Atomic-Level Monte Carlo Modeling of SiN Deposition by PECVD

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Abstract—Plasma-enhanced chemical vapor deposition (PECVD) is a critical technique in integrated circuit manufacturing. As semiconductor devices continue to scale down in advanced technology nodes, the details of PECVD processes are difficult to be captured by traditional Technology Computer Aided Design (TCAD) approaches. In this study, we present a Monte Carlo approach to predict the profile evolution of Si3N4 thin film deposition by PECVD at feature scale. By employing a new transport algorithm for reactive species in vacuum, our method achieves an atomic-level modeling of deposition profile evolution within acceptable computational time. Experimental validation demonstrates that this model achieves a mean prediction errors below 10% for the deposition of trenches with different aspect ratios.

Index Terms—PECVD, Vacuum Transport Algorithm, Monte Carlo Simulation, Profile Evolution Prediction

I. Introduction

As semiconductor devices continue to scale down in advanced technology nodes, FinFETs and GAAFETs have become the dominant logic device structures[1, 2]. This scaling trend increases the complexity of process development, making it more challenging to identify optimal process parameters. Process modeling has been increasingly adopted to help understand the underlying mechanisms and support parameter optimization. However, as the critical dimensions (CDs) shrink into the nanometer regime, microscopic effects and variations have a greater influence on device performance, exposing the limitations of conventional feature scale process models.

In this work, we present an atomic-level simulation based on the Monte Carlo approach to predict the profile evolution of Si_3N_4 thin film deposition by plasma-enhanced chemical vapor deposition (PECVD). The model is first calibrated using experimental data from trenches with varying opening widths. Its predictive capability is then evaluated on different trench structures under the same process conditions.

II. Modeling Flow

We propose an atomic-level Monte Carlo model for PECVD and the workflow is illustrated in Fig.1

A. Construction of the "lattice" on the initial substrate

We employ hexagonal close packing (HCP) lattice to construct the initial substrate. This method is well-suited for modeling actual substrate crystals in 3D epitaxial growth simulation. Using the nearest-neighbor approximation, a particle in a lattice only interacts with its six closest neighbors. The interaction strength is estimated as one half of the chemical bond energies of Si−Si, Si−N and N−N bonds, with values of 0.35 eV, 0.52 eV, and 0.40 eV, respectively[3, 4].

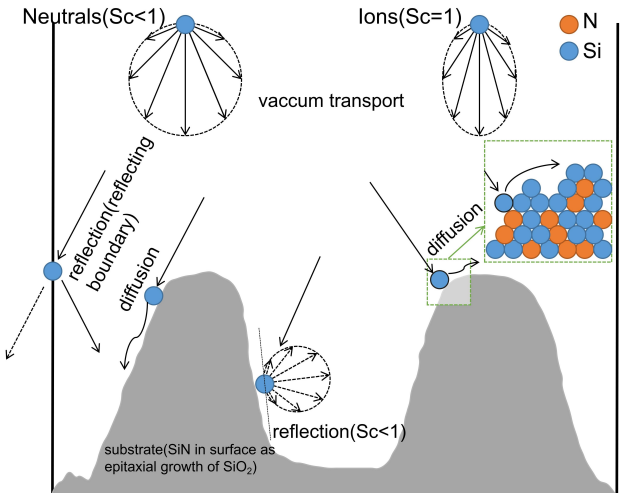

Fig. 1. Particle motion mechanisms in the model.

B. Transport of active particles in vacuum

The fundamental transport in vacuum has been described in our previous work[5]. To improve computational efficiency, given the fact that the interaction region is mathematically simply connected, we have employed a new algorithm (Fig.2) to significantly improve the computational efficiency.

Firstly, we define a data structure termed two-dimensional segment tree — a type of quad-tree

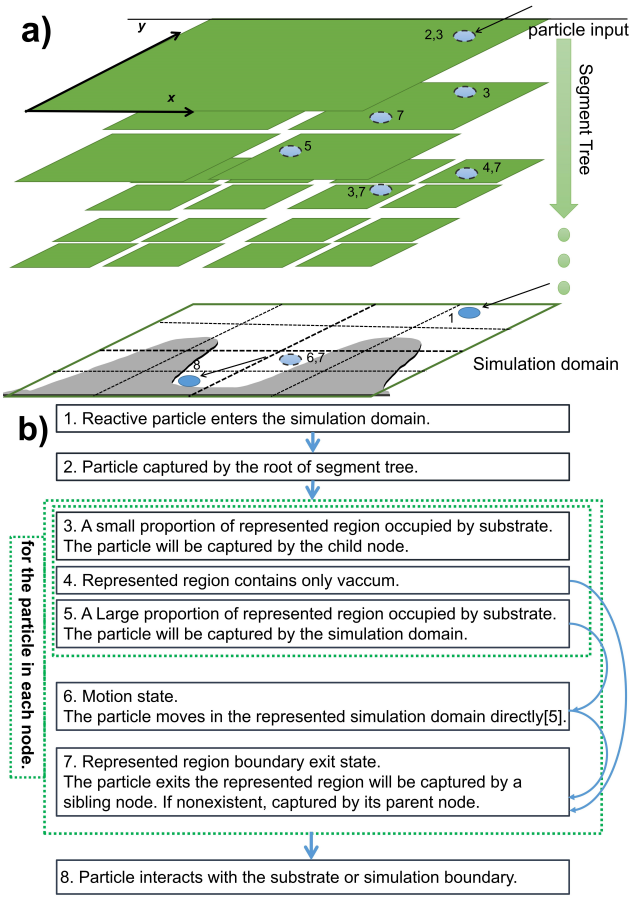

Fig. 2. The illustration of the vacuum transportation algorithm. a) The data structure of the algorithm to capture the vacuum transport process. The labeled numbers beside the particles indicate its state. b) Diagram illustratioon of the finite state machine (FSM) of the algorithm.

structure(Fig.2(a)). The root node of this tree represents the region of the entire simulation domain, including both the substrate and vacuum. The four child nodes represent the top-left, bottom-left, top-right, and bottom-right sub-regions of the region represented by their parent node. Each node records the proportion of its represented region currently occupied by the substrate material, including any SiN thin film grown during the simulation.

The motion of a reactive particle in the quad-tree is determined by a finite state machine (FSM) with 8 types of states (Fig.2(b)) described below:

1) State 1: It is the initial state of the FSM. A reactive particle enters the simulation domain with the initial motion state concluding the initial position and directional vector. The particle travels in a straight-line trajectory through the vacuum.
2) State 2: The particle is captured by the root node of the two-dimensional segment tree.
3) State 3: A small proportion of represented region of current node is occupied by substrate (Coverage $< 90\%$). The particle will be captured by the child node whose represented region contains its position.
4) State 4: The represented region of current node contains only vacuum. As no interaction with the substrate occurs along its motion path, the trajectory can be calculated quickly. Once it moves out of the region, transit to State 7.
5) State 5: A large proportion of represented region of current node is occupied by substrate (Coverage $\geq 90\%$). Transit to State 6.
6) State 6: Motion state. The particle moves in the represented simulation domain directly[5]. Once it exits the represented region, transition to State 7.
7) State 7: Represented region boundary exiting state. The particle exits the represented region will firstly try to be captured by the sibling node of current node. If the sibling node is nonexistent, it will be captured by its parent node.
8) State 8: It is the terminated state of the FSM. Ultimately, the particle will either arrive at the simulation boundary or interact with the substrate, resulting in either chemical reaction or reflection.

Additionally, the model considers only four types of active particles: N-containing neutral particles (e.g., NH_3), Si-containing neutral particles (e.g., SiH_4), plasma-state N particles, and plasma-state Si particles. Once particles enter the simulation domain, their motion is impacted by substrate surface reflections only: Neutral radicals undergo chemical reactions and react with a probability defined by the sticking coefficient $Sc \ll 1$. If a reaction does not occur, particles reflect and resume their transport in vacuum. Plasma-state particles are assumed to always undergo chemical reactions and "stick"[6].

C. Adsorption and diffusion of particles on the substrate surface

Particles that form chemical bonds will diffuse across the surface due to molecular thermal motion. Among all possible surface diffusion mechanisms, only surface vacancy diffusion is considered, as the energy barrier for this process is by far the lowest.

We employed a one-step diffusion model. First, the diffusion length of each adsorbed particle is estimated. Subsequently, the change of energy ΔE of entire substrate associated with moving the particle from current lattice site to each nearest-neighbor vacancy is computed and the diffusion probability P of each direction is estimated by the Arrhenius diffusion formula: $P_i = f \exp(-\Delta E_i / kT)$, where f is a constant and kT represents the thermal energy at the current temperature[7]. The diffusion of the particles is then probabilistically selected based on these values until the estimated diffusion length is reached. Ultimately, the particle tends to remain at a position with a lower surface energy near its initial sticking site on the substrate.

Compared to the Kinetic Monte Carlo (KMC) approach[8], the one-step diffusion scheme used in our model requires less simulation time while reaching comparable accuracy due to the low-pressure and low-temperature conditions of PECVD.

III. Results and Discussion

In this work, we propose an atomic-level MC model for the SiN PECVD process. We calibrate this model using experimental data from a series of trenches with different opening widths. A comparison between experimental and simulated deposition profiles is shown in Fig.3(a) and Fig.3(b). Fig.3(c) shows how the prediction error varies with the sticking coefficient and the plasma-state particle proportion during the calibration phase.

Subsequently, the calibrated model is tested by simulating denser trench structures with different spacing values (Fig.4) and comparing these with TEM images. Additional zoomed-in results of key regions of Fig.3 are shown in Fig.5(a-d). Fig.5(f) compares the thicknesses of the thin film in the TEM image and simulation results at 7 key (Fig.5(e)) locations, indicating the thickness variation trends across trenches with different opening widths.

The model achieves a mean prediction error below 10%, indicating a strong match with experiments. The method presented in this study offers a new approach towards nanoscale PECVD process profile simulation and process parameter tuning.

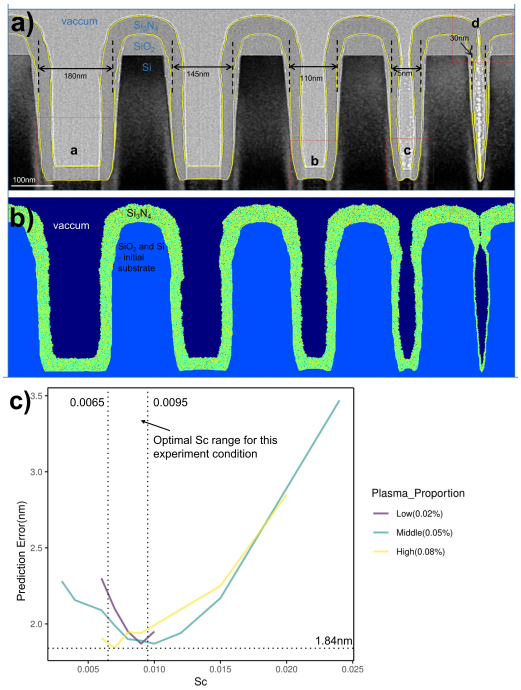

Fig. 3. a) TEM image of a 5-trenches structure with different CDs (180nm, 145nm, 110nm, 75nm, 30nm respectively), b) corresponding simulation result of SiN growth profile, c) the prediction error between a) and the model (by error size/perimeter of the contour) varies as Sc and plasma proportion.

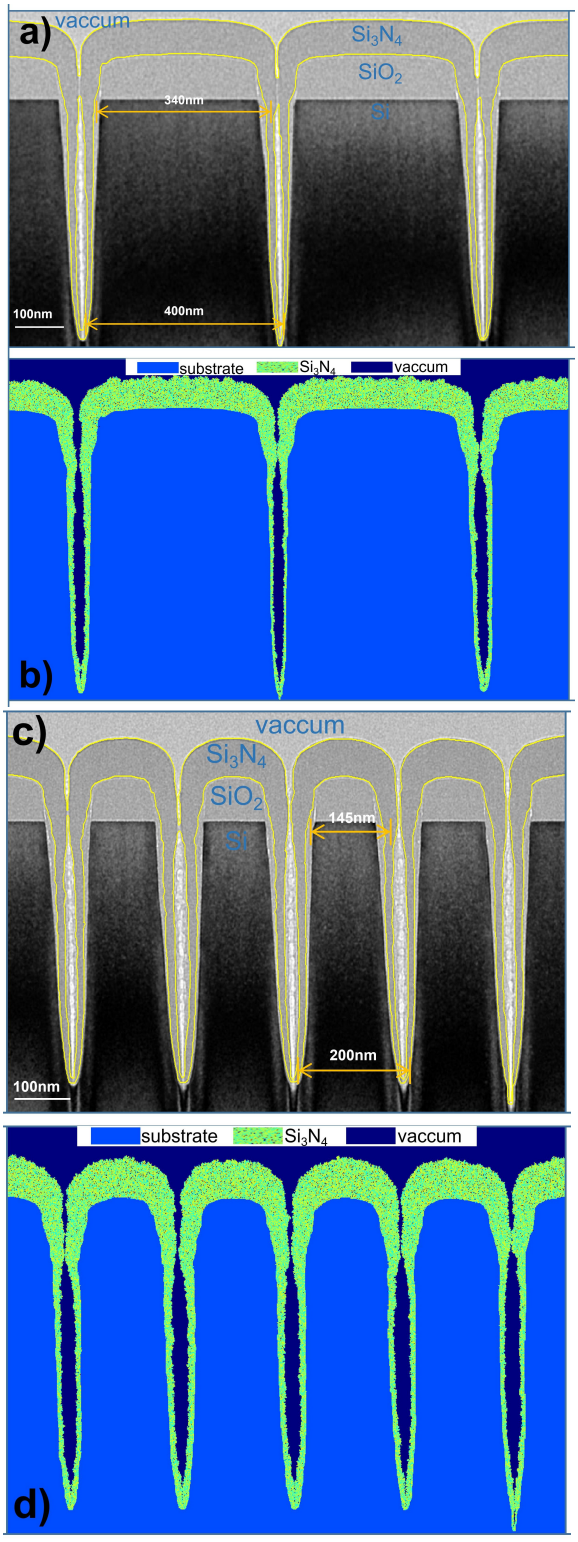

Fig. 4. a) TEM image of structures with dense trenches (pitch/space=400nm/60nm) and b) the corresponding simulation results. c) TEM image of structures with dense trenches (pitch/space=200nm/55nm) and d) the corresponding simulation results.

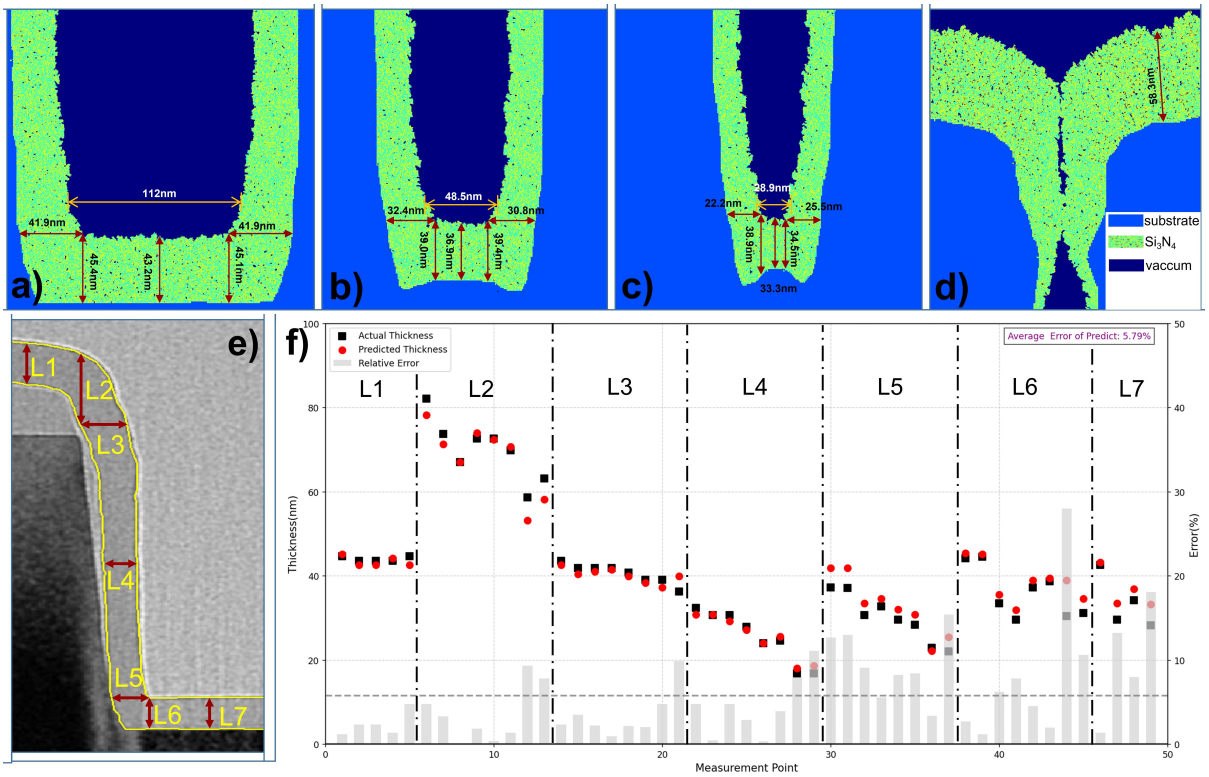

Fig. 5. a-d) Zoomed-in simulation counterparts for Fig.3(a) respectively. e) The selected 7 key film thickness measurement locations. f) Thickness variation trends of TEM image and simulation results across trenches in Fig.3(a).

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