

The Langmuir Reactor Model

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Abstract

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

1 Introduction

The modeling of plasmas for semiconductor processes is challenged by conflicting goals - having detailed, specialized algorithms resolving the particular problems such as iso-dense problems and metal contaminations while also being fast enough to scan a wide parameter space for recipe tuning. The former challenge requires the model as accurate as possible in physics. However, the latter challenge requires the model as fast as possible in computing. Sacrifice and compromise have to be made between these two. The Langmuir Reactor Model is developed to meet these challenges.

2 Geometry and Mesh

The mesh in Langmuir Reactor Model is constructed in 2D space, in which (x, z) are used to represent the 2D coordinates. (to be edited: 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 potential 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

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

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

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

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

$\mu_{e,i}$ = 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,

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

$$= F(n_{e,i}(t), \phi(t))$$

$$[(e\mu_e\Delta t)n_e(t) - \varepsilon]\nabla^2\phi(t+\Delta t) + [(e\mu_e\Delta t)\nabla n_e(t) - \nabla\varepsilon]\cdot\nabla\phi(t+\Delta t) = F(n_{e,i}(t), \phi(t))$$

$$\underline{A(n_e(t))\nabla^2\phi(t+\Delta t) + \nabla B(n_e(t))\cdot\nabla\phi(t+\Delta t)} = F(n_{e,i}(t), \phi(t))$$

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.

$$\tilde{n}_i(t + \Delta t) = n_i(t) + \Delta t \times f_i(n_i(t), \phi(t))$$

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

3.3 Semi-implicit Poisson's equation

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

$$-\nabla \cdot \varepsilon \nabla \phi(t + \Delta t) = e(\sum_{ion} [n_i(t) + f_i(\phi(t + \Delta t))] - [n_e(t) + f_e(\phi(t + \Delta t))])$$

$$-\nabla \cdot \varepsilon \nabla \phi(t + \Delta t) = e(\sum_{e,i} [n_{e,i}(t) + f_{e,i}(\phi(t + \Delta t))])$$

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

$$e(\sum_{e,i} [n_{e,i}(t) + \Delta t \times S_{e,i}(t) + \Delta t \times D_{e,i} \nabla^2 n_{e,i}(t) + \Delta t \times \nabla \cdot (q\mu_{e,i} n_{e,i}(t) \nabla \phi(t + \Delta t))])$$

$$-\nabla \cdot \varepsilon \nabla \phi(t + \Delta t) - \sum_{e,i} \Delta t \times \nabla \cdot (eq\mu_{e,i} n_{e,i}(t) \nabla \phi(t + \Delta t)) = F(n_{e,i}(t))$$

$$\underline{[\sum_{e,i} (eq\mu_{e,i} \Delta t) n_{e,i}(t) - \varepsilon] \nabla^2 \phi(t + \Delta t)} + \underline{[(e \Delta t) \sum_{e,i} \mu_{e,i} \nabla n_{e,i}(t) - \nabla \varepsilon] \cdot \nabla \phi(t + \Delta t)} = F(n_{e,i}(t))$$

$$\underline{A(n_{e,i}(t))} \nabla^2 \phi(t + \Delta t) + \underline{\nabla B(n_{e,i}(t))} \cdot \nabla \phi(t + \Delta t) = F(n_{e,i}(t))$$

The future potential is solved directly, which means that the future potential does not depend on the current potential anymore. All coefficients in this equation are densities at current time. The second term in the LHS is probably (not sure, need additional check) not easy to deal with. It could be rewritten in explicit form and moved to the RHS.

$$\underline{A(n_{e,i}(t))} \nabla^2 \phi(t + \Delta t) + \underline{\nabla B(n_{e,i}(t))} \cdot \nabla \phi(t + \Delta t) = F(n_{e,i}(t))$$

$$\underline{A(n_{e,i}(t))} \nabla^2 \phi(t + \Delta t) = F(n_{e,i}(t)) + \underline{\nabla B(n_{e,i}(t))} \cdot \nabla \phi(t)$$

$$\underline{A(n_{e,i}(t))} \nabla^2 \phi(t + \Delta t) = F(n_{e,i}(t), \phi(t))$$

Now the Poisson's equation retains its Laplacian form, with the source term depending on current potential. The same technique can be applied to Sec. 3.2 as well.