Feature-Scale Modeling of Isotropic SF_6 Plasma Etching of Si

Luiz Felipe Aguinsky[1], Georg Wachter[2], Alexander Scharinger[1], Frâncio Rodrigues[1], Alexander Toifl[1], Michael Trupke[2], Ulrich Schmid[3], Andreas Hössinger[4], and Josef Weinbub[1]

[1] Christian Doppler Laboratory for High Performance TCAD, Institute for Microelectronics, TU Wien, Gußhausstraße 27-29, 1040 Wien, Austria

[2] Faculty of Physics, University of Vienna, VCQ, Boltzmanngasse 5, 1090 Wien, Austria

[3] Institute of Sensor and Actuator Systems, TU Wien, Gußhausstraße 27-29, 1040 Wien, Austria

[4] Silvaco Europe Ltd., Compass Point, St Ives, Cambridge, PE27 5JL, United Kingdom

***Abstract*—Low-bias etching of Si using SF_6 plasma is a valuable tool in the manufacturing of semiconductor and microelectromechanical systems. This kind of etching has strong isotropic tendencies which can be difficult to precisely reproduce in a topography simulation, since experimentally realized surfaces cannot be reproduced by a strictly isotropic velocity model. We present a three-dimensional Monte Carlo particle tracing model for calculating the velocity field in a level-set simulation. We compare it to an experimentally fabricated structure and to conventional models. We show that our model leads to a more accurate description of the final surface by introducing a sticking coefficient and multiple reflections.**

Keywords – Plasma etching, topography simulations, ray-tracing, level-set method, SF_6 plasma

Plasma etching of silicon (Si) using sulfur hexafluoride (SF_6) gases is a standard technology in modern fabrication processes of semiconductors. It has found applications in fabricating memory devices, microelectromechanical systems and as a sub-step in the Bosch process [1,2]. Under low-bias conditions, SF_6 plasma etching is known to have an isotropic behavior [3] yielding profiles similar, but not identical, to those obtained by wet etching. This found applications in, e.g., optics, where cleanliness requirements favor plasma etching [4].

Feature-scale topography simulations are part of process technology computer-aided design (TCAD) workflows which enable the investigation of etched or deposited materials [5]. While two-dimensional feature-scale modeling of SF_6 etching of Si has been reported for anisotropic, high-bias conditions [6], isotropic etching provides a different set of challenges for accurate topography modeling. In this work, we present a three-dimensional feature-scale model tailored to the challenge of the low-bias regime of SF_6 etching of Si. This is achieved using three-dimensional *top-down* Monte Carlo particle tracing [7] including multiple reflections. Our model is contrasted to conventional, strictly isotropic, and bottom-up models [8]. The simulated profile is compared to an experimentally fabricated cavity [4] which is of relevance for the development of optical resonators for quantum science.

To simulate the time evolution of an etched surface, we employ the level-set method [9]. The evolving surface is represented as the zero level-set of the signed distance function. Its propagation is then described by the solution of the following equation for the level set ϕ:

$$\frac{\partial\phi(x,t)}{\partial t} + V(x)|\nabla\phi(x,t)| = 0. \qquad (1)$$

The solution of (1) is performed by Silvaco's three-dimensional process TCAD tool *Victory Process* [10]. The modeling of surface reactions and subsequent local etch rates is achieved by providing the velocity field $V(x)$. As discussed previously [3], under low-bias conditions SF_6 plasma etching is expected to be isotropic, due to the highly reactive and isotropic nature of the F radicals generated in the plasma. However, the precise nature of such isotropic behavior requires accurate modelling. In Fig. 1, we present an illustration of three possible approaches to generate $V(x)$ for an isotropic etchant.

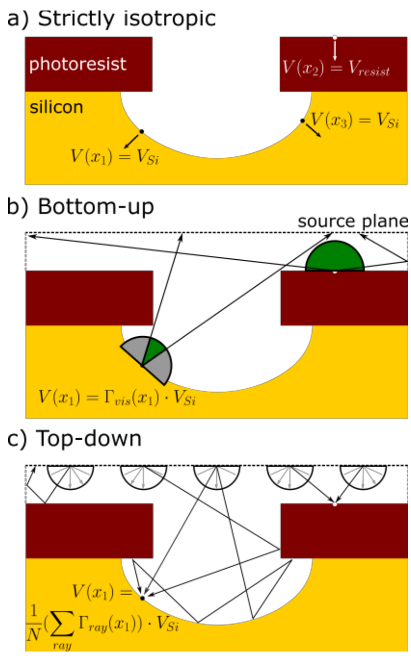

Figure 1. Illustration of models for the local velocity $V(x)$.

The straightforward approach, i.e., strictly isotropic, is represented in Fig. 1.a). In this case, the same constant velocity is applied to all exposed surface elements of the same material. This results in a surface equivalent to that processed by ideal isotropic wet etching [11]. However, since plasma etching is a gas-phase method, the etchant fluxes are expected to be unequally distributed across the surface. A more complex model thus requires estimating the local flux of etchant particles $\Gamma(x)$ to more accurately model $V(x)$. An elementary way of calculating $\Gamma(x)$, represented in Fig. 1.b), assumes that the incoming particle stream originates isotropically from a source plane. Subsequently, the local visibility of this plane is calculated in a bottom-up fashion for the hemisphere above each surface element [8], leading to a local flux $\Gamma_{\text{vis}}(x)$ which is normalized to 1 for a fully-exposed element. The final velocity is a reference V weighted with $\Gamma_{\text{vis}}(x)$. This model allows the capture of some topography-dependent effects; however, it is limited by not including reflections.

We propose a physically richer top-down model, as shown in Fig. 1.c), supporting multiple reflections according to a sticking probability β. This is achieved by Monte Carlo sampling of particles which are generated in the source plane and carry each a flux $\Gamma_{\text{ray}}(x)$. Their trajectories are computed using a ray-tracing method. When a simulated particle hits the surface, it is allowed to isotropically reflect according to β. Finally, the local velocity of the surface is calculated from the normalized sum of all $\Gamma_{\text{ray}}(x)$ and a reference V. This generalizes the previous models, as the strictly isotropic approach is recovered with $\beta \to 0^+$, and the bottom up with $\beta \to 1^-$.

To validate the proposed model, we compare it to a three-dimensional experimental topography of a fabricated structure [4]. A cavity was etched on Si using a two-step SF_6 plasma etching process. The first etch step was performed for $320\ s$, having a photoresist present with a cylindrical opening of $12.4\ \mu m$. After photoresist removal, a second etch step was applied for $48\ min$. The top-down model was manually calibrated to the final topography of the fabricated surface. A two-dimensional cross-section comparing the simulations to experiment is shown in Fig. 2 and calibrated parameters for the top-down simulation are shown in Table 1.

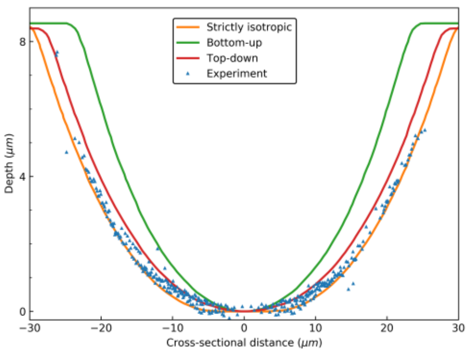

Figure 2. Comparison of cross-section of simulated surfaces to experimental data.

TABLE I. PARAMETERS FOR TOP-DOWN SIMULATION

Parameter	***Calibrated value***
First etch step V_{Si}	$2.151\ \mu m\ min^{-1}$
Second etch step V_{Si}	$0.661\ \mu m\ min^{-1}$
V_{res} [a]	$0.209\ \mu m\ min^{-1}$
β_{Si}	7.5%
β_{res} [a]	6.1%

a. Subscript res refers to photoresist

The results show the failure of the bottom-up model to correctly capture the curvature. The strictly isotropic model has a very similar shape to the experiment and to the top-down model. However, since it applies the same rate to all exposed regions, the area under the original photoresist opening remains flat. Such flat profiles are not observed in the experiment [4] and are unsuited for further numerical investigation [12]. Fig. 3 shows the differences of the simulated surfaces after the first etch step: The bottom-up model does not predict underetching and the strictly isotropic model yields an unrealistic flat bottom.

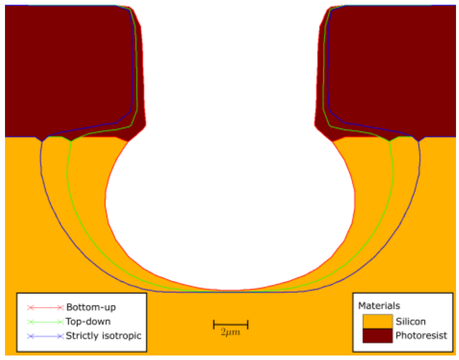

Figure 3. Cross-section of simulations after the first etch.

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