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Impact of High-Aspect-Ratio Etching Damage on Selective Epitaxial Silicon Growth in 3D NAND Flash Memory

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***Abstract*—A physical process model for inductive plasma dry etching is presented and applied to simulate vertical channel hole etching, a critical fabrication step in modern 3D NAND flash memory. A specialized advection algorithm is subsequently applied to simulate the selective epitaxial growth (SEG) of silicon on the bottom source line. The induced etching damage on the bottom silicon substrate, which is included in the etching model, is shown to heavily reduce the quality of the SEG. The removal of this damaged layer is shown to result in highly crystalline epitaxially grown silicon.**

***Index Terms*—Plasma Etching; Plasma-induced damage; Process Simulation; Selective Epitaxial Growth; 3D NAND;**

I. Introduction

Modern three-dimensional flash memory (3D NAND) employs a large number of stacked control gates and insulating layers, comprised of alternating silicon dioxide (SiO_2) and silicon nitride (Si_3N_4) thin films, leading to a recent increase in storage size up to 1.33 TB [1] on a single die [2]. The rapid scaling drives new challenges in the etching of these stacks in order to meet the demands of further increasing memory capacity by adding more stacked layers, thereby dramatically increasing aspect-ratios of the feature sizes. The specific challenge is the dry etching of high-aspect-ratio (HAR) channel holes through these stacks using high energy plasmas. The plasma can often introduce damage in the silicon layers by implanting ions in the silicon substrate which forms the source line [3]. This heavily impacts the subsequent selective epitaxial silicon growth (SEG) of the source contact, severely decreasing its quality and leading to the formation of voids. Recent studies have shown that removing the damaged silicon layer using a post etch plasma treatment can effectively remove impurities, leading to well formed SEG silicon on the bottom [4].

We propose a physical model which is capable of simulating the channel hole dry etch process including the resulting source material damage through ion implantation, leading to undesirable voids in the source contact after SEG. The model uses a level set powered topography simulator in combination with top-down Monte Carlo ray tracing to accurately describe the surface kinetics for multiple materials and 3D geometries, combined and implemented in the ViennaTools software ecosystem [5].

This paper is organized as follows. In Section II we describe the physical process model, starting with the basic idea of level set based surface representations, the applied surface kinetics, describing the surface evolution, the flux calculations using Monte Carlo ray tracing, the modeled ion damage, and the selective epitaxial growth. Section III shortly introduces the plasma chemistry which determines our various model parameters, after which the simulation setup is described in Section IV. The obtained results are then presented in Section V and a conclusion is given in Section VI.

II. Model

A. Level Set Surface Representation

To accurately represent the substrate surface and its time evolution during the etching process, a level set based description is used [6]. In this method, the surface is described implicitly by a level set function $\phi(\vec{x})$, defined at every point $\vec{x}$ in space. This function is obtained using signed distance transforms, containing the surface S as the zero level set:

$$S = \{\vec{x}:\ \phi(\vec{x}) = 0\}. \tag{1}$$

In order to propagate the surface in an advection step, the level set equation

$$\frac{\partial \phi(\vec{x},t)}{\partial t} + v(\vec{x})|\nabla\phi(\vec{x},t)| = 0 \tag{2}$$

is solved given the scalar velocity field $v(\vec{x})$ which describes the surface normal velocity at each point. This is achieved by applying finite difference schemes on a regularly discretized grid, used to store the level set values.

B. Surface Kinetics

To analyze the surface kinetics which describe the etching process, a model based on the theory of active surface sites is used [7]. Three different types of particle species are considered:

1) A reactive etchant forming volatile etch products which dissociate thermally and thus etch the substrate;
2) A passivating species which forms protective polymer layers on the surface;
3) Energetic ions which physically sputter the film and enhance the dissociation of the volatile etch products.

The rates of particle types impinging on the surface can be summed to give coverages ϕ_x of different particle types at all surface sites, φ_x, where x represents etchant (e), polymer (p) or etchant on polymer (pe). Since the etching time is usually much larger than the surface reaction time scales, we can assume that the coverages reach a steady state on the surface and can be expressed by the following equations [7]:

$$\frac{d\varphi_e}{dt}=J_e S_e\left(1-\varphi_e-\varphi_p\right)-k_{ie}J_i Y_e\varphi_e-k_{ev}J_{ev}\varphi_e\approx 0, \quad (3)$$

$$\frac{d\varphi_p}{dt}=J_p S_p-J_i Y_p\varphi_p\varphi_{pe}\approx 0, \quad (4)$$

$$\frac{d\varphi_{pe}}{dt}=J_e S_{pe}\left(1-\varphi_{pe}\right)-J_i Y_p\varphi_{pe}\approx 0. \quad (5)$$

Here, J_x and S_x represent the different particle fluxes and sticking probabilities, respectively. Y_e is the ion-enhanced etching yield for etchant particles, Y_p is the ion-enhanced etching yield on polymer, Y_{sp} gives the physical ion sputtering yield and k_{ie} and k_{ev} are the stoichiometric factors for ion-enhanced etching and evaporation respectively. Solving these equations for the coverages, one can determine etch or deposition rates on the surface. If deposition of polymer dominates, the surface velocity is positive and given by:

$$v=\frac{1}{\rho_p}\left(Y_p J_i\varphi_{pe}-J_p S_p\right), \quad (6)$$

where ρ_p is the atomic polymer density. In this case, polymer material is deposited on the surface, which acts as passivation layer for the chemical etching process. If etching dominates, the negative surface velocity of the substrate is given by:

$$v=\frac{1}{\rho_m}\left[J_i Y_e\varphi_e+J_i Y_{sp}\left(1-\varphi_e\right)+J_{ev}\varphi_e\right], \quad (7)$$

where ρ_m is the atomic density of the etched material and depends on which layer in the stack is being etched. Together, these equations describe the temporal evolution of the surface, given the particle fluxes J_x at each location on the etched substrate.

C. Flux Calculation

The fluxes are calculated using a top-down Monte Carlo ray tracing approach, where a large number of particles are launched from a source plane and traced towards the substrate surface in order to determine the point of impact on the surface. Particles are initialized at random positions on the source plane with random directions according to a particle-specific distributions. Both polymer and etchant particle directions are described by a cosine distribution, while ions are represented with a power cosine distribution, thus being more directional towards the surface.

The ion yield efficiencies on the point of impact are dependent on the ion energy E, as well as the incident angle α between the ion particle and the surface normal. The initial energy for each ion particle is assigned based on the process used. In general, the ion yield efficiency for physical sputtering and ion-enhanced etching upon impact on the surface can be expressed as

$$Y=A(\sqrt{E}-\sqrt{E_{th}})f(\alpha), \quad (8)$$

where A is a process-dependent constant, describing the particle yield per unit of energy, E_{th} is the minimum energy ions must have to etch the substrate, referred to as threshold energy, and $f(\alpha)$ is a function of the incident angle. For the physical ion sputtering this function can be fitted using the expression

$$f(\alpha)=\left(1+B_{sp}\left(1-\cos^2(\alpha)\right)\right)\cos(\alpha), \quad (9)$$

while for the ion enhanced etching, the expression

$$f(\alpha)=\cos(\alpha) \quad (10)$$

is applied, as presented in [7]. If the energy is below the threshold, the ion is reflected specularly, until it reaches a point with a larger incident angle or it leaves the simulation domain.

Polymer and etchant particles, on the other hand, reflect diffusely with varying sticking probabilities at each discretized surface point.

D. Ion Damage

In HAR etching processes, the use of high energy ions is necessary to achieve the desired channel aspect ratios. However, this introduces the problem of high energy ions being able to penetrate into the bottom substrate, consequently leading to a disordered silicon layer on the bottom of the channel hole, thereby destroying the crystal purity. To model this damaged layer in the crystalline silicon substrate, the energy of traced ions is recorded on the substrate surface at each flux calculation step. Since the highest ion energies occur at normal incidence, the recorded energies can be used to model the ion damage in the material directly below the surface. At each surface point, the impinging ion energy E is assumed to decrease through the substrate due to scattering, following an exponential attenuation given by

$$E(d)=E_i e^{-d/\lambda}, \quad (11)$$

where E_i is the initial ion energy upon surface impact and d is the normal distance to the surface inside the material, equivalent to the penetration depth. Given the observed thickness of the damaged layer d_{th} in [4] and the threshold energy for ion enhanced etching E_{th}, the attenuation length λ is determined as

$$\lambda=d_{th}/\ln\left(\frac{E_i}{E_{th}}\right). \quad (12)$$

Subsequently, an ion damage coefficient $D(d)$ is defined and stored for each surface point of the geometry. The coefficient is proportional to the ion energy at a depth d in the substrate:

$$D(d) \propto E(d) - E_{th}. \quad (13)$$

In order for silicon to grow epitaxially, the material must not be damaged and hence, the ion damage coefficient at the surface must fulfill

$$D \leq 0. \quad (14)$$

To remove the damaged layer in a post etch treatment process simulation, the surface is etched using low energy ions. Assuming these low energy ions do not cause any additional implantations in the substrate, the surface is etched until the damage coefficient D at the bottom drops below 0, thereby forming a suitable interface for the subsequent selective epitaxial growth.

E. Selective Epitaxial Growth

In selective epitaxial growth, silicon is grown only on a clean crystalline silicon surface, with growth rates depending on the surface orientation. For the simulation of SEG, the specialized numerical method presented by Toifl et al. [8] is applied. In this approach an additional top layer level set is advected with growth rates as proposed in [9], using the Stencil-Local-Lax-Friedrichs (SLLF) numerical integration scheme.

III. Plasma Chemistry

Etching is modeled as a fluorocarbon based etch process, including Ar and O_2 as inhibitor, as is commonly used for the etching SiO_2/Si_3N_4 layers. The fluorocarbon radicals CF_x^+ together with Ar^+ provide ion bombardment, while the O_2 forms a passivation layer on the substrate. Corresponding parameters are extracted from [10] and summarized in Table I. For the post etch treatment, the chemistry described in [4] is used, where an inductance coupled plasma using low energy CL_2 and NF_3/CH_2F_2 gases is proposed.

IV. Simulation Setup

The structure of the simulation domain is based on the multi-material representation, presented by Ertl and Selberherr [11]. In this approach, the stacked material layers are represented by individual level sets which are connected by sequential union operations. This multi-material representation enables the resolution of thin layer regions (i.e. thickness below a single grid spacing) and thus an additional layer, placed on top of all layers, is used capture any deposited polymer. The etching simulation and post etch treatment process consist of multiple steps of alternating ray tracing and surface advection steps. In the ray tracing step, the required fluxes at each surface point are calculated and used to find the resulting surface velocity which is applied for the subsequent level set advection.

TABLE I
Parameters used for the simulation of the vertical channel hole etching process. Values are extracted from [7] and [10].

Parameter	Value	Description
J_{ion}^{src}	$1 \times 10^{17} \text{cm}^{-2}\text{s}^{-1}$	Source ion flux
J_{etch}^{src}	$5 \times 10^{17} \text{cm}^{-2}\text{s}^{-1}$	Source etchant flux
J_{poly}^{src}	$1 \times 10^{17} \text{cm}^{-2}\text{s}^{-1}$	Source polymer flux
A_{sp}	$0.00339 \text{ eV}^{-1/2}$	Yield coefficient in (8) for physical ion sputtering
A_{ie}^{e}	$0.0361 \text{ eV}^{-1/2}$	Yield coefficient in (8) for ion enhanced etching (substrate)
A_{ie}^{p}	$4A_{ie}^{e}$	Yield coefficient in (8) for ion enhanced etching (polymer)
B_{sp}	9.3	Sputtering yield angular factor in (9)
E_{sp}^{th}	18 eV	Threshold energy for physical ion sputtering
$E_{ie.e}^{th}$	4 eV	Threshold energy for ion enhanced etching (substrate)
$E_{ie.p}^{th}$	4 eV	Threshold energy for ion enhanced etching (polymer)
k_{ie}, k_{ev}	1	Stoichiometric factors
S_e	0.9	Etchant sticking probability
S_p	0.26	Polymer sticking probability
S_{pe}	0.6	Polymer on etchant sticking probability
ρ_{SiO_2}	$2.2 \times 10^{22} \text{ cm}^{-3}$	SiO_2 density
$\rho_{\text{Si}_3\text{N}_4}$	$10.3 \times 10^{22} \text{ cm}^{-3}$	Si_3N_2 density
ρ_{Si}	$5.02 \times 10^{22} \text{ cm}^{-3}$	Si density
ρ_p	$2.0 \times 10^{22} \text{ cm}^{-3}$	Polymer density

V. Results

The geometric profile of the stacked sheets after the etching simulation is shown in Figure 1. The etch process is performed until the via is slightly over-etched in the silicon substrate. On the sidewall one can observe the thin passivation layer in red.

The damage coefficient on a 3D clip of the surface after the etching process is shown in Figure 2. Due to the high directional trajectories of ions and the angle-dependent etching yield, the resulting ion damage is predominately confined to the bottom regions of the via. In the post etch treatment, the surface is etched with low energy ions, until the damaged layer has been removed and the crystalline silicon material underneath is revealed, so SEG can commence properly.

Next, SEG of silicon at the bottom of the channel hole is carried out with the resulting profiles depicted in Figure 3. When the damaged layer is present on the silicon substrate a large void is observed, leading to an ill-formed contact to the silicon source line (Figure 3a). Such defects will heavily impact the bottom select gate characteristics and reduce the overall quality of the memory stack. However, when the silicon substrate is cleaned prior to SEG, the desired SEG growth is obtained with the grown layer providing full contact with the silicon source line, as shown in Figure 3b.

VI. Conclusion

A physical process model is applied to simulate vertical channel hole etching in 3D NAND flash memory layers. The model, based on a level set surface representation and Monte

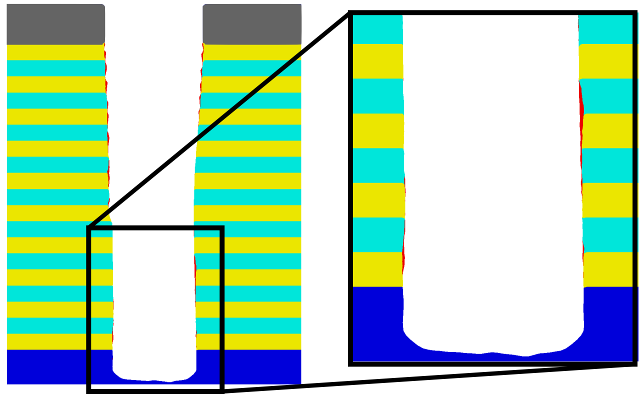

Fig. 1. Final 2D profile slice of the HAR via etching simulation. The alternating SiO_2/Si_3N_4 layers (yellow/cyan) are etched down to a bottom Si layer (blue). The thin sidewall layers (red) represent the deposited polymer formed during the etching process.

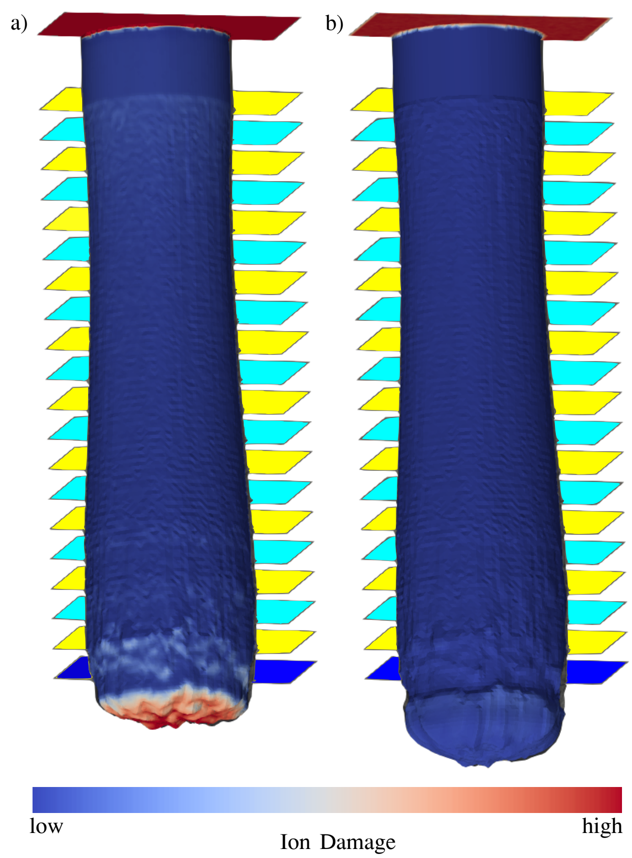

Fig. 2. Clipped 3D surface representation of the ion damage (a) prior to the post etch treatment, and (b) after the post etch treatment.

Carlo ray tracing for flux calculation, is able to simulate the damage induced by ion-enhanced etching. The damage caused on the bottom silicon substrate is modeled using a surface damage coefficient. In a post etch treatment process, the damaged substrate is etched until the crystalline silicon at the bottom is exposed and the subsequent selective epitaxial growth of silicon provides full contact with the source line,

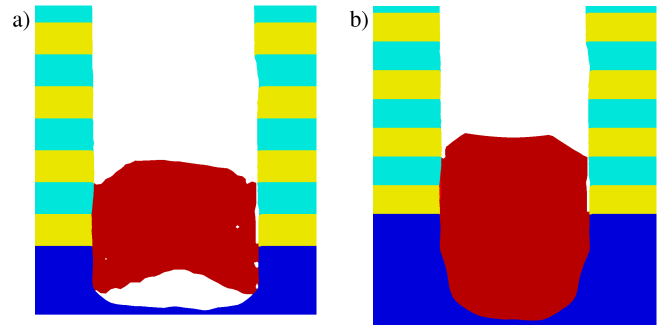

Fig. 3. Results for the selective epitaxial growth of silicon (red) after the etching process, on the bottom of a cropped 2D slice of the trench. In (a) a damaged layer on the surface is covering parts of the Si layer (blue, on the bottom), hence leading to an ill-formed SEG. In (b) the damaged layer has been removed and the SEG covers the entire bottom, leaving no voids.

leaving no undesired voids. This is modeled using the surface damage coefficient which is decreased according to an exponential attenuation during the etching of the bottom substrate.

Due to the physical nature of the presented model, relevant physical effects and underlying etch mechanics are represented appropriately. Therefore, the proposed model allows to analyze the physical behavior of the etch process in order to optimize the fabrication conditions during channel hole etching and the post etch treatment fabrication steps. Therefore, the model serves as a basis for an enhanced understanding of source contact formation in 3D NAND memory cells.

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