Unified Feature Scale Model for Etching in SF$_6$ and Cl Plasma Chemistries

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Abstract—**A novel unified feature-scale model for inductive plasma etching is presented. The model gives an accurate description of passivation layers which form on sidewalls during etch processes, by treating them as independent materials. This allows them to be explicitly included in subsequent etch steps, resulting in a more accurate description of the physical process. Therefore, novel gate stack geometries for advanced nodes can be modelled more rigorously.**

Plasma Etching; Process Simulation; Gate Stack Etching; Levelset; TCAD;

I. INTRODUCTION

Continued CMOS device scaling has introduced increased complexity to the formation of the transistor gate stack. Pattering gate transistors to meet critical dimension requirements, as laid out in the ITRS roadmap [1], has become increasingly challenging. Control over sidewall tapering has been attained by using several, individual etch steps for each gate stack layer and the simultaneous deposition of a passivation layer during most of these etch processes [2]. The two etch steps during polysilicon etching are: main etch (ME) and over etch (OE). Both of them provide a polymer layer, which protects the polysilicon during subsequent etching. We propose a unified feature scale model for the simulation of complex etching processes, as used in the patterning of modern transistor gate stacks, which was implemented into ViennaTS [3], a levelset powered topography simulator. This simulation tool can therefore be used to treat the different materials independently and accurately, which is especially important in understanding the behaviour of the deposited polymers and their interaction with other materials in complex geometries.

II. UNIFIED FEATURE SCALE MODEL

Our model assumes that, in any complex plasma etch process, there are four fundamental types of particles: neutral, etchant, depositing polymer particles and ions [4]. Due to the long etch times, compared to surface reaction time scales, we can safely assume that each of these substances' concentrations will reach a steady state on the surface. Therefore, the surface coverages of all involved particle types φ_x, where x represents etchant (e), polymer (p), etchant on polymer (ep), and ions (i), are expressed by the following equations:

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

$$\frac{d\varphi_p}{dt} = J_p S_p - J_i Y_p \varphi_p \varphi_{pe} \approx 0 \quad (2)$$

$$\frac{d\varphi_{pe}}{dt} = J_e S_{pe}\left(1-\varphi_{pe}\right) - J_i Y_p \varphi_{pe} \approx 0 \quad (3)$$

J_x and S_x are the fluxes and sticking probabilities. The values k_x are stoichiometric factors for ion-enhanced etching (k_{ie}) and evaporation (k_{ev}), while the Y_x describe the ion-enhanced etching yields for polymer (Y_p) and etchant (Y_e) as well as the sputtering yield (Y_s). The above equations can be solved to obtain the concentrations at any given point on the surface. From these, the surface rates are determined. If deposition dominates (surface rate is positive), instead of etching, a deposition rate is applied to the material given by:

$$v = \frac{1}{\rho_d}\left(Y_p J_i \varphi_{pe} - J_p S_p\right) \quad (4)$$

Therefore, a new material represented as an independent levelset grows on top of the old material, which is currently being etched. If etching dominates, the following etch rate is applied to the top most material:

$$v = \frac{1}{\rho_m}(J_i Y_e \varphi_e + J_i Y_s\left(1-\varphi_e\right) + J_{ev}\varphi_e \quad (5)$$

ρ_d and ρ_m are the densities of the polymer and the material being etched, respectively. The parameters in Equations (4) and (5) can be adjusted systematically to create a set describing a specific etch process, without changing the underlying model. The levelset approach applied in this work, allows for the tracking of complex deformation, separation, and merger of surfaces, essential to represent the thin passivation layers often formed in modern etching techniques. These layers are tracked as separate materials, which is achieved by introducing new surfaces where passivation layers build up and applying deposition only to those. If this new surface is removed during the process, the exposed sections of the underlying material are etched again. This seamless integration of different materials and processes into one model enables efficient and robust simulations of these complex processes, while being able to record deposited polymer layers separately. This is especially useful for sequential simulations, where different passivation layers form on top of one another. Since the materials involved in etch processes interact strongly, the simulated surfaces must not be interpreted as strict boundaries, but rather as rough guides indicating the concentrations of different materials at the interface.

III. ETCHING IN SF_6 PLASMA

Since Sulphur Hexafluoride (SF_6) chemistries are often used to etch Silicon (Si) and SiO_2, detailed knowledge about the characteristics of this process is imperative. However, the details of plasma etching in Sulphur and Fluoride chemistries is complex, since both elements are highly volatile, which our model circumvents by assuming a steady state flux from the reactor, impinging on the surface, thereby drastically simplifying the problem.

IV. ETCHING IN CL PLASMA

Chlorine (Cl) based chemistries are mainly used for titanium etching and can show similar behaviour to SF_6 chemistries. However, Cl chemistries can also lead to different geometries depending on the additional gases used during etching, being almost isotropic with high selectivity against Si while also being highly directional and uniform using other additives. The main influencing factors are captured in the few variables described earlier, which enables an accurate representation of the different behaviour of various etch chemistries.

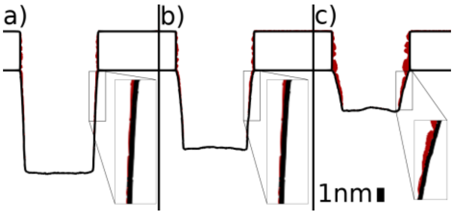

Figure 1. Two-dimensional trenches formed by etching Silicon (black), varying the polymer (red) fluxes to the same mask geometry. Etchant and Ion fluxes were kept constant at 10^{15} cm^{-2}s^{-1} and $1.3\cdot10^{16}$ cm^{-2}s^{-1}, respectively. Trenches were etched for 25s while the polymer concentration was varied: a)$5\cdot10^{15}$, b)10^{16}, and c) $5\cdot10^{16}$ cm^{-2}s^{-1}.

V. RESULTS

Sample simulations in Figure 1 show how the polymer flux influences the final shape and depth of the etched trenches. A higher polymer flux results in slower etching, and strongly slanted profiles. The figure also shows the different ways the polymer can be treated in the model: While the passivation layer has an associated thickness in some regions, there is no extra layer noticeable in others, although its influence can be seen in the final shape. Etching dominates in the latter, meaning the polymer is removed as soon as it is deposited and therefore cannot form a thick layer. However, this does not mean that there are no polymerising materials on the surface, only that there are too few to form a thick layer.

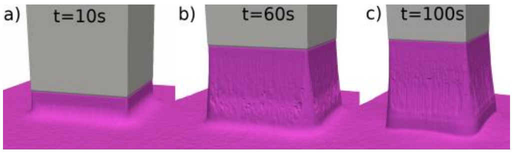

Figure 2. Three-dimensional simulation of Silicon (purple) in a gate stack using a rectangular mask (grey), where a) shows the start of the main etch, b) the start of the over etch step, and c) the end of the Silicon etching. Passivation layers are not shown for clarity.

Sequential simulations, depicted in Figure 2, show the different characteristics of the etch processes in detail: SF_6 etching results in thick passivation layers and therefore leads to strongly slanted profiles of the polysilicon substrate. An intermediate over etch step is applied, which is highly selective in order not to damage the TiN underneath [5]. The subsequent Cl based etch steps are very selective but less directional leading to a complex final shape noted in Figure 3. Here, we clearly demonstrate the ability of the unified model to simulate intricate and sequential etching processes including those essential for the fabrication of advanced node gate stacks.

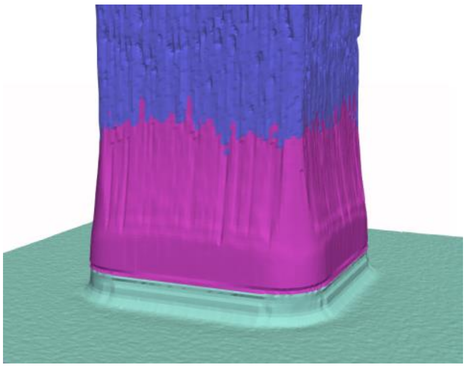

Figure 3. Final profile of a complex gate stack etching simulation. TiN (green) is etched last with an isotropic chemistry resulting in a concave profile, while Silicon (purple) is etched using highly directional chemistries resulting in a tapered profile and deposition of a passivation layer (blue).

VI. CONCLUSION

A unified feature scale model, implemented in a process simulator, is used to describe many chemically different etch processes effectively. This enables simulations of complex geometries involving many layers and several sequential etch steps. In addition, newly deposited elements, such as passivation layer forming polymers, can be represented as separate materials, enhancing simulation accuracy for complex, nanoscale fabrication processes.

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