

The Langmuir Feature Model

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Abstract

In this document, a feature scale model is developed and used for recipe tuning. The detailed physical mechanisms and numerical algorithms are introduced and discussed.

1 Introduction

The Langmuir Feature Model uses particle-based Monte Carlo methods to simulate the evolution of etch features when exposed to plasma discharges. The model uses pseudo-particles to represent the incoming species, including electron, ions and neutral particles. All these pseudo-particles are tracked for their trajectories and interactions with materials. The materials in the model are represented by a structured mesh of voxels or cubes. Each voxel or cube represents a macro solid material, which consists of hundreds of atoms or molecules. The mesh can be initialized in an arbitrary shape with surface conditions, which may include multiple materials and features within the each domain. This allows the simulation of complex structures and steps in the fabrication process, such as finFET structure.

A pseudo-particle is also a macro particle, which consists of atoms or molecules with the same number as in the materials. The pseudo-particles are launched with specified flux, angle and energy, which are often derived from a reactor scale model, which is, within the Langmuir Model, the Langmuir Reactor Model. Without the reactor model, the Langmuir Feature Model can also self generate generic functions of flux, angle and energy. The coupling of feature scale model to reactor scale model allows the Langmuir Model to explore the process recipe with the etch result, or to be used to study fundamental physics. This versatility makes the Langmuir Model a strong tool for recipe tuning and optimization, as well as new physics investigation.

2 Mesh

The mesh in Langmuir Feature Model is constructed in 2D space, in which (x, z) are used to represent the 2D coordinates and infinity is assumed in y direction. The model discretizes the 2D space into a rectangular computational cells. The cell center is marked as a node, which determines the location (x, z) of the cell. Each cell has a volume of $\Delta x \times \Delta z$, where Δx and Δz are the resolutions in x and z directions, respectively. Usually, square cells, where $\Delta x = \Delta z$, are used. Non-square cells, which are used for high aspect ratio domain for memory saving, need future test and validation. The computational complexity increases with reducing resolution as approximately $O(n^3)$, where n is the number of cells per side in the simulation domain. The choice of resolution also affects the time weighting of each pseudo-particle, which will be described later.

Each cell, representing a solid material, is assigned a material property. The material