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A Compound Semiconductor Process Simulator and its Application to Mask Dependent Undercut Etching

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This paper describes a process simulator that is designed to describe the etching and deposition processes used in constructing compound semiconductors, which have at least two different atomic species. This nature dictates a very different response to compound semiconductor process from the silicon process. One of the most remarkable processes in compound semiconductors is the reverse-mesa formation. This simulator successfully represents the mesa and the reverse mesa profiles that are often observed after chemical etching. The mask material dependence of the undercut etching can also be simulated with a good agreement between the experimental and the simulated shapes.

Keywords: process simulation, compound semiconductor, etching, undercut, mesa, reverse-masa

INTRODUCTION

Process simulators are widely used in silicon LSI fabrication, but do not yet play an important role in compound semiconductor processing. At present, the compound semiconductor process depends solely on the expertise of experienced operators. However, integrated optical devices and the highly functional optical devices being developed now require very precise shape reproduction. For this reason, a strong demand is emerging for simulators that can precisely describe these shapes.

In optical device processes, where the compound semiconductor is dominantly used, crystal orientation is important. Because optical devices transmit light as well as current, more attention has to be given to process damage. Chemical etching still plays an important role in the compound semiconductor process, therefore the chemical etching process as well as the physical etching process is required to be simulated. The shapes produced by chemical etching very much depend on the crystal orientation. This is especially true for the mesa and reverse mesa. The latter is a characteristic shape in compound semiconductors and is produced because of its binary nature. Thus, detailed representations of the mesa and the reverse mesa are indispensable for the process simulation.

COMPOUND SEMICONDUCTOR PROCESS SIMULATOR

A block diagram of the simulator is shown in Fig. 1. It has a modular construction and consists of three user-interface modules and three calculation modules. The calculation modules, the "Gas Distribution Module" (GDM), the "Crystal Orientation Module" (COM) and the "Surface Reaction Module" (SRM), determine the time evolution of the etching and deposition

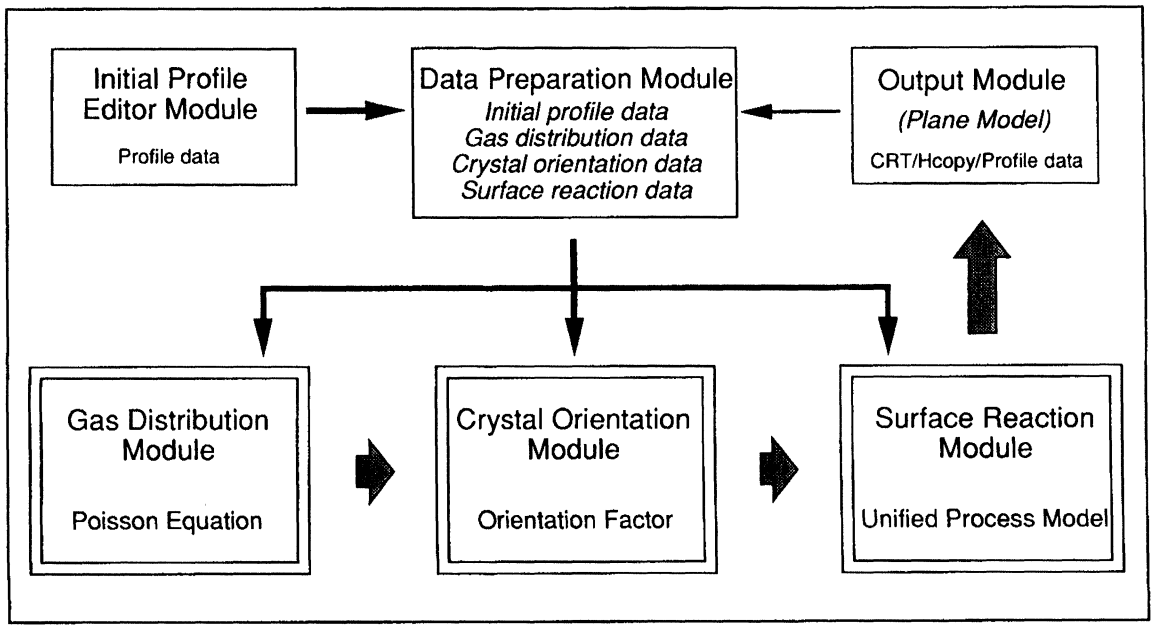

FIGURE 1 Block diagram of this simulator

processes. GDM and COM supplement the SRM and enhance the accuracy of its applications.

In this simulator, surface velocity plays a dominant role: It describes the time evolution of the processed surface of the specimen. SRM determines the surface velocity while the other two work to make adjustments to the surface velocity. The surface velocity is given by a unified process model using 6 simulation parameters (A, B, C, D, n, E), which are defined by the angle dependence of the reaction as well as the angle distribution of the incident particles. The simulation parameters thus correspond to the physical properties of the reaction. A describes the isotropic reaction, B and C the reaction caused by direct incident ions, D and n the reaction caused by the direct incident neutral particles, and E the reaction caused by the indirect incident particles. These parameters can be extracted from the actual etching or deposition profile of the reference sample, which has simple ridge structure. GDM calculates the correction coefficient of the surface velocity to represent the nonuniform gas distribution. The coefficient is determined by solving the Poisson equation. This module gives the detailed representation of the micro loading effect as well as the horizontal diffusion effect of the reactive gas. COM calculates the correction coefficient of the surface velocity to describe the crystal orientation dependence of the process. The crystal orientation dependence is given by the slow surface velocity for given surface orientations and angles near these orientations. This module reproduces the orientation dependence of the process. The characteristic mesa- and reverse mesa-face formation process is described by this module. Residual gas due to the nonuniform etching or deposition is also taken into account in the calculation.

MESA AND REVERSE MESA FACE REPRESENTATION

As described above, the crystal orientation is a key factor in the compound semiconductor process. The most noticeable manifestation of crystal orientation

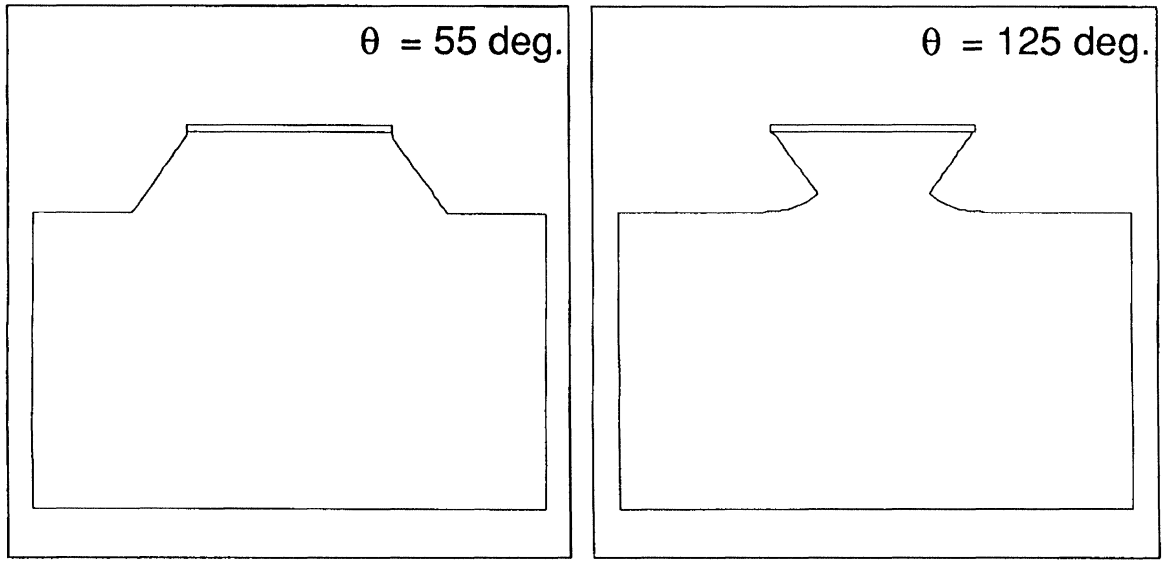

FIGURE 2 Simulated mesa and reverse mesa faces

dependence is in mesa and reverse mesa face formation. Figures 2(a) and 2(b) respectively show simulated etching profiles for mesa and reverse mesa faces. In this case ridge formation on (100) substrate was simulated in the pure isotropic reaction. The characteristic orientations were assumed to be 55 degrees for Fig. 2(a), and 125 degrees for Fig. 2(b), respectively. In this calculation, the GDM was bypassed and the residual gas re-distribution was ignored for the sake of simplicity. It can be seen from the figure that both the mesa and the reverse mesa shape were simulated successfully.

ACTUAL APPLICATION

Using this simulator, we simulated the mask dependence of the etching profile. It is often observed that the undercut etching profile is strongly affected by the mask. Figures 3(a) and 3(b) respectively show the experimental wet etching profiles of InP substrates with two different mask materials: SiO2 and SiN. The SiO2-masked InP has a large undercut etching, while the SiN-masked InP shows a smaller undercut. The difference is due to the difference in the adhesivity of the mask materials to the semiconductor surface. The deposition method as well as the mask material itself play significant roles in determining the adhesivity. This is difficult to simulate because the difference is not due to the etching characteristics of the mask material. To simulate these phenomena, we must include the adhesivity in some manner. For this purpose, we propose the virtual metamorphic layer model. A very thin virtual layer is employed below the mask material. This virtual layer acts as metamorphized interface and has a different etching rate from the mask and substrate material. The etching rate represents the adhesive strength of the interface. By introducing this layer, a less adhesive interface is effectively represented by the preceding etching of the thin interface region. This model is also applicable to the case where the interface is metamorphized by the upper layer deposition process.

The simulation results are presented in Figs. 4(a) and 4(b). The simulation conditions for both figures are the same except for the etching rate of each metamorphic layer. The etching rate of the metamorphic layer under the SiO2 mask (Fig. 4a) is assumed to be

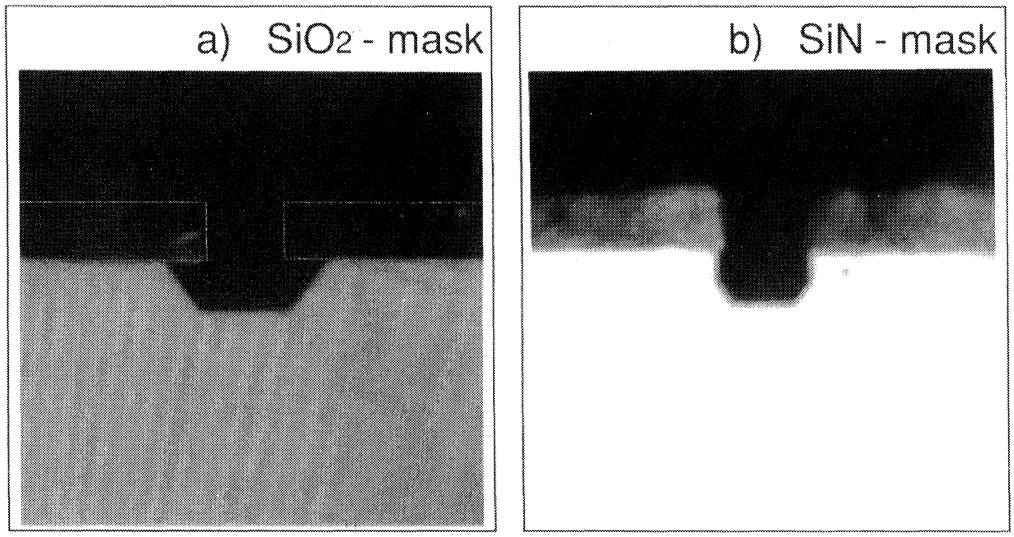

FIGURE 3 Wet etched profiles: (a) SiO2-masked InP. (b) SiN-masked InP

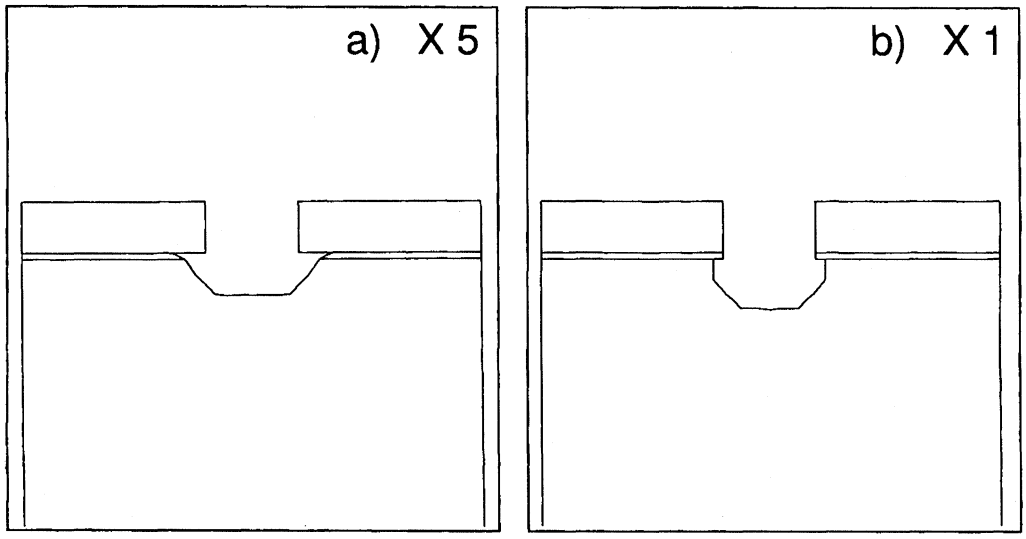

FIGURE 4 Simulated profiles: (a) Etching rate of the virtual metamorphic layer is taken to be 5 times the substrate. (b) Etching rate of the virual metamorphic layer is taken to be the same as that of the substrate

5 times that of the substrate material, while that under the SiN mask (Fig. 4b) is assumed to be same as the substrate material. The mask etching rate is taken to be zero. Good agreement between the results in Figs.3 and 4 can be seen which means this model works effectively.

CONCLUSION

In summary, a process simulator has been developed that describes the complicated etching processes on compound semiconductors. Using this tool, the crystal orientation dependence and the gas distribution

dependence of the process can be simulated precisely. As an actual application, we proposed the virtual metamorphic layer model and simulated the mask-dependent undercut etching, and got a good agreement between the experimental and simulated results.

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