

Twisting in High Aspect Ratio Etching with Charging Effects as a Stochastic Mechanism

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Abstract— Twisted profiles in high-aspect-ratio etching are anomalous features that significantly affect device performance. In this paper, we investigate the charging effect on the twisted profiles as a stochastic phenomenon using an in-house voxel-based Monte Carlo dry-etching simulator. We develop a novel algorithm for charged-particle transport that drastically reduces computational cost and makes it possible to run multiple simulations over a large parameter space. As a demonstration, we introduce the quantitative definitions that characterize the strength of twisting, and discuss the dependence of the polymer-deposition probability on the twisting. Our quantitative analysis reveals that the strength of the twisted profile depends on the polymer-deposition probability, and is suppressed once the probability exceeds a critical threshold. Our work shows that the twisted profile emerges as a stochastic mechanism and provides support for process development of advanced three-dimensional semiconductor devices.

Keywords—HARC, Topography, Voxel, Twisting

I. INTRODUCTION

The dry-etching process is a critical step in microelectronics fabrication. The typical target of the process is the high-aspect-ratio (HAR) etching of holes and trenches in dielectric layers. In current technology, the diameter of the holes is about ten nanometers, and the aspect ratio exceeds 70 for memory cells in large arrays. The high aspect ratio makes controlling vertical etching a major challenge. Several anomalous features appear during HAR etching, and they affect device performance. Therefore, their fundamental origins must be thoroughly understood.

Twisting is one of the anomalous features, and randomly emerges after a significant fraction of the feature has been etched. One of its origins that has been proposed so far is non-uniformity of macroscopic parameters - such as ion- and neutral-energy-angular distributions and fluxes- which can be

controlled by changing the reactor parameters. The patent literature [1] explains that the careful choice of frequencies and powers in multifrequency capacitively-coupled plasma can reduce the incidence of twisting. A small feature opening to the plasma may also contribute to twisting. For a smaller size of the mask opening, the number of radicals and ions entering the feature becomes small, leading to statistical variations. Once charging effects become active, the statistical fluctuations of charged particles entering the feature become even more important. This produces an asymmetric surface-charge profile and electric field. Since ion trajectories are bent by the asymmetric electric field and the ion interacts with surface materials, the twisted profile appears. Electrons also play an important role in neutralizing charge. In [2], they discussed that the high energy electrons suppress the twisting. Recent multiscale modeling [3] combined chamber-scale plasma simulations with a feature-scale model to capture charging-induced tilting and twisting, providing a predictive tool for 3D NAND optimization.

To investigate twisting as a stochastic phenomenon, we develop a voxel-based Monte-Carlo (MC) dry-etching simulator that includes charging effects using a low-cost algorithm for charged-particle transport, enabling us to run more than 1000 statistically independent simulations. We also demonstrate the parameter dependence of the occurrence frequency of twisting.

II. MODEL DESCRIPTIONS

Our dry-etching process simulator is based on the voxel method. In the method, the numerical domain is divided into three-dimensional cubes, called voxels, and the structure is expressed by the number of material particles in each voxel. The voxel size Δ determines the resolution of the structure. In our voxel method, each voxel can contain up to N_{max} material particles. The simulation flow of the simulator is summarized in Fig.1. In the beginning of the simulation, data

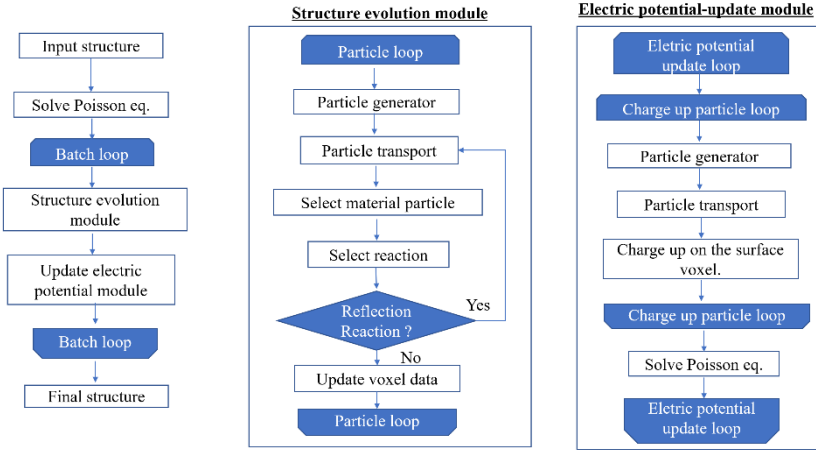


Figure 1: Simulation Flow

of the initial structure is loaded, and expressed as voxels. When the boundary condition of electric potential is non-trivial, the source-free Poisson's equation is solved, and the electric-potential profile is obtained. After that, the dry-etching simulation module starts. The module can be divided into two sub-modules.

A. Structure evolution module

In the module, neutral or charged particles are selected by a MC method using the gas fluxes at the source positions, and their trajectories are computed until they intersect a material surface. The initial velocity of each particle is calculated from the energy and angular distribution. The energy angular distribution of ions in plasma has been well studied. Reference [5] shows that the angular distribution with small-angle limit can be approximated by Gaussian function:

$$f(\theta) \propto e^{-\frac{\theta^2}{2\sigma^2}}. \quad (1)$$

Instead of using the Gaussian function, we use the following angular distribution function:

$$f(\theta) \propto \cos^m \theta, \quad (2)$$

where m is the exponent that characterizes the strength of particle anisotropy. For large m , Eq.(2) has similar profile as the Gaussian profile with small-angle limit. On the other hand, for small m , it shows the isotropic angular distribution.

For neutral particles, the trajectories are straight lines and are computed with a Digital Differential Analyzer (DDA) algorithm. On the other hand, charged particles are deflected by the electric field and obey Newton's second law:

$$M\ddot{\vec{x}} = q\vec{E}, \quad (3)$$

where M is the ion mass, q is ion electric charge, and $\vec{E}$ is the electric field:

$$\vec{E} = -\vec{\nabla}\phi. \quad (4)$$

The electric potential ϕ is obtained from the Poisson-solver sub-module (described later).

In the conventional algorithm of the charged particle transport with voxel method, the electric field is assumed to be constant inside the voxel. With the assumption, the particle trajectory in the voxel is expressed as a quadratic function of time:

$$\vec{x} = \frac{q}{2M}\vec{E}t^2 + \vec{v}_0t + \vec{x}_0, \quad (5)$$

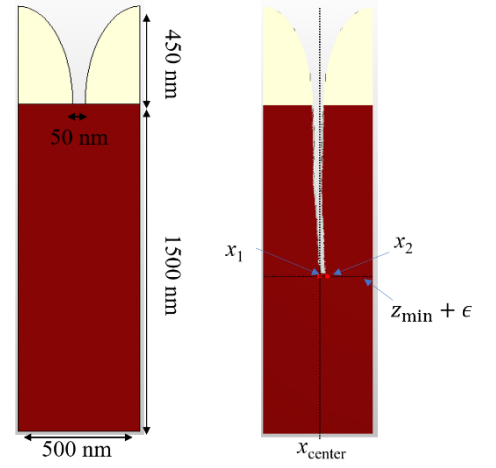


Figure 2: Left panel shows the initial structure of the simulation. Right panel shows the example of twisted hole.

where $\vec{E} = (E_x, E_y, E_z)$ is the electric field inside the voxel, $\vec{v}_0 = (v_{0x}, v_{0y}, v_{0z})$ is the particle velocity and $\vec{x}_0 = (x_0, y_0, z_0)$ is the position when the particle enters the voxel. t denotes the time since the particle entered ($t = 0$ at entry). To identify the next voxel at which the particle reaches, we calculate the intersection between the trajectories Eq.(5) and each voxel boundary. For example, the intersection with the voxel bottom boundary which vertices are $(x_b, y_b, z_b), (x_b + \Delta, y_b, z_b), (x_b, y_b + \Delta, z_b), (x_b + \Delta, y_b + \Delta, z_b)$ can be calculated by solving the following equation for t :

$$z_b = \frac{q}{2M}E_z t^2 + v_{0z}t + z_0. \quad (6)$$

If real roots exist, we define the intersection time t_{-z} as the positive smaller root among the two solutions, and check x and y coordinate of the intersection point is in the voxel boundary:

$$x_b \leq \frac{q}{2M}E_x t_{-z}^2 + v_{0x}t_{-z} + x_0 \leq x_b + \Delta, \quad (7)$$

$$y_b \leq \frac{q}{2M}E_y t_{-z}^2 + v_{0y}t_{-z} + y_0 \leq y_b + \Delta. \quad (8)$$

If these two inequalities are satisfied, it is one candidate of the intersection point. We can calculate other intersection times for other voxel boundaries by same way, and the intersection with the smallest intersection time corresponds to the actual intersection, and update the voxel including the particle. This step is executed iteratively until the particle reaches the surface voxel. Since this algorithm is complicated, it is computationally expensive.

In our particle transport algorithm [4], instead of using the quadratic function, the particle trajectory is assumed to be a straight line in the voxel:

$$\vec{x} = \vec{v}_0t + \vec{x}_0. \quad (9)$$

In this case, it is relatively easy to calculate the intersection point using the same algorithm as DDA. For example, if all components of the velocity vector are positive ($v_{0x} > 0, v_{0y} > 0, v_{0z} > 0$), the intersection time can be calculated by the following equation:

$$t = \min\left(\frac{x_b + \Delta - x_0}{v_{0x}}, \frac{y_b + \Delta - y_0}{v_{0y}}, \frac{z_b + \Delta - z_0}{v_{0z}}\right). \quad (10)$$

The next voxel which the particle enters also can be identified. The velocity is updated by calculating the impulse acting on the particle while it moves inside the voxel:

$$\vec{v}_0 \rightarrow \vec{v}_0 + \frac{q}{M} \vec{E} t. \quad (11)$$

Although the resolution of the integration is low, we found that the final structure is almost same as the native algorithm, and computational time can be drastically reduced.

The above algorithm becomes low resolution when the electric field is enough large for the particle direction to change in a voxel. Our patent [4] describes the further improvement of the algorithm.

When particle reaches a surface voxel, reaction judgements are executed. In the reaction judgement, one material particle in the voxel is randomly selected, and the possible reaction between gas particle and the material particle is randomly selected based on the reaction probabilities. The reactions between the gas particle and material particle are user input parameters. In our simulator, specular reflection, diffuse reflection, adsorption, etch, sputter, and depo reactions are implemented. Based on the selected reaction, the material particles in the voxels are updated. When the surface voxel storing electric charge becomes air voxel by etch or sputter reaction, the electric charge is redistributed into near voxels.

B. Electric-potential-update module

Electric-potential update module is divided into two sub-modules, charge-up and Poisson-solver. In charge-up sub-module, ions and electrons are generated based on their fluxes, and their particle trajectories are calculated. The electron flux is automatically decided from neutralization condition. When they hit a surface voxel, the electric charge of the voxel is updated. In our simulator, ions in the module do not change the structure, and only contribute to charge accumulation on the surface voxel.

In Poisson-solver sub-module, we solve the Poisson's equation using the charge density ρ and permittivity ϵ :

$$\vec{\nabla} \cdot \epsilon \vec{\nabla} \phi = -\rho, \quad (12)$$

and update the electric potential. After the potential is updated, the charge-up sub-module is called again. This iteration continues until the total number of ions and the electrons in the module reaches the prescribed number. In our simulations, the bottom boundary condition of the electric potential is Dirichlet boundary condition with $\phi = 0$, and the top boundary condition is Neumann boundary condition with

$$\frac{d\phi}{dz} = 0. \quad (13)$$

The boundary conditions in the x- and y-directions are reflective boundary conditions. The execution frequency of the electric potential update module is user-defined parameter, and the number of executions determines the temporal resolution of charging simulations. Ideally, the Poisson-solver sub-module would be executed after each single-particle insertion in the charge-up sub-module. However, since the Poisson-solver is computationally expensive, we update after every 5-10 ions or electrons are processed in the charge-up sub-module.

Our simulator alternately executes the structure evolution module, and electric potential update modules, and obtains the etched structure including the charging effects.

III. RESULTS & CONCLUSION

We performed 6000 ion-assisted etching simulations with sidewall-protection-film depositions while varying the random seed of the MC method. Although our simulator can calculate three-dimensional etching simulations, we focus on two-dimensional simulations by assuming a geometrically thin structure for computational simplicity. The left panel in Fig.2 shows the initial structure. It consists of SiO₂ (dark red) and dome shaped photoresist (light yellow).

In order to simplify the plasma source and complex reaction sets, we employ two neutral gases A_g and B_g, and charged ion I_g. The flux of neutral gas A_g is 0.02 [mol/m²sec], and the flux of neutral gas B_g is 0.007[mol/m²sec]. Ion's flux is 0.0008 [mol/m²sec]. Since the neutral gases have isotropic angular distribution, their exponents are 1. On the other hand, the ion has an anisotropic angular distribution, and its exponent is 10000. Ion electric charge is 1[e], and its mass is 1 amu. We assume that the ion energy distribution is uniform between 0 eV and 200 [eV].

For simplicity, we use minimum reaction set for ion-assisted etching. As a first step, neutral gas A_g reacts with SiO₂, and SiO₂ converts to SiA as an adsorption reaction. Neutral gas B_g reacts with SiA, and produces Poly (the polymer layer) with probability p. When the charged ion I_g hits the surface with SiA or Poly, the impacted material is sputtered.

The right panel in Fig.2 shows one of our simulation results, where a twisted etched profile is clearly visible. We define

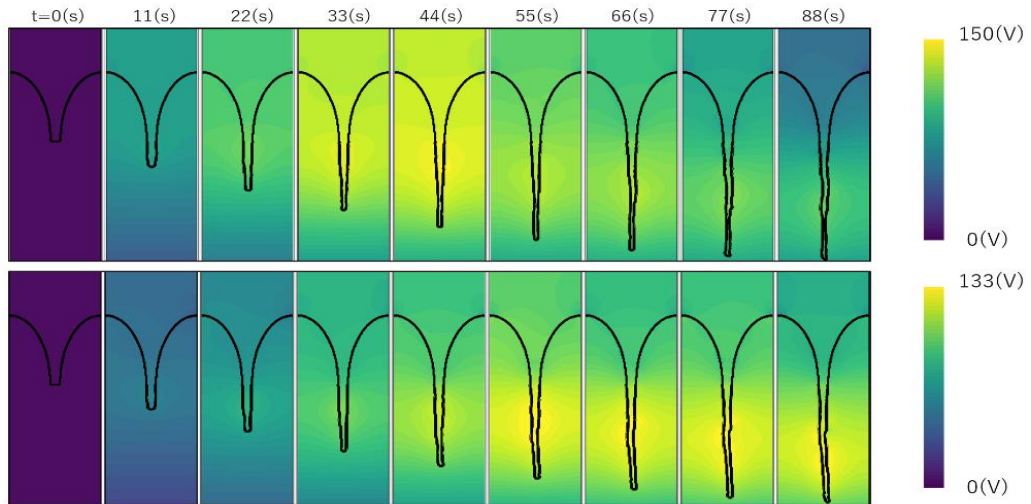


Figure 3: Top panel shows the snapshot of the electric potential without the twisted profile. Bottom panel shows the snapshot of the electric potential with the twisted profile.

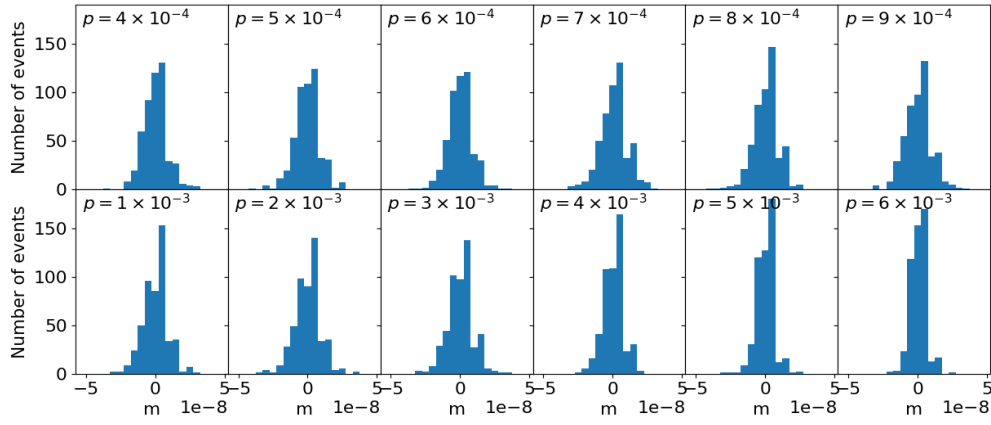


Figure 4: Histogram showing the distribution of the twist.

the strength of the twist as follows. Geometrically, the twisting can be characterized as the difference between the center of mask opening, and the center of bottom of etched profile. We identify the bottom z-coordinate $z_{\min}$ of the etched profile, and extract the intersection points between the etched profile and horizontal line defined as $z = z_{\min} + \epsilon$ (see the right panel in Fig.2), where ϵ is small value which is typically the size of a voxel. In general, there are two intersection points x_1 and x_2 , and the center of these two points is bottom center. We can also obtain the center of mask opening x_{center} from the initial structure. Using these measurement results, we define the twist as following equation:

$$\text{twist} = \frac{x_1 + x_2}{2} - x_{\text{center}} \quad (14)$$

By varying the MC seed, we obtain twisted features as statistical variations. Figure 3 shows the two examples of the snapshots of the electric potential in time. Top panel is the results in which the twist does not emerge, and bottom panel is the results in which the twist emerges.

We performed several simulations, and analyze the polymer-deposition probability dependence of the twist. For small deposition probability, ions can enter the bottom of the trench, and sputter the materials. On the other hand, for large deposition probability, Poly clogs the trench, preventing ions from reaching the bottom and effectively suppressing the sputtering reactions. In our setup, the typical critical deposition probability is $p_{\text{crit}} \simeq 4 \times 10^{-3}$. For $p > p_{\text{crit}}$, the deposition reaction dominates, and clogging occurs. Using the twist definition, we summarize the histogram of frequency distributions for different deposition probabilities. (see Fig.4). The figure shows that the twisted feature has a statistical variance. Figure 5 shows the dispersion of the twist.

These results show that the polymer-deposition probability is important factor governing twist formation. It suggests that operating the process above the critical deposition threshold suppresses the twist and enables uniform HAR etching. The intuitive and physical understanding is as follows. For large deposition probability, the gas region through which ions can

pass becomes narrow. The deflected trajectories only etch the polymer, and cannot contribute to etch the hole. On the other hand, the relatively straight trajectories can enter the narrow gas region, and they contribute the vertical etching.

It is promising that the statistical simulation framework with our proposed charged-particle-transport algorithm provides a practical tool to predict and mitigate twisted profiles in advanced three-dimensional semiconductor manufacturing.

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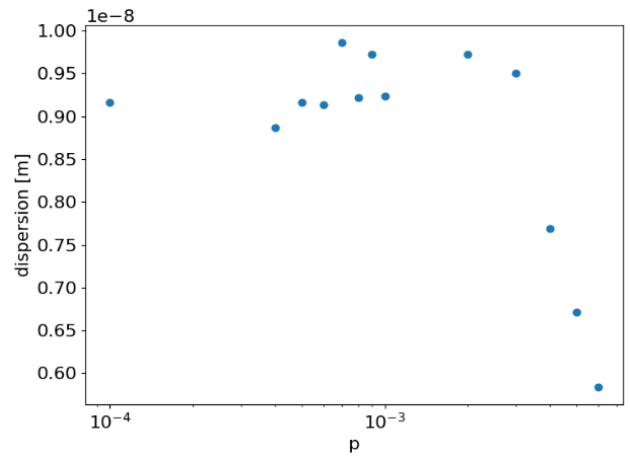


Figure 5: Dispersion of the twist as function of deposition probability