High-Fidelity and Efficient Epitaxial Growth Simulations Using Hybrid Meshing and BVH-Based Ray Tracing

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***Abstract*—Epitaxial growth simulations are critical for understanding and optimizing semiconductor fabrication processes, particularly in logic devices, such as source/drain (S/D) contact fabrication for high-aspect-ratio structures. In this work, we propose novel computational methods to enhance both the accuracy and efficiency of simulations. These methods include an optimized ray-tracing approach using Bounding Volume Hierarchies (BVH), a high-fidelity surface mesh generation technique based on Alpha-Wrapping, a hybrid mesh method combining atomic structure and continuum mesh, and a ray-splitting method for efficient ray trajectory computations. Our simulation results demonstrate significant improvements in simulation time and accuracy.**

***Index Terms*—Epitaxial Growth, Bounding Volume Hierarchy (BVH), Alpha-Wrapping, Hybrid Mesh Generation, Ray-Splitting Method**

I. Introduction

Epitaxial growth processes are fundamental to semiconductor manufacturing, especially in logic devices, where precise control over source/drain (S/D) contact formation is critical. Simulating these processes becomes particularly challenging due to the need for atomic-scale accuracy while maintaining computational efficiency. This paper introduces novel computational approaches designed to overcome these limitations and achieve both fidelity and efficiency. We introduce ray-tracing gas transport simulations as well as the Kinetic Monte Carlo (KMC) simulation using the bond-counting model [1], [2].

Previous studies assumed homogeneous gas densities and gas flux distributions near the surface [1]–[3]. The molecular gas flux, also known as the Knudsen flux, is expressed by (1), where P is the pressure, m is the molecular mass, k_B is the Boltzmann constant, and T is the temperature.

$$F = \frac{P}{\sqrt{2\pi m k_B T}} \tag{1}$$

Inhomogeneous gas density must be considered for complex and high-aspect-ratio structures, which have been used in real semiconductor devices and processes in recent years. It is clear that the homogeneous gas density assumption is not valid for isolated voids in device structures, as shown in Fig. 1. This study focuses on the ray-tracing and mesh generation aspects of epitaxial growth simulations. Inhomogeneous gas density is

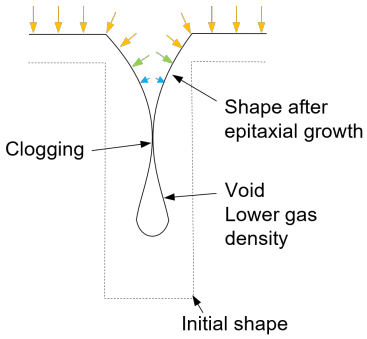

Fig. 1. Inhomogeneous gas densities near the surfaces.

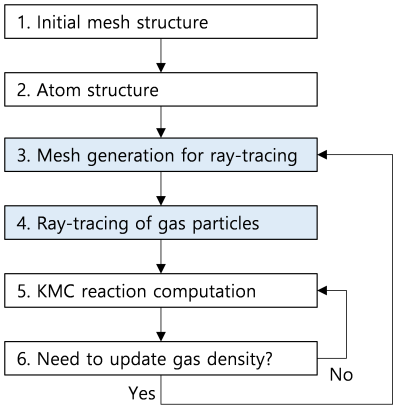

Fig. 2. Schematics of the entire simulation flow.

a key factor in void formation for practical applications, which cannot be adequately addressed by KMC simulations alone.

TABLE I
SIMULATION CONDITIONS

Items	***Values***
Gas molecule model type	neutral
Angular distribution at the source surface	Knudsen cosine
Scatter angular distribution	Knudsen cosine
Surface orientation	[0, 0, -1]
Flat orientation	[1, -1, 0]
Lattice constant	0.5431 [nm]
Boundary conditions	Periodic for x and y

II. METHODS AND RESULTS

In this study, the KMC part computes the surface reaction rate using (2). Here, the surface reaction refers to the reaction of precursor gas molecules binding to the surface.

$$r = f \cdot F \cdot \nu^0 \nu_{\text{bc}} \exp\left(-\frac{E^0_{\text{act}} + \Delta E_{\text{bc}}}{kT}\right) \tag{2}$$

where f is a global scaling factor, F is the molecular gas flux, ν^0 and E^0_{act} are the baseline prefactor and activation energy. ν_{bc} and ΔE_{bc} are the prefactor multiplier and activation energy shift with the bond-count model [1].

Figure 2 shows the schematics of the entire simulation flow. To perform ray-tracing computations, meshes must be generated from the KMC atomic structure. Repeated mesh generations and ray-tracing computations are necessary because the gas density near the surface changes due to geometry changes. These repetitive ray-tracing computations and mesh generations constitute the most time-consuming part of the entire simulation. To apply the simulations to practical applications, reducing the computational cost of mesh generation and ray-tracing while maintaining high-fidelity atomic structure shapes is the biggest challenge. To address these challenges, we introduce four methods, which are explained in the following subsections. These methods are not mutually exclusive but are designed to be used in conjunction, enhancing overall performance when combined.

The details of the simulation conditions are summarized in Table I.

A. Bounding Volume Hierarchy (BVH) Method

Ray-tracing computations are essential for modeling the transport of precursor gas molecules from the source to the epitaxial growth surfaces. We developed a Bounding Volume Hierarchy (BVH)-based ray-tracer using the Embree library [3]. Surface triangle mesh elements were used as geometric primitives for the BVH method. Figure 3 shows the initial structure and the time evolution of the Silicon surface profile during epitaxial growth. Repetitive mesh generation and ray-tracing were performed 47 times during the entire simulation. In each ray-tracing simulation, a total of 100 million rays were emitted from the source surface. Four of them are shown in Figure 3. The BVH method reproduced the diamond shape of Silicon, which is commonly observed in experimental measurements for S/D epitaxial growth [1]. We also confirmed that the BVH method reduces computation time by an order of magnitude compared to the volume-mesh-based ray-tracing method. The epitaxial growth profiles of both methods were almost identical.

B. Alpha-Wrapping Surface Mesh Generation

Accurate epitaxial growth simulations require high-fidelity surface meshes. To address this, we adopted the Alpha-Wrapping method [5] to generate precise surface meshes from KMC atomic structures. Figure 4 (a)-(c) show the initial structure, the time-evolved growth profiles of KMC atomic structures, and the corresponding surface mesh generated by the Alpha-Wrapping method. Repetitive mesh generation and ray-tracing were performed 151 times during the entire simulation. In each ray-tracing simulation, a total of 9 million rays were emitted from the source surface. Four of them are shown in Figure 4. The example includes bridging and merging of surface fronts originating from multiple epitaxial growth seeds. It can also include void formations. The method produces smooth surfaces robustly while maintaining the higher geometric accuracy of the KMC atomic structures. Figure 4 (d) shows the time evolution of flux distributions. It is evident that the flux exhibits a spatial distribution at any given time and that its magnitude changes dynamically over time.

C. Hybrid Mesh Generation

We developed a hybrid mesh method that uses atomistic surface meshes for active regions and continuum-based initial meshes for non-active areas. Figure 5 illustrates the workflow and results. The initial mesh structure, comprising all solid material regions, is depicted in Fig. 5 (a). Figure 5 (b) illustrates the gas region of the initial structure. Using the Alpha-Wrapping method, we generated a surface mesh from the KMC atomic structure for the Silicon material region, as shown in Fig. 5 (c). Combining the gas region of the initial

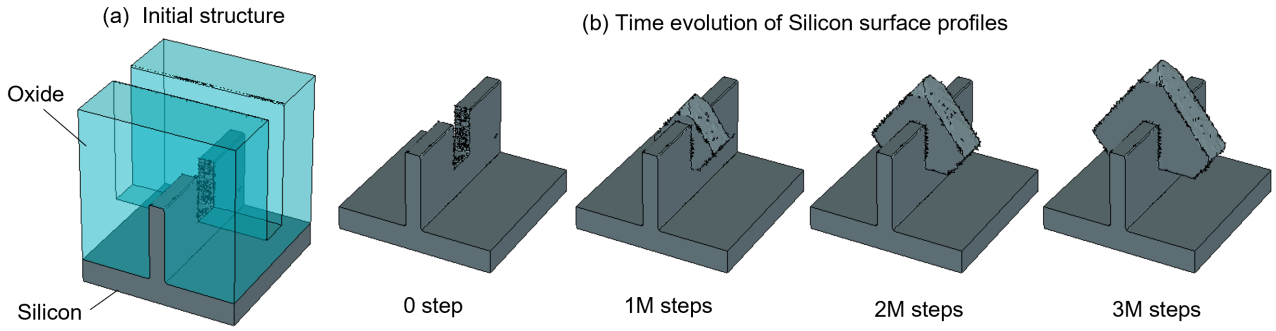

Fig. 3. Silicon surface profile evolutions with BVH ray-tracing method.

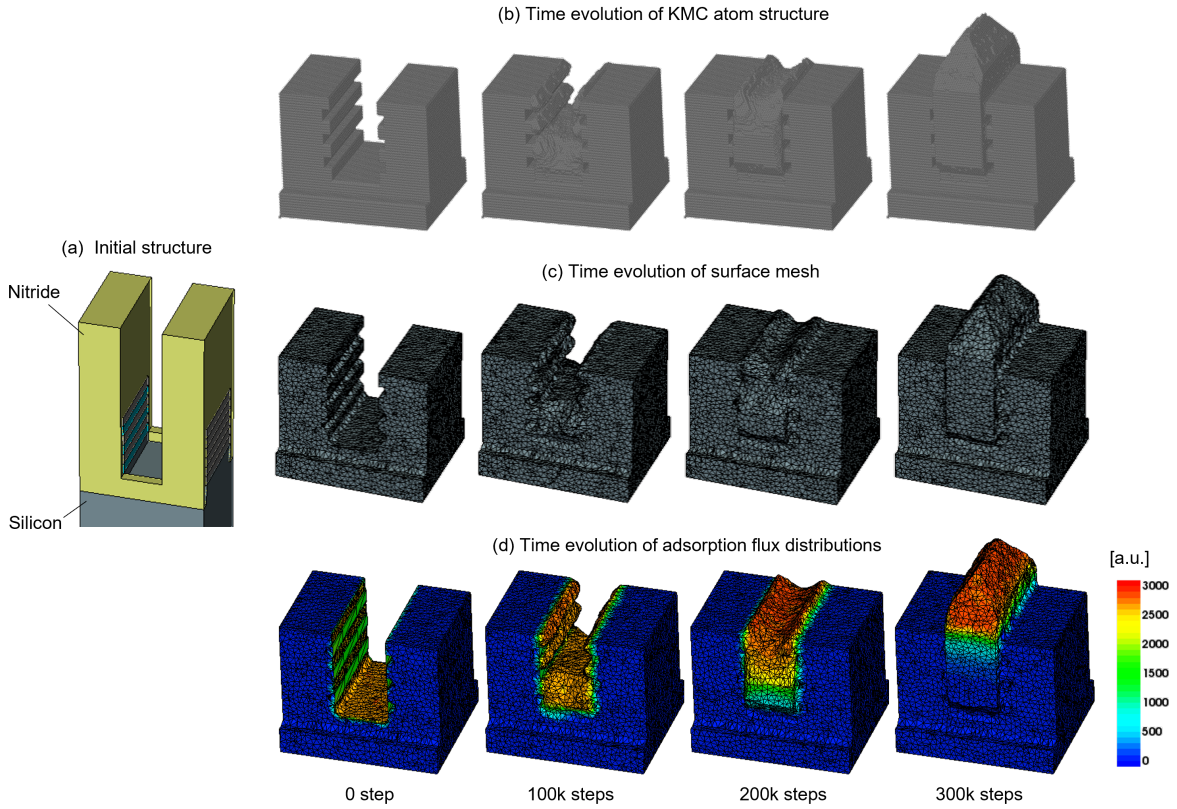

Fig. 4. Time-evolved Silicon surface profiles.

structure with the surface mesh of the Silicon region yields the integrated structure presented in Fig. 5 (d). The integrated structure is used for ray-tracing simulations. The proposed hybrid method ensures atomic precision in critical areas while reducing surface irregularities at the atomic scale and limiting excessive mesh generation in non-active regions. The method can also maintain the sharp corners of the original mesh structure without compromising them by using the atomic structure.

D. Ray-Splitting Method

To further reduce ray-tracing simulation time for high-aspect-ratio structures, we introduced a ray-splitting method inspired by trajectory-splitting techniques used in Monte Carlo ion implantation simulations [6], [7]. Figure 6 (a) illustrates the algorithm of the ray-splitting method. An incoming ray with weight 1.0 hits a surface mesh element. The method splits the ray into two rays. The sticking coefficient of the elements material is 0.1. One ray adsorbs on the element with weight 0.1, while the other ray with weight 0.9 scatters

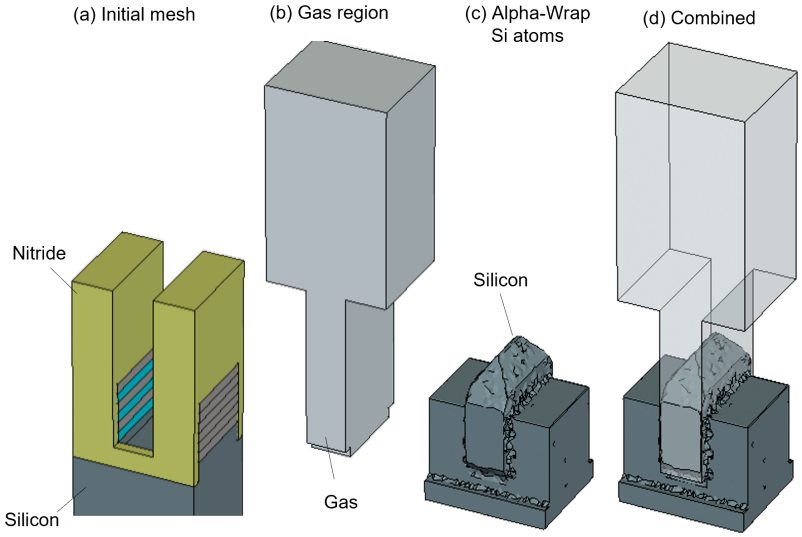

Fig. 5. Hybrid mesh workflow and results.

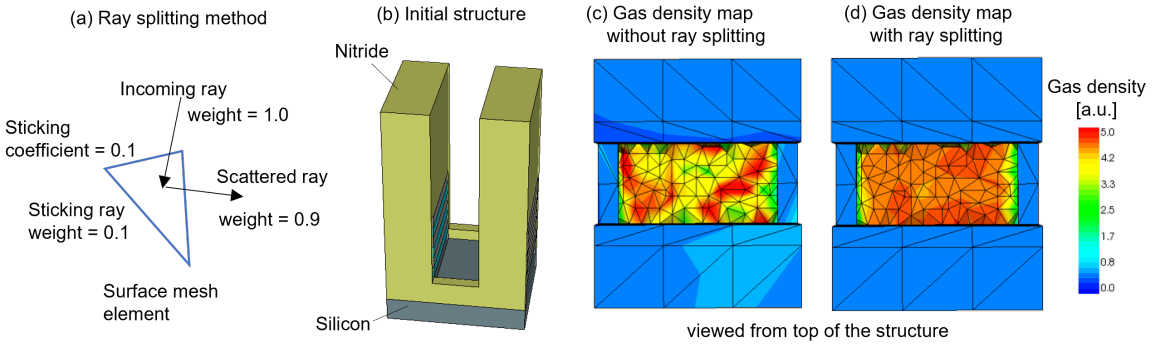

Fig. 6. Ray-splitting method and gas density maps.

on the surface. Ray-splitting achieves a tenfold reduction in simulation time, maintaining a similar level of statistical accuracy. Figure 6 (c) shows the gas density distribution without the ray-splitting method. Figure 6 (d) shows the gas density distribution with the ray-splitting method. The results demonstrate the effectiveness of the methods in balancing accuracy and computational efficiency. The number of rays split on surface mesh elements can exceed two, and the weights can be adjusted for performance optimization.

III. Conclusions

This work presents critical advancements in epitaxial growth simulation methodologies: (i) a BVH-accelerated ray-tracer achieving an order of magnitude speedup, (ii) Alpha-Wrapping-based mesh generation for high-fidelity surfaces, (iii) a hybrid atomic-continuum mesh method optimizing computational costs, and (iv) a ray-splitting method improving simulation efficiency. These innovations collectively enable faster and more accurate simulations, which are vital for process development and device reliability optimization.

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