

The Langmuir Reactor Model

Wei Tian

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TSMC

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.

3 Poisson Equation

3.1 Explicit Poisson's equation

With explicit method, the potenital in the Poisson's equation is determined by the current charge density, which is impacted by the previous potential.

$$-\nabla \cdot \varepsilon \nabla \phi(t) = e \left(\sum_{ion} n_i(t) - n_e(t) \right)$$

$$-\nabla \cdot \varepsilon \nabla \phi(t + \Delta t) = e \left(\sum_{ion} n_i(t + \Delta t) - n_e(t + \Delta t) \right)$$

$$\frac{\partial n_{e,i}}{\partial t} = D_{e,i} \nabla^2 n_{e,i}(t) \pm \nabla \cdot (\mu_{e,i} n_{e,i}(t) \nabla \phi(t)) + S_e(t)$$

$$n_{e,i}(t + \Delta t) = n_{e,i}(t) + \Delta t \times f_{e,i}(\phi(t))$$

$$-\nabla \cdot \varepsilon \nabla \phi(t + \Delta t) = F(\phi(t))$$

where

$$\phi = \text{potential}$$

$$\varepsilon = \text{permittivity}$$

$$e = \text{elementary charge}$$

$$n_{e,i} = \text{electron, ion density}$$

$$\mu_{e,i} = \text{electron, ion mobility}$$

with the derivation above, the future potential is determined by the current potential.

3.2 Semi-implicit electron with predictor-corrector ions

The timestep is limited to as small as a few picoseconds, which is not practical for any useful simulations. Implicit method can theoretically remove the limit of the timestep, with the cost of solving for the reversed matrix. The matrix solver could be much expensive as well. A semi-implicit method is, therefore, proposed to increase the timestep and meanwhile reduce the cost of matrix solver. The principal is shown as below,

$$-\nabla \cdot \varepsilon \nabla \phi(t + \Delta t) = e \left(\sum_{ion} n_i(t + \Delta t) - n_e(t + \Delta t) \right)$$

$$\frac{\partial n_e}{\partial t} = D_e \nabla^2 n_e(t) - \nabla \cdot (\mu_e n_e(t) \nabla \phi(t + \Delta t)) + S_e(t)$$

$$n_e(t + \Delta t) = n_e(t) + \Delta t \times f_e(\phi(t + \Delta t))$$

$$\begin{aligned}
\frac{\partial n_i}{\partial t} &= D_i \nabla^2 n_i(t) + \nabla \cdot (\mu_i n_i(t) \nabla \phi(t)) \\
n_i(t + \Delta t) &= n_i(t) + \Delta t \times f_i(\phi(t)) \\
-\nabla \cdot \varepsilon \nabla \phi(t + \Delta t) &= e \left(\sum_{ion} [n_i(t) + f_i(\phi(t))] - [n_e(t) + f_e(\phi(t + \Delta t))] \right) \\
-\nabla \cdot \varepsilon \nabla \phi(t + \Delta t) &= \\
e \left(\sum_{ion} [n_i(t) + \Delta t \times f_i(\phi(t))] - [n_e(t) + \Delta t \times S_e(t) + \Delta t \times D_e \nabla^2 n_e(t) - \Delta t \times \nabla \cdot (\mu_e n_e(t) \nabla \phi(t + \Delta t))] \right) \\
-\nabla \cdot \varepsilon \nabla \phi(t + \Delta t) + e \times \Delta t \times \nabla \cdot (\mu_e n_e(t) \nabla \phi(t + \Delta t)) &= F(n_{e,i}(t), \phi(t)) \\
\left[-\nabla \varepsilon \cdot \nabla \phi(t + \Delta t) - \varepsilon \nabla^2 \phi(t + \Delta t) \right] + \left[(e \mu_e \Delta t) \nabla n_e(t) \cdot \nabla \phi(t + \Delta t) + (e \mu_e \Delta t) n_e(t) \nabla^2 \phi(t + \Delta t) \right] \\
&= F(n_{e,i}(t), \phi(t)) \\
\left[(e \mu_e \Delta t) n_e(t) - \varepsilon \right] \nabla^2 \phi(t + \Delta t) + \left[(e \mu_e \Delta t) \nabla n_e(t) - \nabla \varepsilon \right] \cdot \nabla \phi(t + \Delta t) &= F(n_{e,i}(t), \phi(t)) \\
\underline{A(n_e(t))} \nabla^2 \phi(t + \Delta t) + \underline{\nabla B(n_e(t))} \cdot \nabla \phi(t + \Delta t) &= F(n_{e,i}(t), \phi(t))
\end{aligned}$$

underline – emphasis

The electron density is solved using implicit method, where the future electron density is determined by the future potential, while the ion density is still solved using explicit method, where the future ion density is determined by the current potential. In this scenario, electron density and potential get quickly convergent with large timestep. A further attention needs to be paid to the ion density, which could oscillate. The predictor-corrector method is used for ion density.

$$\begin{aligned}
\tilde{n}_i(t + \Delta t) &= n_i(t) + \Delta t \times f_i(n_i(t), \phi(t)) \\
n_i(t + \Delta t) &= n_i(t) + \Delta t \times \frac{1}{2} (f_i(n_i(t), \phi(t)) + f_i(\tilde{n}_i(t + \Delta t), \phi(t + \Delta t)))
\end{aligned}$$

3.3 Semi-implicit Poisson's equation

The ion density can use implicit method as well. In this case,

$$\begin{aligned}
-\nabla \cdot \varepsilon \nabla \phi(t + \Delta t) &= e(\sum_{ion} [n_i(t) + f_i(\phi(t + \Delta t))] - [n_e(t) + f_e(\phi(t + \Delta t))]) \\
-\nabla \cdot \varepsilon \nabla \phi(t + \Delta t) &= e(\sum_{e,i} [n_{e,i}(t) + f_{e,i}(\phi(t + \Delta t))]) \\
-\nabla \cdot \varepsilon \nabla \phi(t + \Delta t) &= \\
e(\sum_{e,i} [n_{e,i}(t) + \Delta t \times S_{e,i}(t) + \Delta t \times D_{e,i} \nabla^2 n_{e,i}(t) + \Delta t \times \nabla \cdot (q\mu_{e,i} n_{e,i}(t) \nabla \phi(t + \Delta t))]) & \\
-\nabla \cdot \varepsilon \nabla \phi(t + \Delta t) - \sum_{e,i} \Delta t \times \nabla \cdot (eq\mu_{e,i} n_{e,i}(t) \nabla \phi(t + \Delta t)) &= F(n_{e,i}(t)) \\
\underline{[\sum_{e,i} (eq\mu_{e,i} \Delta t) n_{e,i}(t) - \varepsilon] \nabla^2 \phi(t + \Delta t)} + \underbrace{[(e\Delta t) \sum_{e,i} \mu_{e,i} \nabla n_{e,i}(t) - \nabla \varepsilon] \cdot \nabla \phi(t + \Delta t)} &= F(n_{e,i}(t)) \\
\underline{A(n_{e,i}(t)) \nabla^2 \phi(t + \Delta t)} + \underline{\nabla B(n_{e,i}(t)) \cdot \nabla \phi(t + \Delta t)} &= F(n_{e,i}(t))
\end{aligned}$$

The future potential is solved directly, which means that the future potential does not depends on the current potential anymore. All coefficients in this equation are densities at current time.