Feature Scale Modeling of Fluorocarbon Plasma Etching for Via Structures including Faceting Phenomena

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With the continuous miniaturization of electronic device structures which is necessary to improve performance, plasma etching challenges continue to evolve in the semiconductor industry [1]. Higher aspect ratios and higher density features are required for new device technologies and the precise modeling of etching processes can greatly aid manufacturing [1]. To that end, we have implemented a modeling methodology for feature scale fluorocarbon reactive-ion-etching (RIE) and integrated it into Silvaco's Victory Process [2] simulator for evaluation purposes. The methodology (Fig. 1) integrates a bottom-up ray-tracing scheme [3] for the simulation of the fluxes associated with impinging plasma species. The fluxes feed a Langmuir set of surface coverage equations [4] (Figs. 2-4), which outputs either a substrate etching rate or a polymer deposition rate. The rates are provided to a level-set [5] topography engine which updates the geometry accordingly. We also implemented different angular yield functions for RIE and physical sputtering mechanisms (Fig. 5) to enable the reproduction of faceting phenomena [6]. We applied the developed methodology to a typical via etching of SiO_2 with an Ar/C_4F_8 plasma chemistry, adapting parameters from [4]. The simulated via (Fig. 6) was etched for 25s and exhibits a polymer sidewall; the shape and maximum thickness (17nm) agree with experimental data [4]. The faceting is observed at the mask material as expected (Fig. 6) and the tapering angle agrees with the experimentally observed angle of 45º [6]. The developed methodology can be extended to different materials and can be fully incorporated into TCAD workflows.

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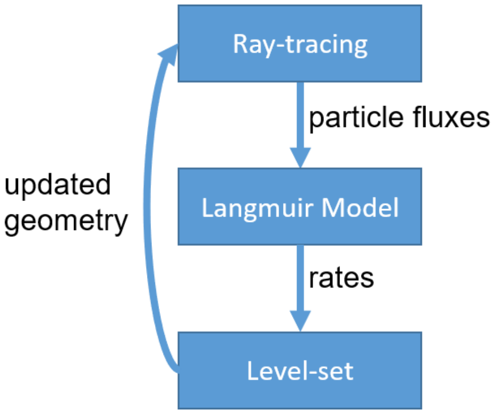

Fig. 1: Flow diagram of the developed methodology. Bottom-up ray-tracing is used to evaluate the flux of neutral, polymer, and ion particles for different geometries and source distributions. The set of equations (Fig. 3) is solved and outputs an etching or deposition rate to the level-set engine which evolves the surface accordingly.

Symbol	Description
Θ_x	Coverage
J_x	Flux
S_x	Sticking coefficient
Y_x	Yield of ion related mechanisms
k_x	Stoichiometric coefficient
R	Rate of deposition or etching
ρ	Density of substrate material

Fig. 2: Variables used to describe the coverage equations (Fig. 3). The coverages represent the fraction of the surface that is covered by a given species. The subscript x identifies either an evaporation mechanism (ev) or the involved chemical species: neutrals (n), polymers (p), ions (i), and neutrals over polymers (n/p).

$$\frac{d\Theta_n}{dt} = \underbrace{J_n S_n (1 - \Theta_n - \Theta_p)}_{\text{adsorption}} - \underbrace{J_i Y_n k_n \Theta_n}_{\text{RIE}} - \underbrace{J_{ev} k_{ev} \Theta_n}_{\text{evaporation}} \approx 0 \quad (1)$$

$$\frac{d\Theta_p}{dt} = J_p S_p - J_i Y_{n/p} \Theta_p \Theta_{n/p} \approx 0 \quad (2)$$

$$\frac{d\Theta_{n/p}}{dt} = J_n S_{n/p} (1 - \Theta_{n/p}) - J_i Y_{n/p} \Theta_{n/p} \approx 0 \quad (3)$$

$$\Theta_p = \frac{J_p S_p}{J_i Y_{n/p} \Theta_{n/p}} \quad (4)$$

Fig. 3: For each surface element and time step the system of equations for neutrals and polymer coverage (1)-(3) is solved under a steady-state condition. Each term represents a mechanism of addition or removal of species into the surface. The steady-state condition is applicable because the coverage mechanisms reach equilibrium much faster than the etching rate time scales [4].

$\Theta_p > 1$ results in a deposition rate given by:

$$R_{dep} = \frac{J_i Y_{n/p} - J_p S_p}{\rho_p} \quad (5)$$

$\Theta_p < 1$ results in an etching rate given by:

$$R_{etch} = \frac{1}{\rho_{sub}} \Big(\underbrace{J_i Y_n \Theta_n}_{\text{RIE}} + \underbrace{J_i Y_s (1 - \Theta_n - \Theta_p)}_{\text{sputtering}} + \underbrace{J_{ev} k_{ev} \Theta_n}_{\text{evaporation}} \Big) \quad (6)$$

Fig. 4: The value of the polymer coverage given by (4) determines whether a deposition or etching rate is applied to the local surface element. When Θ_p is larger than 1, the surface is covered in polymers, the set of equations simplifies to equation (3) and polymer deposition occurs (5). Otherwise, an etching rate (6) is applied.

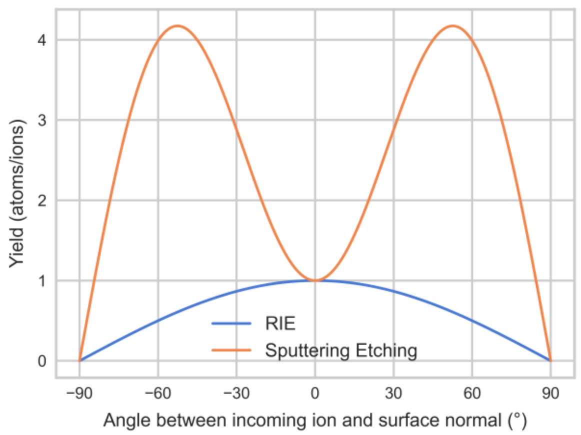

Fig. 5: Angular yield dependencies of RIE and sputtering etching mechanisms. The difference in angular dependencies between mechanisms influences the shape of the via and gives rise to faceting observed at the mask material (Fig. 6) [6].

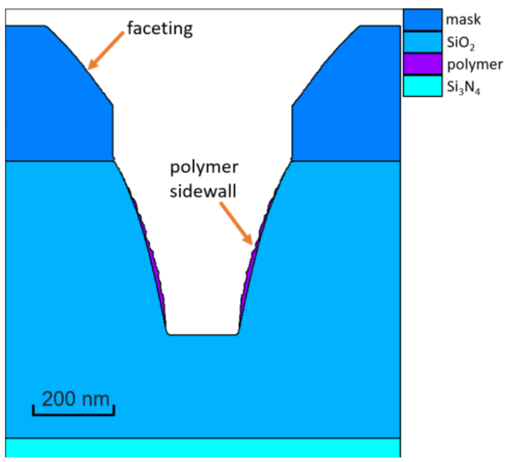

Fig. 6: The resulting SiO_2 via after 25s of etching by an Ar/C_4F_8 plasma. The maximum polymer sidewall thickness of 17nm agrees with experiments [4]. The faceting of 45° at the mask is expected for materials for which the main etching mechanism is sputtering [6].

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