Feature-Scale Simulations for Multi-Step Plasma Processing

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Plasma materials processing becomes ever more complex as technology advances, and simulations are often an integral part of process development. We present a set of simulations for processes that involve the challenge of multi-step processing. To demonstrate the capability of our simulations, we present results of simulations for two very different processes. The first is the Bosch process, which is a high etch-rate (in the range of 1000 A/s or more) etching for features with dimensions in the range of 1 micron to 100s of microns. The second is the Atomic Layer Etching, in which etching is done by a single atomic layer per cycle, allowing maximal processing accuracy but with an etch rate in the range of one to a few A/min. Both of these processes involve multiple cycles of the etching and passivation (or deposition) steps. Results of both 2D and 3D modeling are presented.

1. Introduction. Feature Scale Simulator FPS3D.

Semiconductor technology is advancing quickly; for the last forty years, it has followed Moore's law, which predicts that the number of transistors per area doubles every two years. Accordingly, features have decreased in size, and requirements for accuracy in processing have become much more stringent. This has led to improvements in plasma processing equipment and to much higher complexity of materials and processing chemistry. While experimentation is still the traditional way of finding optimal process parameters, the increased number of variables has led to the development of simulation methods which assist in finding optimal parameters and in guiding process engineers.

At Tokyo Electron [1], we have developed a powerful feature-scale simulator FPS3D [2-3] capable of 2D and 3D simulations. The advantage of having a single simulator operating with the same assumptions algorithms, and reaction sets in both 2D and 3D cases is significant; 2D simulations can be computed quickly to investigate a larger set of parameters of interest, while 3D simulations could then be applied to a more narrow set of parameters to capture the 3D effects of geometries.

Our calculations have demonstrated that features such as trenches can be accurately simulated as 2D objects, while 2D and 3D simulations of most other features, such as vias, produce different results. Correspondingly, 2D simulations for those cases can only be used as a rough approximation to investigate trends.

Multi-step processing has now become a standard method both for IC fabrication and for micromachining, especially in cases for which deep etching is required. By multi-step processing, we mean materials processing, such as etching or deposition of materials, that is carried out in several time-steps, typically in cycles. Each time-step has its own parameters such as time of application, chemical composition of incoming fluxes, and energy and angular distributions of species.

Development of a feature-scale simulator is a challenging task which has been attempted for over 40 years. Early methods, such as a string model [4-5], method of characteristics [5-7], or the level-set method [8-9] relied upon local etching or deposition rates. These rates were used as the local velocities with which the surface of the profile was advanced at each position. Those local reaction rates are proportional to the corresponding fluxes and are functions of the energy of incoming species, their angle of incidence, and the local surface coverage by various species.

However, it is not a trivial task to calculate local fluxes for those methods, especially due to potential re-emission of species from various parts of the profile. Such calculations require significant computational time, and moreover, to account for possible shading, the local fluxes must be recalculated upon each slight change of the profile.

Another group of feature-scale simulators [10-17] was based on a very different approach, using the so-called cellular model. In this model, the full simulation space is divided into 2D or 3D rectangular cells, with each cell representing a particular material or a vacuum. Removing some material cells (converting them into a vacuum) represents etching of solid materials, while adding some cells (giving them material identity) represents deposition. This is a general and flexible approach, which can easily describe complex 2D and 3D geometries. We have used the cellular model in developing FPS3D.

In FPS3D, we do not use the typically applied simplifying assumptions either requiring each cell to contain only one type of molecule or the same number of molecules. In our approach, a material cell may contain any number of different molecules, from a single molecule up to the maximum number of molecules, calculated from the given volume of the cell and the number densities of the corresponding materials.

The number of molecules, ions, radicals, and photons coming to the surface could be too large for direct simulation of interaction of each of them with solid materials. For the sake of computational efficiency, these species are grouped into computational particles, each containing from a single to a large number of the same species. In FPS3D, incoming particles can be chosen to contain significantly fewer species than the number of molecules in a cell. This improves the statistical accuracy of resulting reactions and helps to avoid the artificial roughness of simulated profiles.

2. Simulation of Bosch Processing

The two most well-known high-etch-rate techniques for deep silicon etching are cryogenic etching [18] which requires temperatures to be in the range of -110°C during etching, and the so-called Bosch etching [19-20]. Bosch etching requires high density inductively coupled plasmas and uses alternating steps of isotropic etching by SF_6 and wall passivation (polymer deposition) by c-C_4F_8 to obtain vertical profiles.

Many other schemes for efficient deep silicon etching were proposed and investigated. These sometimes used gases other than the usual SF_6 and c-C_4F_8 , or used mixtures of gases, and did not necessarily require high density inductively coupled plasmas [21-22]. A similar technique to that used in Bosch processing was sometimes called gas chopping [21-22] or time multiplexed deep etching [23].

There are many publications which provide specific information on particular experiments which use the same chemistry as does the Bosch process; they suggest a set of main reactions (see, for example, [24-25]). We have used some of this data but only to put the reaction parameters in the right range.

In simulations presented in this article, the following parameters were used. During the polymer deposition time-step, the flux of the main polymer depositing species CF_2 was set to $2.4*10^{19}$ $cm^{-2}s^{-1}$ for the duration of 4 s. An intermediate transitional time-step of 1 s was set, during which the fluxes gradually change from the deposition regime to the etching regime. For the etching time-step, the fluxes of the main species, F radicals and SF_3^+ ions, were respectively set to the values of $5.4*10^{19}$ and $8.4*10^{16}$ $cm^{-2}s^{-1}$. After the etching step, an intermediate transitional time-step was set again during which the fluxes change back to the polymer deposition regime. These four time-steps represent a single cycle. During Bosch processing, this cycle was repeated many times.

The incident fluxes of reactive species to the wafer change over time in cycles, as shown for the main species, CF_2, CF_3+ and F, in Fig. 1.

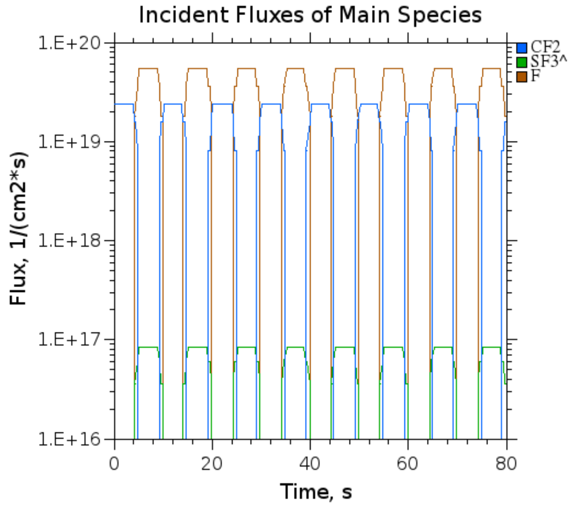

Fig 1. Time variation of species fluxes.

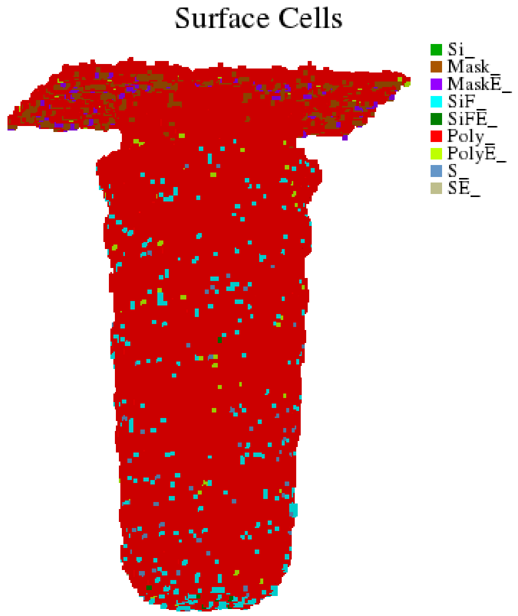

Fig 2. Surface cells during the polymer deposition.

Bosch etching was simulated for a via with a diameter of 1 μm. Fig. 2 presents the view of surface cells in the via at the moment at which most of its internal surface is covered by the teflon-type polymer (shown in red). To see more clearly the cells’ structure inside and outside of the via, Fig. 3 shows a mid 2D cross-section of it.

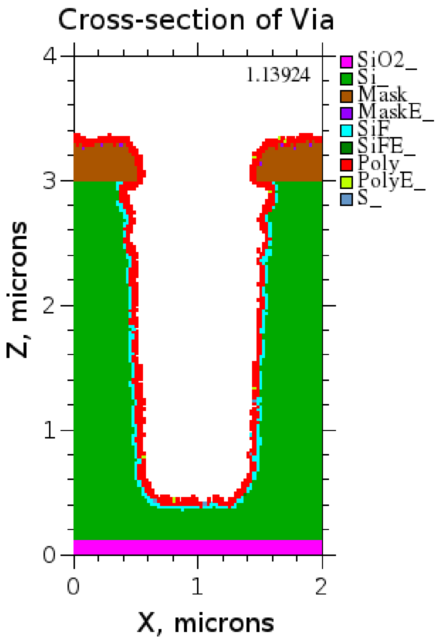

Fig 3. Cross-section of via corresponding to Fig 2.

The scales (or ripples) on the sides of the via correspond to process cycles. This is a typical feature of the Bosch process. The bottom of the via is periodically covered with the polymer, which is removed during the etching steps, as shown in Fig 4.

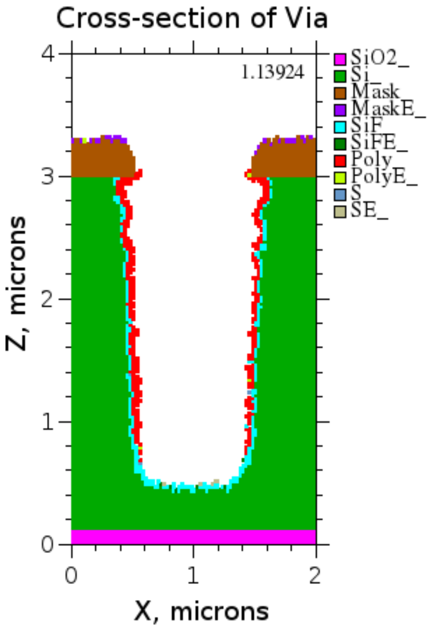

Fig 4. Cross-section of via during the etching step.

In Bosch etching, the height of the bottom of the via decreases periodically, as shown in Fig 5. The polymer deposition steps cause small increases in height, while etching steps sharply reduce the height.

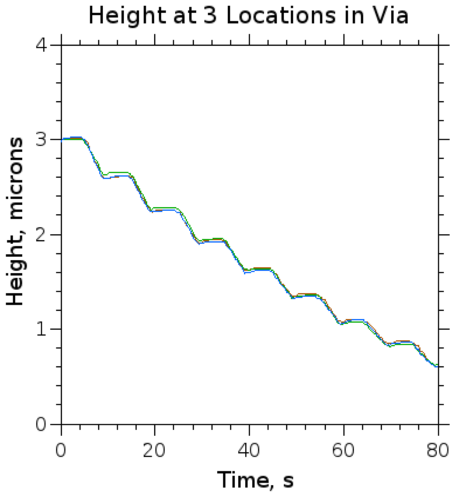

Fig 5. Height change at the bottom of the via.

The instantaneous etch rate was recorded at three locations near the bottom of the via and is shown in Fig 6. The gradual decrease in etch rate with each new cycle is due to the etch rate's dependence on the aspect ratio of the via, which grows over time as the via deepens.

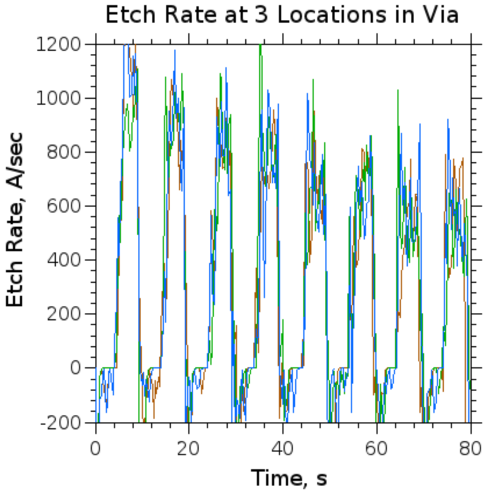

Fig 6. Instantaneous etch rate in the via.

The positive values in Fig. 6 correspond to etching, while the negative ones correspond to deposition.

3. Simulation of Atomic Layer Etching

Atomic Layer Etching (ALE) [26-31] is an advanced etching method allowing much more precise and conformal etching than attainable via traditional methods. ALE has been explored since beginning of the 1990s, but still has significantly fewer applications than its counterpart, Atomic Layer Deposition (ALD) [32-33], which has found numerous applications in technology.

Here we present FPS3D simulations of ALE, in which ALE is applied to smooth an initially rough profile. The ALE cycle consists of two time-steps. The first step corresponds to the application of low-energy Ar+ ion flux with a narrow ion energy spectrum (between 25 and 27 eV) for the duration of 100 s. During the second step, which lasts for 20 s, Cl_2 gas is applied to the previously activated Si surface to chlorinate it, producing $SiCl_2$ surface species. The ion energy in the first step is such that it is enough to etch the $SiCl_2$ monolayer, but not enough to sputter Si from the bulk.

Fig. 7 shows an initial profile obtained after Si sputtering by high energy Ar+ ions (at 1 keV). The significant roughness of the profile is evident.

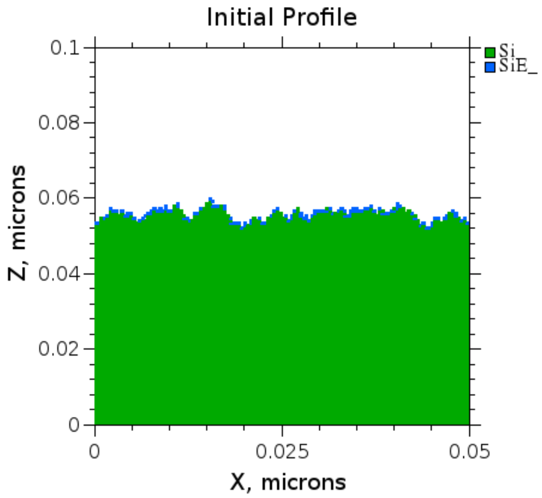

Fig 7. Profile after Si sputtering by Ar+ ions.

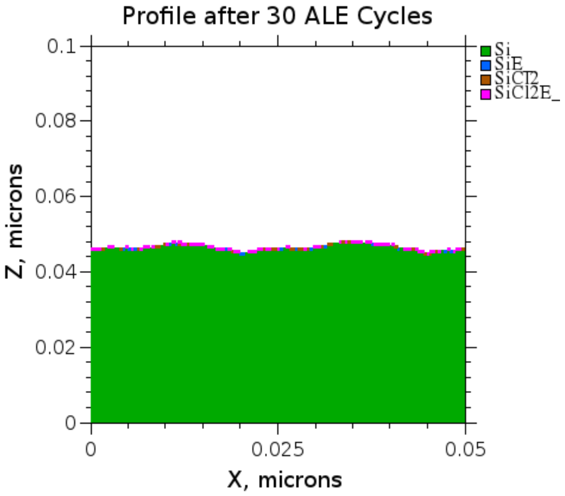

Fig 8. Profile smoothing after 30 ALE cycles.

Fig. 8 demonstrates the effect of smoothing that profile by application of 30 ALE cycles as described.

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