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Framework to model neutral particle flux in convex high aspect ratio structures using one-dimensional radiosity

Paul Manstetten [a,*], Lado Filipovic [b], Andreas Hössinger [c], Josef Weinbub [a,b], Siegfried Selberherr [b]

[a] Christian Doppler Laboratory for High Performance TCAD, Institute for Microelectronics, TU Wien, Gußhausstraße 27-29/E360, 1040 Wien, Austria
[b] Institute for Microelectronics, TU Wien, Gußhausstraße 27-29/E360, 1040 Wien, Austria
[c] Silvaco Europe Ltd., Compass Point, St Ives, Cambridge PE27 5JL, United Kingdom

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ABSTRACT

We present a computationally efficient framework to compute the neutral flux in high aspect ratio structures during three-dimensional plasma etching simulations. The framework is based on a one-dimensional radiosity approach and is applicable to simulations of convex rotationally symmetric holes and convex symmetric trenches with a constant cross-section. The framework is intended to replace the full three-dimensional simulation step required to calculate the neutral flux during plasma etching simulations. Especially for high aspect ratio structures, the computational effort, required to perform the full three-dimensional simulation of the neutral flux at the desired spatial resolution, conflicts with practical simulation time constraints. Our results are in agreement with those obtained by three-dimensional Monte Carlo based ray tracing simulations for various aspect ratios and convex geometries. With this framework we present a comprehensive analysis of the influence of the geometrical properties of high aspect ratio structures as well as of the particle sticking probability on the neutral particle flux.

1. Introduction

High aspect ratio structures are essential for the fabrication of various semiconductor devices, where the aspect ratio (AR) of the structure is defined as *depth/diameter* in case of cylinders and as *depth/width* in case of trenches. One particular example is negative-AND (NAND) flash cell fabrication [1], where three-dimensional multi-layer designs (3D-NAND) involve vertical holes which require aspect ratios above 40. Significant pressure on control of the fabrication process as well as on modeling and simulation techniques originates from these high aspect ratio structures.

One process to fabricate high aspect ratio structures is ion-enhanced chemical etching (IECE) [2]. In this process, the surface is exposed to reactive atoms and molecules from the plasma, which chemically react with the surface to form a volatile product. However, not only volatile products are created in this reaction, but also non-volatile by-products which hinder subsequent surface reactions and therefore decrease the etch rate. This chemical sealing is frequently desired on the vertical sidewall of high aspect ratio structures. To maintain a high etch rate at the bottom region of a structure, the surface is additionally bombarded with vertically accelerated ions, with the purpose of removing the non-volatile by-products on exposed areas. This makes a highly anisotropic chemical etching possible, supporting the fabrication of high aspect ratio structures.

To simulate an IECE process, a common approach is to model the reactive atoms and molecules of the plasma as electrically neutral particles that diffuse into the domain. In contrast, the accelerated ions are modeled as a directed source. A general simulation sequence for a single time step is to (a) calculate the local neutral particle flux and the local ion flux adsorbed on the surface, (b) model the local surface reaction using the obtained flux rates, and (c) calculate the new surface positions.

Common approaches for three-dimensional flux calculation are Monte Carlo ray tracing [3] and radiosity based [4] methods. When applying these methods to high aspect ratio structures, the computational costs for the neutral flux calculation dominates the simulation. The local neutral flux originating from multiple reflections becomes the dominant component towards the bottom of the structures; this multiplies the computational effort by the number of considered reflection events, compared to the costs for the computation of the direct flux.[1] Also, the flux rates can easily vary by orders of magnitude along the structure depth; this increases the

* Corresponding author.
E-mail address: manstetten@iue.tuwien.ac.at (P. Manstetten).

[1] The flux which originates from direct visibility of the source area.

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number of particles necessary to obtain an acceptable signal-to-noise ratio when using a ray tracing approach. For spatial resolutions typically desired for practical simulation cases, this leads to high computational costs for the full three-dimensional computation of the local neutral flux using Monte Carlo ray tracing or radiosity based methods.

We suggest to use a one-dimensional approximation for the calculation of the local neutral flux inside high aspect ratio structures. Our approach, initially introduced in [5], is radiosity based and is applicable to simulations of convex rotationally symmetric holes and convex symmetric trenches with a constant cross-section.

The adsorption of the neutral particles is modeled with a sticking probability s as a locally constant parameter of the surface. All sources and reflections are treated as ideal diffusive, which is a common assumption for neutral particles [6]. Molecular flow (ballistic transport) is assumed for the neutral particles. The sum of these assumptions allows for the computation of the neutral flux distribution using a radiosity approach, which was originally used in the context of heat transfer [7] and later adopted in computer graphics to compute global illumination [8].

The surface of the structure is discretized into elements along the line of symmetry. Assuming a constant flux and a constant sticking probability s over each surface element, we reformulate the discrete radiosity equation to obtain a *receiving* perspective, which allows for fully adsorbing surface elements.

We establish a general formulation to compute the view factor between two elements of a convex rotationally symmetric hole, based on a formula for the view factor between two coaxial disks of unequal radius. The view factors between two elements of a convex symmetric trench with a constant cross-section is derived using the crossed-strings method [7].

The framework is validated using a three-dimensional Monte Carlo ray tracing based simulator [9] by comparing results for different aspect ratios and sticking probabilities. Furthermore, we study the influence of geometric variations along the wall, as well as the variations of the particle sticking probability, on the flux distribution.

Kokkoris et al. [6] also proposed a framework to approximate the neutral flux in long trenches and holes by exploiting symmetry properties of the structures: The three-dimensional problem is reduced to a line integral and the Nyström method [10] is used for discretization, where a special numerical treatment is needed to avoid singularities. Spikes and oscillations of the solution near corners of the structure were reported, when the resolution is not refined (compared to the resolution required by the Nyström method) at these critical spots. Assumptions for the neutral flux, which are the same for our framework, are the ideal diffuse sources/reflections, the locally constant sticking probability, and molecular flow (ballistic transport without considering inter-particle collisions) of the neutral particles.

In the following sections we first define the simulation domain and introduce the surface model (Section 2). Then, we derive the *receiving* perspective for the discrete radiosity equation (Section 3) and describe the computation of the view factors for holes and trenches (Section 4). Finally, we present the results of the validation and the effects of geometric variations on the wall (Section 5).

2. Simulation domain

For cylindrical holes, the simulation domain is a rotationally symmetric closed convex surface. For trenches, the simulation domain is a trench with a closed convex symmetric cross-section. The neutral flux source is modeled by closing the structures at the top. This leads to a disk-shaped source and a strip-shaped source for holes and trenches, respectively. Fig. 1a and b illustrates the cross-sections of domains with vertical walls and with a kink at one half of the depth, respectively.

The surface adsorption is modeled using a locally constant sticking probability s. The received flux R is split according to s into an adsorbed flux A and a re-emitted flux RE as depicted in Fig. 1c. Source areas additionally emit flux E independent of R.

For the remainder of this work, a sticking probability $s_s = 1$ is used for source areas which to not have any reflections originating from these artificial areas; the bottom is modeled as a fully adsorbing area with a sticking probability $s_b = 1$. A constant sticking probability s_w is used for the walls of the structures. These choices represent a reasonable approximation to the prevalent conditions for the neutral particles in an IECE environment.

3. Radiosity equation

Our assumptions, particularly that all sources and surfaces are ideal diffuse and that the transport of the neutral particles is ballistic, allows for the use of a radiosity formulation.

By assuming a constant flux and a constant sticking probability over each surface element, the problem can be formulated using the discrete radiosity equation: for a surface element i the equation reads

$$B_i = E_i + (1 - \alpha_i)\sum_j (F_{ji}B_j), \tag{1}$$

where B is the radiosity (sum of emitted and reflected energies), E is the self-emitted energy, α is the absorptance, and F_{ji} is the view factor (proportion of the radiated energy, which leaves element j and is received by element i). We adapt (1) to our problem by substituting the absorptance α with the sticking probability s and identifying the adsorbed flux as the adsorbed energy A. The radiosity B is then related to the adsorbed energy A by

$$A_i = (B_i - E_i)\frac{s_i}{1 - s_i}. \tag{2}$$

Since we are also interested in the adsorbed flux at the fully adsorbing areas, (1) and (2) are not applicable because $\lim_{s_i \to 1} A_i = \infty$. For this reason we use the following formulation for the received flux R:

$$R_i = \sum_j (E_jF_{ji}) + \sum_j ((1 - s_j)R_jF_{ji}), \tag{3}$$

where the relation to the adsorbed flux is

$$A_i = R_is_i. \tag{4}$$

Rewritten in matrix notation and resolved for the vector of the received flux R we obtain

$$\begin{aligned} \mathbf{F}^T \cdot E + \mathrm{diag}(1 - s)\mathbf{F}^T \cdot R &= R, \\ (\mathbf{I} - \mathrm{diag}(1 - s)\mathbf{F}^T) \cdot R &= \mathbf{F}^T \cdot E, \end{aligned} \tag{5}$$

with the vector of emitted flux E, a vector of sticking probabilities s, and a matrix of view factors $\mathbf{F}$ (where F_{ij} corresponds to the view factor $i \to j$).

We approximate the solution of the resulting diagonally-dominant linear system of Eq. (5) using the Jacobi method. Each iteration of the Jacobi method can be imagined as a concurrent diffuse re-emission of each element to all other elements. The adsorbed flux A is obtained by multiplying the entries in the solution for R with the corresponding sticking probability s of the element (4). The relation $\|A\| - \|E\| = 0$, which holds for closed surfaces, can be used to test the implementation and to define a stopping criterion for the Jacobi iterations.