Modeling on Tilting and Twisting Distortions of 3D NAND High-Aspect-Ratio Etching

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***Abstract*—Plasma etching plays a key role in forming high-aspect-ratio (HAR) structures critical for modern three-dimensional memory technologies. In this study, a multiscale modeling framework is developed to investigate tilting and twisting distortions during HAR plasma etching of SiO_2/Si_3N_4 multilayer structures. The model integrates two-dimensional chamber-scale plasma simulations with a feature-scale etching profile evolution model to capture plasma characteristics and their impact on etching profiles at the feature scale. Simulation results demonstrate that ion incidence angle governs profile tilting, while stochastic charge accumulation on trench sidewalls induces profile twisting. This integrated approach offers a predictive tool to understand and optimize plasma etching processes for advanced semiconductor fabrication.**

Keywords—3D NAND, Multiscale Modeling, High-Aspect-Ratio Etching, Tilting, Twisting

I. Introduction

The plasma etching process of dielectric materials with high-aspect-ratio (HAR) features plays an essential role in manufacturing cutting-edge 3D memory devices[1], such as 3D NAND, as shown in Fig.1(a). As device dimensions shrink and structural complexity increases, precise control of feature profiles becomes critical to ensure functionality and yield[2].

However, feature distortions often occur due to complex physico-chemical mechanisms during plasma etching[3]. Among them, tilting and twisting are two commonly observed defects, illustrated in Fig.1(b). While both represent deviations from the ideal vertical structure, their causes and characteristics differ[4]. Tilting refers to the inclination of the feature sidewall, mainly caused by non-uniform ion angular distributions across the wafer, which originates from asymmetries in the plasma sheath. In contrast, twisting is a rotational deformation of the feature profile along its depth, driven by asymmetric surface charging and the resulting lateral electric fields[5].

To investigate these phenomena, we developed a multiscale modeling framework that integrates chamber-scale plasma simulations with feature-scale profile evolution modeling. This approach captures the ion angular distribution from equipment simulations and incorporates charging effects into the feature-level etching model, enabling a better understanding of the origins and mitigation strategies for tilting and twisting defects.

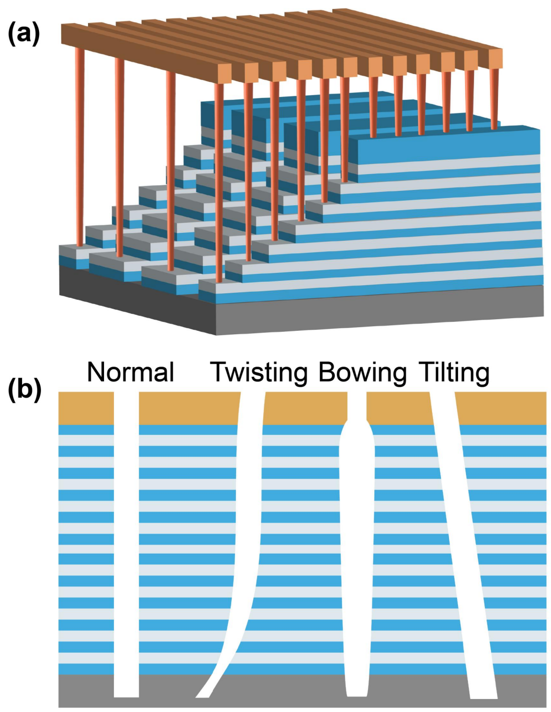

Fig.1 (a) 3D NAND structure, (b) Common Defects in HAR etching: Normal, Twisting, Bowing, Tilting

II. The Description of Multiscale Modeling

In this work, we established a multiscale modeling framework that bridges the gap between chamber scale and the feature evolution scale. As illustrated in Fig.2, this integrated approach consists of two main modules.

A. Chamber-scale plasma simulations

To reproduce realistic plasma conditions within the reactor chamber, a two-dimensional axisymmetric model of a Capacitively Coupled Plasma (CCP) reactor was developed using the finite element method. This model couples multiple physics interfaces, including plasma, laminar flow, heat transfer, and charged particle tracing. By coupling these physics, the model captures the interplay between plasma species, thermal fields, and fluid dynamics, which collectively influence plasma behavior. The simulation output includes detailed particle fluxes as well as their angular and energy distributions, which serve as inputs for the feature-scale model

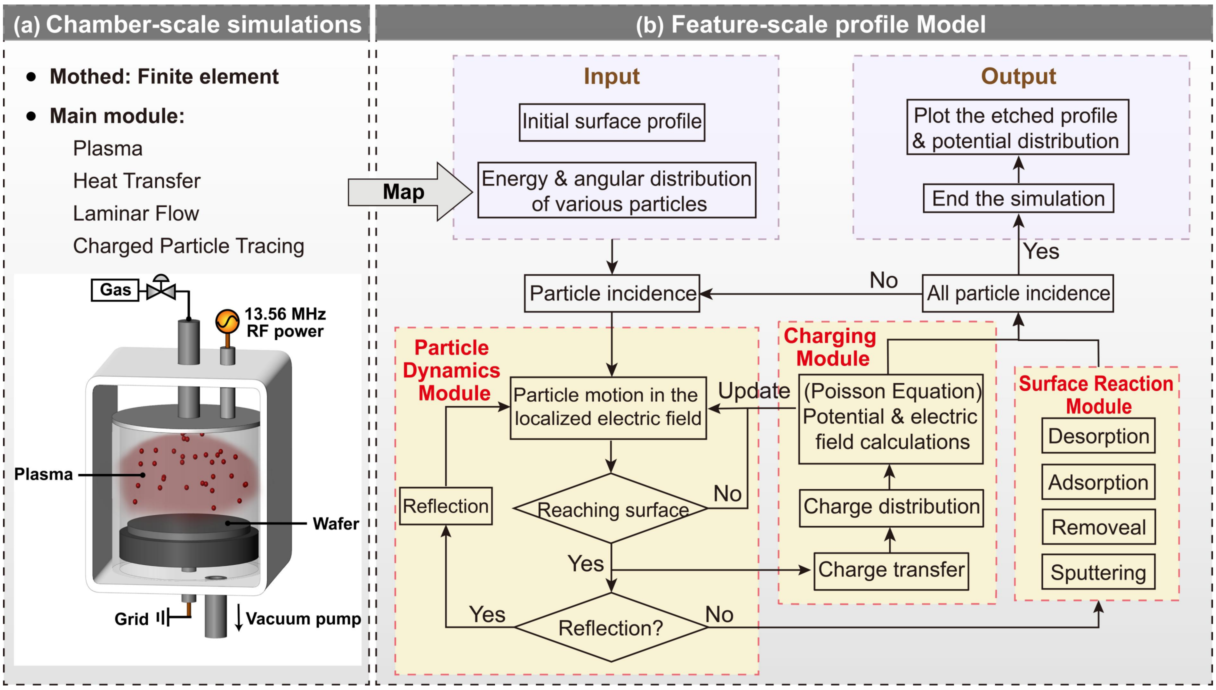

Fig. 2. Workflow of the multiscale model: (a) Chamber-scale plasma simulations capturing plasma dynamics and particle flux distributions; (b) Feature-scale profile model simulating the profile evolution under plasma etching.

B. Feature-scale profile evolution

The feature-scale model combines the cellular automaton and Monte Carlo methods to address the etching behavior of high aspect ratio (HAR) structures considering the charging effect.

- Input: The initial surface profile is imported and discretized using the cellular method, with each cell representing different materials, as shown in Fig.3. The angular and energy distributions of incident particles are mapped from the results of the chamber-scale simulation results. The Monte Carlo method is then used to particles' initial positions and velocity vectors based on these distributions, establishing realistic boundary conditions for particle incidence[6].

- Particle Dynamics Module: Particles trajectories follow Newton's second law under local electric fields. Upon surface contact, ions reflect nearly specularly with partial energy loss, while neutral particles undergo diffuse scattering.

- Charging Effects Module: Charge accumulation on dielectric surfaces alters the local electric potential, which in turn affects particle trajectories and surface reactions. The potential distribution is obtained by solving Poisson's equation. This dynamic feedback loop between charging and particle motion ensures realistic evolution of surface potentials during etching.

- Surface Reaction Module: Surface reactions are simulated using Monte Carlo methods to capture their stochastic nature. The module includes four key surface reactions: adsorption, chemical removal, desorption, and sputtering. Among these, sputtering is treated as a physical erosion mechanism, with its probability depending on the energy and collision angle of incoming particles.

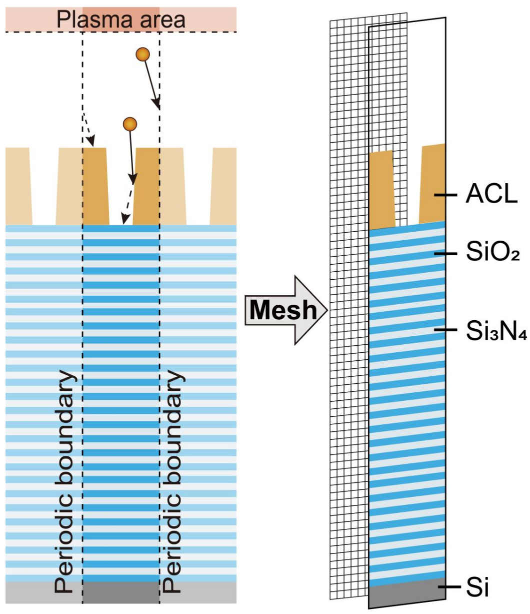

Fig.3 Initial surface profile discretized for feature-scale simulation.

III. RESULTWS AND DISCUSSION

In this study, we simulated HAR plasma etching in SiO_2/Si_3N_4 multilayers structure using a CCP reactor with $C_4F_8/Ar/O_2$ gas mixtures. The initial surface profile in the feature-scale model was established with an open critical dimension (CD) of 50 nm, and each underlying layer had a thickness of 40 nm, resulting in a total stack thickness of 1840 nm.

A. Tilting

Fig.4 presents the simulation results of the CCP simulation under specific process conditions, including (a) the electron density distribution, (b) the potential distribution, and (c) the lateral electric field. Notably, an uneven lateral electric field is observed near the wafer surface, particularly near the wafer edge. This asymmetry influences ion trajectories, resulting in angular deviations that affect etching uniformity.

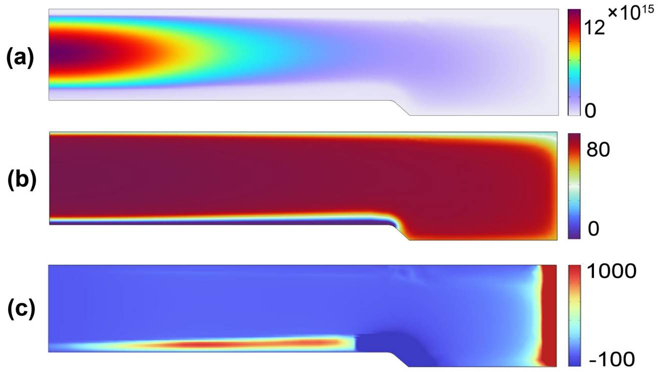

Fig.4 The results of CCP simulation under specific process conditions: (a) electron density, (b) potential distribution, and (c) lateral electric field.

To further investigate this effect, three representative points were selected along the wafer radius: Point A at the center, Point B at mid-radius, and Point C near the edge, as illustrated in Fig.5(a). Ion incidence angular distributions extracted at these points (Fig. 5(b)) reveal that ions near the wafer edge (Point C) exhibit larger deviations from the surface normal, consistent with the stronger lateral fields in that region.

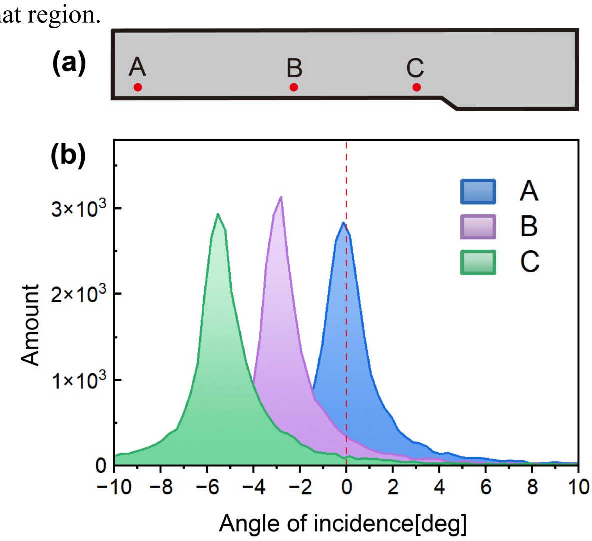

Fig. 5. (a) Schematic of selected points A, B, and C along the wafer radius. (b) Ion incidence angular distributions at points A, B, and C.

To assess the impact of these angular deviations on feature-scale etching, the ion energy and angular distribution data from Points A, B, and C were incorporated into a feature-scale etching model. The resulting etched profiles are shown in Figs.6(a)-(f), where Figs.6(a), (c), and (e) correspond to the ion distributions at the three points, and Figs. 6(b), (d), and (f) show the respective etched features. A clear tilting of the etch profiles is observed, particularly at Point C, where the ion incidence angle exhibits the largest deviation from normal incidence. Fig.6(g) quantitatively compares the ion incidence angles with the measured profile tilt angles, revealing a strong correlation. This suggests that the ion incidence angle plays a dominant role in determining the direction and degree of profile tilting during etching.

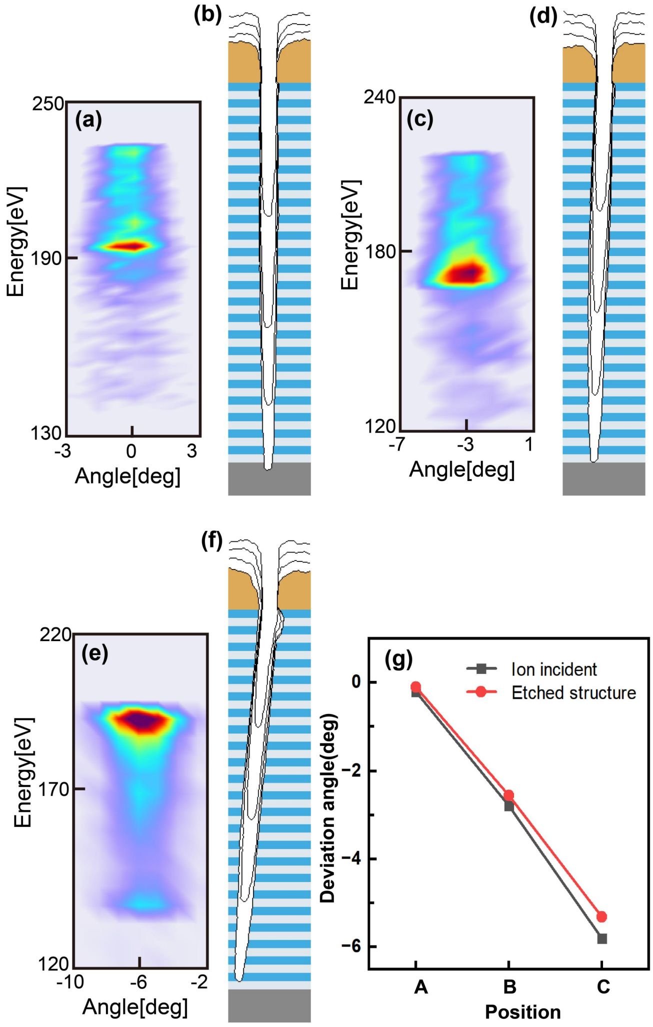

Fig. 6. Ion energy and angular distributions at points A, B, and C [(a), (c), (e)] and their corresponding etched profiles [(b), (d), (f)]. (g) Comparison between ion incidence angles and resulting profile tilt angles at the three positions.

B. Twisting

To eliminate the effect of ion incidence angle, we mapped the plasma simulation results from point A into the feature-scale model. Figs.7 and 8 show the simulation results for the vertical feature and twisting feature, respectively.

During the etching of the vertical feature, the potential distribution remains nearly symmetric on both sides of the trench throughout the process (Fig.7). This symmetry ensures that ions are guided predominantly vertically, minimizing lateral ion deflection and preserving a straight profile. Such behavior is typical under idealized, uniform conditions.

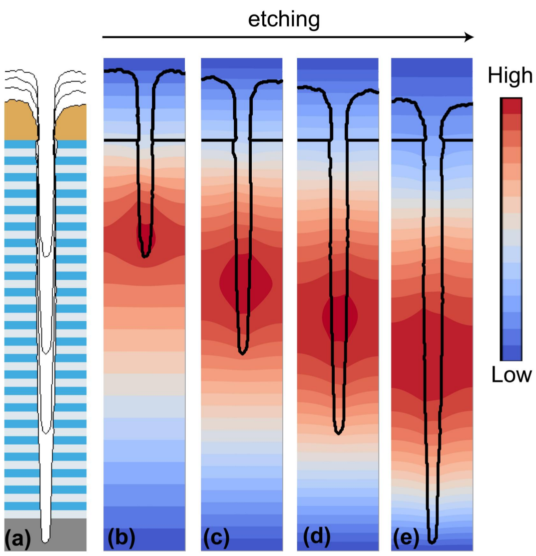

Fig. 7 Simulation results for the tilting feature: (a) etched profile evolution; (b)-(e) time-resolved potential distribution within the feature throughout the etching process.

However, in realistic conditions, the stochastic nature of particle incidence causes uneven charge accumulation on the trench sidewalls. This local charge imbalance distorts the potential distribution, breaking the symmetry and generating lateral electric fields. These fields deflect incoming ions sideways, causing random twisting of the etched profile. Fig. 8 illustrates this effect, showing that after multiple simulation runs, the potential becomes uneven across the trench, which correlates with observed twisting in the feature profile.

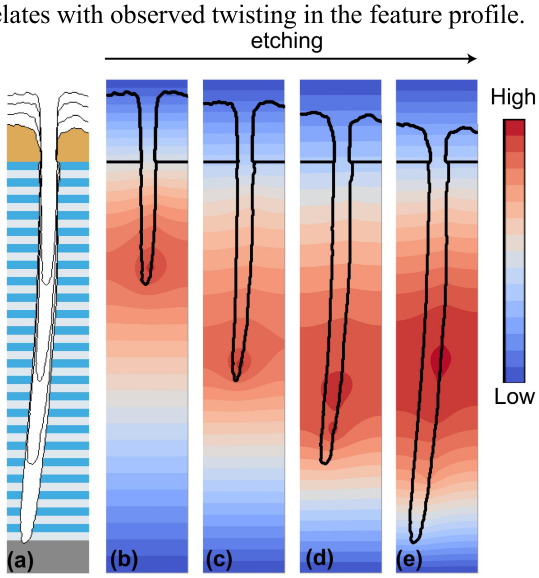

Fig. 7 Simulation results for the twisting feature: (a) etched profile evolution; (b)-(e) time-resolved potential distribution within the feature throughout the etching process.

IV. Conclusion

In this study, we developed a comprehensive multiscale modeling framework that effectively bridges chamber-scale plasma dynamics and feature-scale etching profiles in SiO_2/Si_3N_4 multilayer structures. The chamber-scale CCP simulations provided detailed ion energy and angular distributions, capturing non-uniform electric fields near the wafer surface. By integrating these results into a feature-scale model that accounts for particle dynamics, charging effects, and surface reactions, we successfully reproduced key etching phenomena such as profile tilting and twisting. Simulation results demonstrate that the ion incidence angle strongly affects the profile tilting, whereas random charge accumulation on the sidewalls leads to distortion through localized electric field asymmetry. This work provides valuable insights into plasma etching mechanisms and offers a predictive tool for optimizing HAR etching processes in semiconductor manufacturing.

Acknowledgements

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