Kinetic Monte Carlo Simulation of Etching Profile Evolution for Low Dielectric Constant Inorganic Materials in Fluorocarbon Containing Plasma

Workshop
April 15, 2004
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2003-04 Main Objectives

- To develop a two dimensional profile simulator based on Kinetic Monte Carlo (KMC) methods for low dielectric etching in a fluorocarbon discharge. (Milestone 4)
- Profile simulator development and refinement is ongoing continuously. The goal is to have the first version of the KMC based simulator at the end of the third year.
- During the first year, we aim to have the general KMC model in place and capture the most important phenomena necessary to capture the range of experimental observations in the literature. These include (but not limited to):
  - The balance between etching and deposition which controls the side wall angle.
  - Dependence of the etch deposition rate on the ion energy.
  - Roughening of the sidewalls.
  - Ion activated polymer deposition and etch stop.

2 Kinetic Monte Carlo Simulation Geometry and First Cell Representation

- All solid cells that are not at surface would still contain $N$ particles. A cell is removed when the number of particles in cell reaches less than lower limit (e.g., $N/5$).
- A new cell is added when the number of particles in cell reaches more than upper limit (e.g., $2N$).

3 The Problem

- Position of the dielectric-vacuum interface is governed by the interface evolution equation where $ER = \frac{\partial \phi}{\partial t}$ is the right hand side that involves fluxes and energy and angle distributions.
- The profile simulator satisfies the equation

$$\nabla \cdot (E \phi) = 0. \nabla \cdot (E \phi) = 0
$$

4 Elements of Profile Evolution Simulations by KMC

Each particle trajectory is independently treated because intermolecular collisions can be neglected at the ion pressures (40 mTorr), the mean free path of molecules is ~1 cm and the feature dimension is ~1 µm.

- Each cell in the simulation is assigned a memory structure that contains the identity of the cell ($r$, $\theta$, $z$), total particle count and the composition of the cell.
- The thin film consists of 20 to 50 cells, in which the number of particles in 20±5 cells differ less than the number of particles in 25±5 cells (e.g., 2h cell). Each cell represents many atoms.
- Each cell is assumed to be perfectly mixed and particles are allowed to react with incoming neutrals and ions. Number of atoms and the composition of each cell is updated at each Monte Carlo step.
- Reactions can take place in a cell or in cells determined by the probability of reactions (parameters).
- We aim to model surface reactions that correspond to chemical etching in an ion-assisted etching. Further refinements will include polymeric depositions.
- Neutral species (e.g., $\text{CF}_2$, $\text{CF}_3$) formed as a result of these reactions in the cells are removed from the cell and cell changes identity (e.g., from dielectric to vacuum) if the number of particles in the cell falls below a threshold value.
- Time is advanced based on the rates of randomly selected processes.
- KMC and cellular representation permit the modeling of stochastic processes, such as surface roughening due to etching of porous structures that are impossible to model by deterministic methods.

5 Flow Chart of Simulation

- Neutral Trajectory Computation & Surface Interactions

6 Surface Interactions

- Ion Trajectory Computation & Surface Interactions

7 Calculation of Surface Normal and Collisions with the Surface

- Surface normal calculation for neutral and ion scattering events require different accuracy. Accurate surface normal calculation is required for ion because ion induced etching and scattering are strong functions of the incident angle. The other hand, it is not necessary to calculate the surface normal accurately for neutral scattering.
- Four points calculation for the neutral scattering.
- Least square method for the ion scattering.

8 Results: Where are we going?

- Process development and analysis are being carried out to make comparisons between the experimental SEM data and the profile simulations.
- We have made adjustments to the profile simulations using the feedback between the experimental SEM data and the profile simulations.
- We aim to have first version at the end of the first year.
- Year I: Process and single wafer etching and make comparisons to make our simulations.
- Year II: Procure patterned wafers and etch them to make comparisons of the results.
- Year III: Couple reactor scale simulations with profile scale simulations.
- Year IV: Incorporate effects of feature charging in coupled reactor scale and feature profile simulations.
- Year IV: Compare profile simulations with experimentally obtained profiles in the center of and off axis.

9 Future Goals

- Profile simulator development and refinement will go on continuously. We aim to have first version at the end of the first year.
- Year I: Process optimization and single wafer etching and make comparisons between the experimental SEM data and the profile simulations.
- Year II: Make adjustments to the profile simulations using the feedback from the experiments, MD simulations and reactor scale simulations.
- Year III: Procure reactor scale simulations with profile scale simulations.
- Year IV: Incorporate effects of feature charging in coupled reactor scale and feature profile simulations.
- Year IV: Compare profile simulations with experimentally obtained profiles in the center of and off axis.

Acknowledgment