb drive resonator

Figure 7 shows the simulation result for structure of comb drive resonator.

This resulting is a final profile structure on the wafer after simulation in accordance with the user-defined layout and process procedure. The simulation region is used the size 257 μm × 234 μm × 2 μm. This structure has total 120,276 (257 × 234 × 2) cells. This structure is constructed moving comb, anchor, folded beam and stationary comb. The comb drive resonator is suspended by two folded beam flexures to form a mechanical mass-spring damper system.

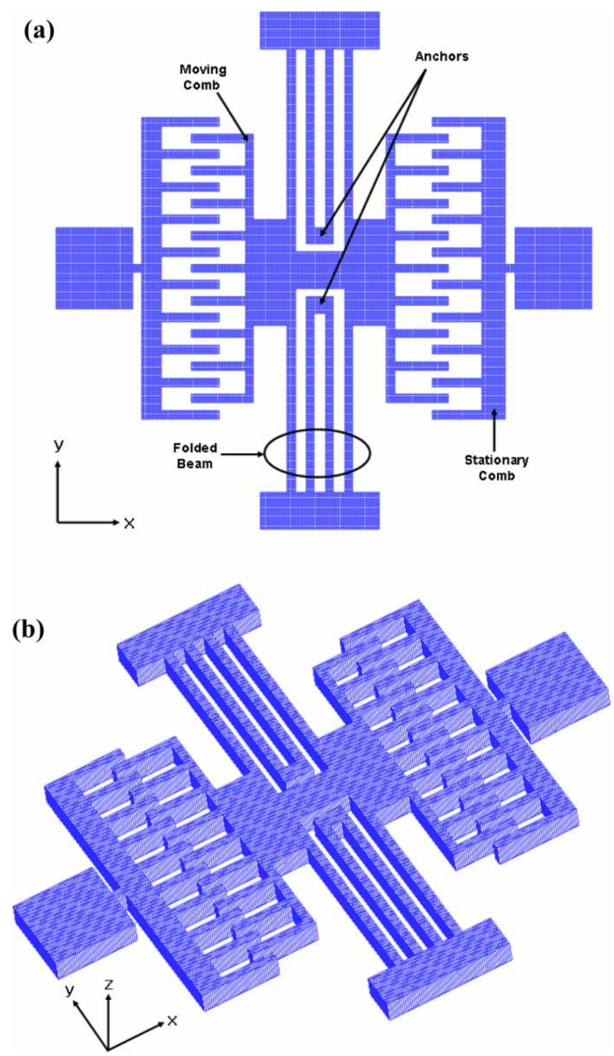

Figure 7. The simulation result of a comb drive resonator: (a) side view of $x-y$ plane direction, (b) bird-eye's view.

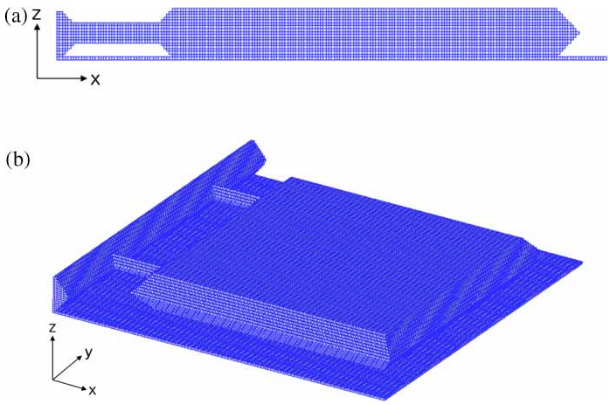

Figure 8. Simulation result of a spring-mass system (part of an acceleration sensor: (a) side view of x–y plane direction, (b) bird-eye's view.

3.3 Spring-mass system

The processing of anisotropic wet chemical etching which is the typical application of bulk micromaching technology of silicon. But bulk micromaching of silicon processing requires long etching times, since the substrate has to be etched in its whole thickness. Also, the geometric of MEMS device is required an accurate predictive simulation due to the anisotropic nature of the etching that is taking place. The accurately designed MEMS device structures derived from realistic simulations, which play an essential role to avoid waste of device development time and costs.

Figure 8 shows three-dimensional simulation results of the typical spring-mass system. This resulting is simulated with our simulation tool. The simulation parameter of typical spring-mass system is used ⟨100⟩-oriented wafer surface and KOH of 35 wt% and 60°C. The simulation region is used the size 200 μm × 200 μm × 25 μm. This structure has total 1,000,000 (200 × 200 × 25) cells.

4. Conclusion

In conclusion, we develop a simulation tool for the three-dimensional anisotropic wet etching of single-crystal silicon. Our simulation tool provides the capability of considering the etching properties of various materials and structuring techniques. And the developed simulation tool guarantees for the detailed analysis of complex three dimensional MEMS structures. Several simulation results demonstrate our simulation tool which is quite efficient for the design and development of bulk micromachining technology. Thus, it is considered that our simulation tool is very suitable to figure out the profile during the anisotropic wet chemical etching process.

Acknowledgements

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