

Impact of Surface Charging on Feature Profile Evolution in 3D NAND Pillar Etching

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Abstract—This work presents a reactor-coupled Particle Monte Carlo study of surface charging during high Aspect Ratio (HAR) ONO stack plasma etching for 3D NAND fabrication. The simulations reveal that surface charging reduces etch depth by approximately 55% through ion flux redistribution and profile distortion. Increasing substrate bias power enhances ion energy but also intensifies surface charge accumulation, whereas higher chamber pressure suppresses charging via enhanced charge neutralization. Surface charging further reduces ion reflections by nearly threefold under low pressure and high substrate bias conditions. The results demonstrate that etch evolution in HAR structures is governed by the coupled effects of ion transport, surface charging, charge neutralization, and ion reflection. These findings provide physical insight into charging induced transport mechanisms and offer guidelines for optimizing plasma etching processes for future high density 3D NAND flash technologies.

Index Terms—3D NAND, High Aspect Ratio Etching, Surface Charging, Particle Monte Carlo, Plasma Etching, Ion Reflection, ONO Stack, Feature Profile Evolution

I. INTRODUCTION

High Aspect Ratio (HAR) plasma etching is a cornerstone process in the fabrication of advanced three dimensional (3D) NAND flash memory, where deep channel holes must be etched through multilayer stacks of alternating oxide and nitride films extending several micrometers in thickness [1]. As device architectures continue to scale toward higher stack counts, maintaining profile fidelity and critical dimension (CD) control becomes increasingly challenging [2]. Consequently, understanding the physical mechanisms governing feature-scale evolution is essential for ensuring high device performance, reliability, and manufacturing yield [3], [4].

Despite significant advances in plasma processing technology, HAR etching remains susceptible to profile anomalies arising from complex plasma-surface interactions. Defects such as incomplete bottom etching, bowing, microtrenching, and twisting continue to limit etch performance and process reliability [5]. Among the mechanisms responsible for these distortions, surface charging remains one of the most critical yet underexplored phenomena [6]. As illustrated in Fig. 1, differences in the transport characteristics of ions and electrons create a local charge imbalance within the trench, leading to non uniform surface charge accumulation and the formation of localized electric fields. These electric fields deflect ion trajectories, redistribute ion flux, and ultimately govern

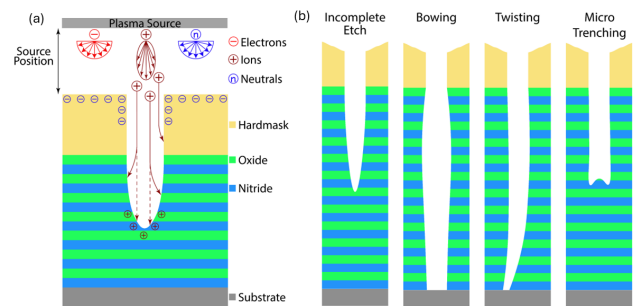


Fig. 1. (a) Schematic of differential surface charging arising from angular distribution of incident electrons and ions, leading to non uniform charge accumulation and deflection of ion trajectories within the trench (b) Resulting etch profile distortions due to surface charging, including incomplete etch, bowing, twisting and microtrenching.

feature profile evolution. In addition to deflecting ion trajectories, charging induced electric fields modify the energies, reflection characteristics, and angular distributions of incident ions within HAR features. These changes alter the spatial distribution of ion flux, degrade etch anisotropy, and promote profile distortions, particularly in structures with extremely high aspect ratios. Furthermore, plasma operating conditions, including substrate bias power and chamber pressure, strongly influence ion energy distributions, electron transport, and charge neutralization, thereby establishing a complex interplay between plasma characteristics, surface charging, and feature profile evolution.

To investigate these effects, a multiscale simulation framework integrating reactor scale plasma simulations with feature scale Particle Monte Carlo transport and self consistent surface charging module was developed. The framework captures the coupled evolution of ion transport, charge accumulation, electrostatic potential, ion reflection, and etch profile evolution, enabling a systematic investigation of the effects of substrate bias power and chamber pressure on HAR ONO etching.

II. METHODOLOGY

A reactor-coupled Particle Monte Carlo (PMC) framework was implemented using Synopsys Sentaurus Topography [8] to investigate the influence of surface charging on feature profile evolution during HAR 3D NAND ONO stack etching. The simulated 3D NAND structure, shown in Fig. 2, consists of

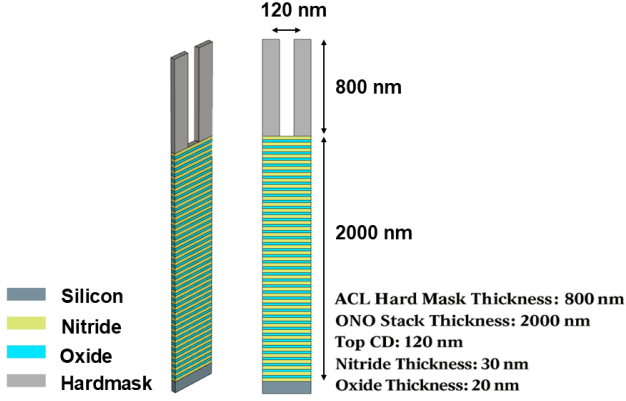


Fig. 2. 3D NAND stack structure used for etch simulations, comprising Amorphous Carbon Layer (ACL) hard mask, and ONO layers with defined thicknesses.

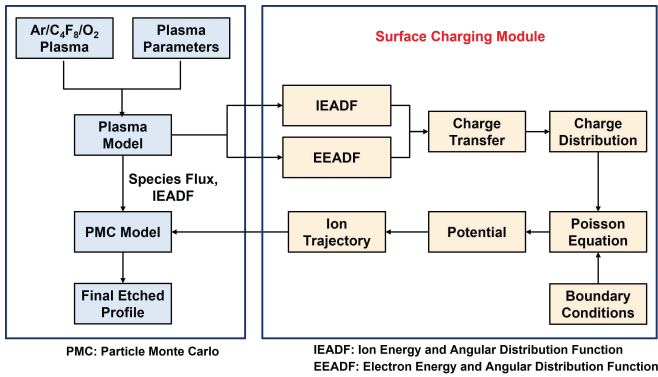


Fig. 3. Flowchart illustrating the simulation methodology used in this study. The plasma and Particle Monte Carlo (PMC) models are coupled with the surface charging module to simulate Ar/C₄F₈/O₂ plasma etching using Synopsys Sentaurus Topography. [8]

an 800 nm amorphous carbon layer (ACL) hard mask and a 2000 nm ONO stack comprising alternating 20 nm oxide and 30 nm nitride layers with an initial top critical dimension of 120 nm.

The overall simulation workflow is illustrated in Fig. 3. The inductively coupled plasma (ICP) reactor model computes the species fluxes along with the ion and electron energy and angular distribution functions (IEADFs/EEADFs) [7], which are directly coupled to the feature scale PMC model. The baseline plasma operating conditions employed throughout this study are summarized in Table I. The PMC solver models stochastic transport of ions and neutrals within the evolving feature, incorporating chemical etching, sputtering, deposition, and reflection through a voxel based surface evolution algorithm.

To account for surface charging effects, a self consistent surface charging module is coupled to the Particle Monte Carlo (PMC) transport solver. The surface charge density is updated from the incident ion and electron fluxes according to the relation:

$$\frac{\partial \sigma}{\partial t} = e(\Gamma_i - \Gamma_e), \quad (1)$$

TABLE I
PLASMA OPERATING PARAMETERS

Parameter	Value
Chamber Type	ICP
Reactor Radius	5 cm
Reactor Height	3 cm
Chamber Pressure	25 mTorr
C ₄ F ₈ /Ar/O ₂ Gas Flow Rate	75/375/50 sccm
ICP Power	2500 W
Substrate Bias Power	250 W
Bias Frequency	13.56 MHz

TABLE II
ELECTRICAL PARAMETERS AND BOUNDARY CONDITIONS

Parameter	Value
Relative Permittivity of Oxide	3.9
Relative Permittivity of Nitride	7.0
Relative Permittivity of ACL	3.5
Top Boundary Condition	0 V
Bottom Boundary Condition	0 V

where σ is the surface charge density, e is the elementary charge, and Γ_i and Γ_e are the incident ion and electron fluxes, respectively. The electrostatic potential is obtained by solving Poisson's equation using the accumulated surface charge distribution as the source term:

$$\nabla \cdot (\epsilon \nabla \phi) = -\rho_s, \quad (2)$$

where ϵ is the dielectric permittivity, ϕ is the electrostatic potential, and ρ_s is the equivalent surface charge density. The corresponding electric field is obtained from:

$$\mathbf{E} = -\nabla \phi, \quad (3)$$

and is subsequently coupled to the PMC solver to update charged particles trajectories through the Coulombic force, thereby capturing charging induced ion deflection, reflection, and flux redistribution. The procedure is iterated until a steady state solution is achieved. The dielectric properties used in the electrostatic calculations are summarized in Table II, where relative permittivities of 3.9, 7.0, and 3.5 are assigned to Oxide, Nitride, and ACL, respectively. Dirichlet boundary conditions are imposed at the top and bottom boundaries for solving the electrostatic potential distribution.

III. RESULTS AND DISCUSSION

Figure 4 illustrates the impact of surface charging on profile evolution under the baseline operating conditions listed in Tables I and II. Without charging, ions propagate nearly vertically and efficiently reach the trench bottom, resulting in deeper and more anisotropic etching. In contrast, surface charging produces localized positive charge accumulation that generates electrostatic fields, deflects ion trajectories, and redistributes the ion flux. Consequently, the ion flux reaching the trench bottom is reduced, leading to an approximately 55% decrease in etch depth together with critical dimension broadening and profile distortion.

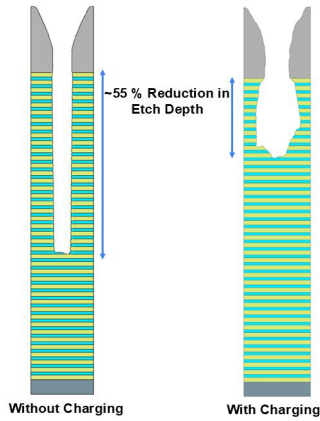


Fig. 4. Comparison of etch profiles obtained without and with surface charging, demonstrating a significant reduction of approximately 55% in etch depth under charging conditions.

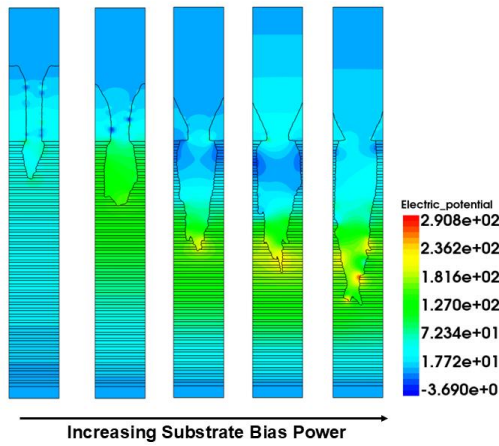


Fig. 5. Effect of substrate bias power on profile evolution and electric potential distribution, showing increased surface charge accumulation and higher electric potential within the trench with increasing bias power.

To understand how process conditions influence charging-induced profile evolution, substrate bias power was systematically varied from 100 W to 500 W. As shown in Fig. 5, increasing the substrate bias power results in greater positive charge accumulation near the trench bottom, accompanied by a corresponding increase in the electrostatic potential. The underlying mechanism responsible for this behavior is illustrated in Fig. 6. As the substrate bias power increases, the ion energy spread (ΔE) increases, indicating that ions enter the feature with higher kinetic energies. The more energetic ions promote greater positive charge accumulation within the trench, generating stronger electrostatic fields that modify ion transport and redistribute the ion flux. Consequently, the profile becomes increasingly susceptible to critical dimension broadening and microtrenching.

The influence of chamber pressure was subsequently investigated. As shown in Fig. 7, increasing chamber pressure reduces the electrostatic potential within the trench. At lower

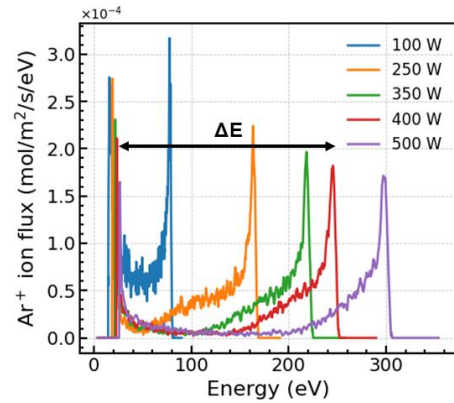


Fig. 6. Ar^+ Ion Energy Distribution Functions (IEDFs) at different substrate bias powers, showing a shift toward higher ion energies with increasing bias power.

pressures, the longer ion mean free path allows ions to retain higher energies, resulting in greater positive charge accumulation. With increasing pressure, the ion energy spread decreases from approximately 160 to 130 eV, while the electron flux to the trench surfaces increases (Fig. 8), enhancing charge neutralization and suppressing surface charging. Although the incident ion energy decreases, the higher plasma density at elevated pressures increases the ion flux reaching the feature, resulting in greater etch depth. In contrast, the increase in etch depth with substrate bias power is primarily driven by the higher incident ion energy, since the ion flux remains nearly unchanged. Figure 9 summarizes the variation of the maximum

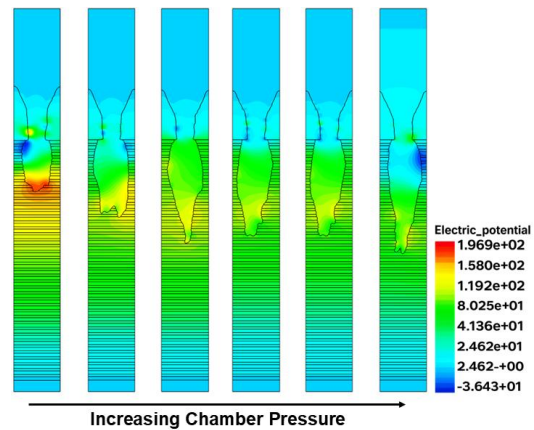


Fig. 7. Evolution of the etched profile and electric potential distribution with increasing chamber pressure, showing a gradual reduction in charge accumulation within the trench.

surface potential at the trench bottom with substrate bias power and chamber pressure. Increasing the substrate bias power from 250 to 500 W raises the maximum surface potential from approximately 160 to 290 V, whereas increasing the chamber pressure from 10 to 70 mTorr reduces it from approximately 200 to 130 V, demonstrating the opposing influence of these process parameters on surface charging.

The variation in surface charging also influences ion reflections within the trench. As shown in Fig. 10, incorporating surface charging reduces the average reflected ion fraction from approximately 6% to 1.9% for bias power variation and from approximately 4.5% to 1.5% for pressure variation, corresponding to a threefold reduction in ionic reflections. In the absence of surface charging, ions undergo repeated sidewall collisions, resulting in a higher probability of reflection. In contrast, charging induced electric fields modify ion trajectories, reducing the probability of repeated sidewall interactions and subsequent reflections. These results demonstrate that charging induced electric fields strongly influence ion reflection and species transport in HAR structures.

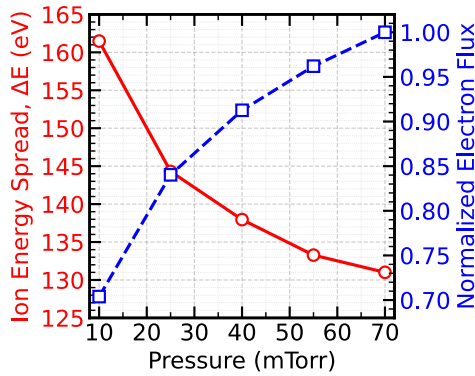


Fig. 8. Variation of ion energy spread and normalized average electron flux distribution with chamber pressure, showing reduced ion energy and increased electron population at higher pressures.

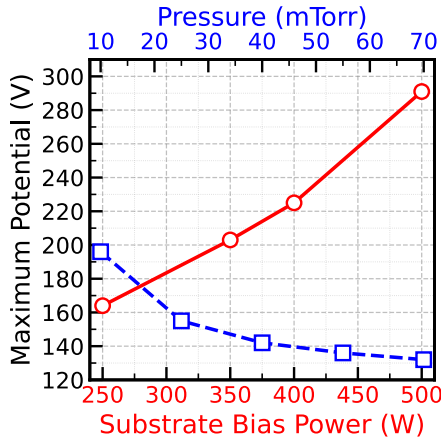


Fig. 9. Dependence of the maximum surface potential at the trench bottom on substrate bias power and chamber pressure, illustrating enhanced charge accumulation with increasing bias power and reduced charging with increasing pressure.

IV. CONCLUSION

A reactor-coupled Particle Monte Carlo (PMC) framework incorporating a self-consistent surface charging model was developed to investigate charging-induced transport during HAR

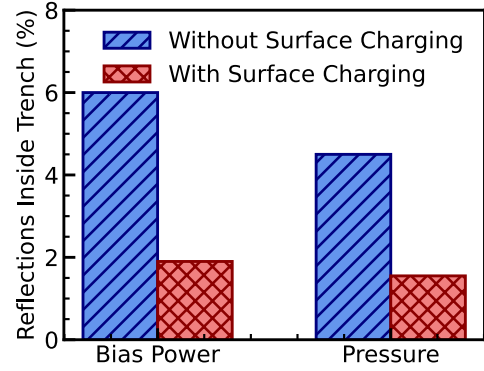


Fig. 10. Comparison of the average ion reflection percentage inside the trench with and without surface charging under substrate bias power and chamber pressure variations, showing a significant reduction in reflections due to surface charging.

ONO stack etching for 3D NAND fabrication. Surface charging generates localized electrostatic potentials that alter ion transport, resulting in approximately 55% lower etch depth, critical dimension broadening, and microtrenching. Increasing substrate bias power intensifies charge accumulation and electrostatic potential, whereas increasing chamber pressure suppresses surface charging through enhanced electron flux. Surface charging also reduces ion reflections by nearly three times, highlighting its significant influence on species transport within HAR features. These findings establish the relationship among plasma operating conditions, surface charging, and feature evolution, providing a predictive framework to optimize HAR plasma etching for future high density 3D NAND technologies.

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