TWO-DIMENSIONAL NUMERIC MODELING OF PLASMA ETCHING

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ABSTRACT

Plasma etch is the most suitable technique for advanced micro- and nanofabrication. The comprehension of plasma behavior is of great importance to develop models which can predict fabricated structures. A two-dimensional numeric model of plasma using the Vlasov equation has been developed. This model allows for the analysis of low density plasma, composed of particles which are not subject to collisions. The simulation method applied is the particle-mesh and is carried out with SCILAB. Both, unidimensional and bidimensional plasmas with classic interaction cases are studied.

1. INTRODUCTION

Pattern transfer by plasma etching is an integral part of advanced microelectronics fabrication. Wet etching has several limitations, including poor adhesion of the masking layer to the substrate, inability of liquid etchants to penetrate narrow and high-aspect-ratio features. So plasma etching has great advantages, such as: high etch rate, uniformity of etch rate across the surface, high selectivity of the layer to be etched with respect to both the masking material and to the underlying layers, a residue-free surface after etch and others [1].

In etching processes by high-density plasma it is possible to achieve characteristics such as large etching depth, high anisotropy and low surface roughness, which are sought after characteristics in micro- and nanofabrication. Among other advantages, one could mention: better quality and control; the reagents can be monitored with spectrometric methods, allowing for the determination of the process end. Hence, it is very important to understand the interactions and phenomena that occur with plasma in certain applications.

Due the importance of the plasma mentioned before, this work presents a method for numeric modeling of plasma etching. The idea is consider a computational mesh with forbidden regions. The forbidden regions are regions in which the particles are not allowed to enter. In this work, the chamber walls are hard forbidden regions, and the material to be etched is a soft forbidden region. For the soft forbidden region, if a particle reaches it with energy higher than a minimum, the particle will penetrate this region, and after this event, this corresponding region mesh will become allowed. This means that an etching event occurred. For particles with energy below minimum or reaching a hard forbidded region, the conservation of energy and moment is applied. An illustration of the mesh is presented in Figure 1.

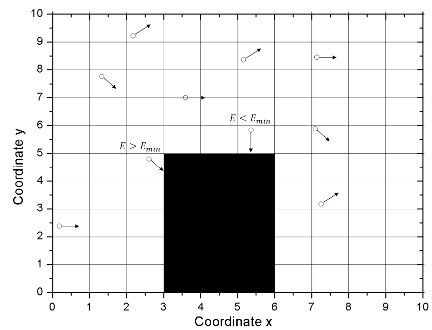

Figura 1: Illustration of the model proposed for the simulation of plasma etching, where the darkened region corresponds to a forbidden region, which will be etched depending on the energy with which the particles collide to this specific region.

Due to the easiness of altering plasma parameters and conditions in a computational model, such as temperature, oscillation frequency, number of particles, charge density and initial conditions, it becomes faster and more feasible to study the plasma behavior via a computational model instead of by experimentation.

The simulation model to plasma used is the particle-mesh, which exploits the force-at-a-point formulation and a field equation for the potential and a NGP (Nearest-Grid-Point) scheme for the plasma was obtained. Since the model is based on the Vlasov equation, the particles are not subject to collision.

This work begins with a brief introduction. Then, the plasma phenomena and equations are presented. After, simulations results are presented and discussed. Finally the conclusions.

2. PLASMA

Plasma is an ionized medium composed by free electrons, ions and neutral atoms in varying proportions and exhibits a collective behavior. The quantity of charged particles depends on the temperature and creation method. The three main phenomena that characterize matter in plasma state are: emission of electromagnetic radiation, Debye shielding, and collective oscillations due to coulombian forces.

The electric field shielding phenomenon or Debye shielding is related to the system equivalent charge, which exponentially decays with a time constant given by the Debye length, as follows:

$$\left(q_{eq} = q_0 . e^{\frac{-x}{\lambda_D}} \right)$$

This explains the *quasi*-neutrality of plasma, in which a disturbing electric field that might eventually appear in its interior must nullify itself to distances much longer than the Debye length.

Besides this *quasi*-neutrality, other criteria for the existence of plasma exist. The number of particles inside the Debye sphere must be sufficiently large for the electric field shielding to be efficient and the frequency of collisions between the charged particles and the gas' neutral atoms must be smaller than the frequency of the plasma oscillation.

3. PHYSICAL ANALYSIS OF THE SYSTEM

The mathematical model that was considered for the plasma holds a limited subset of the phenomena that occur in real plasma. Assuming conservation of charge, no collisions (kinetic energy much greater than potential energy), and velocity of the electrons are much smaller than the speed of light and extending the system in reference [2] for two dimensions, the bidimensional physical model is obtained. In this model, the energy dissipation is neglected.

$$\frac{df}{dt}=\frac{\partial f}{\partial t}+v_x\frac{\partial f}{\partial x}+v_y\frac{\partial f}{\partial y}+\frac{F_x}{m}.\frac{\partial f}{\partial v_x}+\frac{F_y}{m}.\frac{\partial f}{\partial v_y}=0$$

$$F_x = qE_x$$

$$F_y = qE_y$$

$$\rho(x)=q\int f dv+\rho_0$$

$$\nabla^2\phi=\frac{-\rho}{\varepsilon_0}$$

where $\vec{v}=(v_x,v_y)$, $\vec{x}=(x,y)$, $f(\vec{x},\vec{v},t)$ and $\phi=\phi(x,y,z)$.

The equations for the Debye length and the frequency of plasma oscillation are respectively [2]:

$$\lambda_D=\sqrt{\frac{\varepsilon_0 k_B T}{nq^2}} \qquad \omega_p=\sqrt{\frac{nq^2}{\varepsilon_0 m_e}}$$

4. DISCRETIZATION OF THE MATHEMATICAL MODEL

For the implementation of the computational algorithm it is necessary to discretize the equations of the proposed physical model. Due to computational reasons it is not feasible to accomplish the model for all of the plasma's particles, thus superparticles are used. Each superparticle is constituted of a reasonably large number of particles and the number of superparticles in the system is so that it keeps the physical characteristics of the system.

4.1. Equations of motion

Using the same analysis done in the direction x [2] holds for the direction y since they can be solved separately due to the decoupling, the discretized equations of motion of the bidimensional system's superparticles, where N_S is the number of electrons of the plasma per unit of length in the direction z, are given by:

$$\frac{x_i^{n+1}-x_i^n}{DT}=v_{x_i}^{n+\frac{1}{2}} \qquad \frac{v_{x_i}^{n+\frac{1}{2}}-v_{x_i}^{n-\frac{1}{2}}}{DT}=\frac{F(x_i^n)}{N_S m_e}$$

$$\frac{y_i^{n+1}-y_i^n}{DT}=v_{y_i}^{n+\frac{1}{2}} \qquad \frac{v_{y_i}^{n+\frac{1}{2}}-v_{y_i}^{n-\frac{1}{2}}}{DT}=\frac{F(y_i^n)}{N_S m_e}$$

For the approximations and the system to respond satisfactorily, some conditions must be met. The number of superparticles in a Debye length must be sufficiently large so that the moment fluctuations are small. The value of DT must be chosen so that the plasma oscillations can be followed adiabaticaly.

$$\omega_p DT << 2$$

4.2. Equations for the potential and the electric field

The computational mesh is the region of space in which the model simulation occurs. In the case of two dimensions, the computational mesh of area A is split in cells of area H^2. The points where the calculations of the potential, the electric field and the charge density are performed are called mesh points, which correspond to the midpoint of each cell in the computational mesh [2]. Therefore all of the superparticles inside a given cell are subject to the same potential and electric field. Let N_x be the number of points in the direction x and N_y the number of points in the direction y, then the area of the computation mesh is given by:

$$A=(N_x+N_y)H^2$$

The walls of the mesh are considered to be hard and conductive, and the length in the direction x and in the direction y must be longer than the Debye length.

Using the techniques for discretization [2], Poisson's equation in two dimensions assumes the form:

$$\phi(x_{p+1},y_k)+\phi(x_{p-1},y_k)+\phi(x_p,y_{k+1})+\phi(x_p,y_{k-1})+$$
$$-4\phi(x_p,y_k)=-\frac{H^2}{\varepsilon_0}\rho(x_p,y_k)$$

where $\rho(x_p,y_k)$ is the charge density in the cell of mesh point (x_p,y_k).

So the electric field equation in two dimensions assumes the form [2]:

$$E_x(x_p,y_k)=\frac{\phi(x_{p-1},y_k)-\phi(x_{p+1},y_k)}{2H}$$

$$E_y(x_p,y_k)=\frac{\phi(x_p,y_{k-1})-\phi(x_p,y_{k+1})}{2H}$$

4.3. Charge assignment and force interpolation

Using the method used in [2] to two dimensions, the discretized equation of charge density inside a cell of mesh point (x_p,y_k) is given by:

$$\rho(x_p, y_k) = \frac{qN_S}{H} \sum_{i=1,j=1}^{Np} W[(x_i, y_j) - (x_p, y_k)] + \rho_0$$

Where the function W is defined as:

$$W(x, y) = 1, \text{ if } |x| \le \frac{H}{2} \text{ e } |y| \le \frac{H}{2}$$

$$W(x, y) = 0, \text{ otherwise}$$

Since the forces of the superparticles depend on the value of the electric field to which they are submitted and the electric field is calculated in the midpoint of each cell, then all of the superparticles inside a given cell will feel the same intensity of force.

Thus the calculation of the force is obtained with the following expressions, using the function W:

$$F_x(x_i, y_i) = N_S q . \sum_{p=1,k=1}^{N_x, N_y} W[(x_i, y_j) - (x_p, y_k)].E_x(x_p, y_k)$$

$$F_y(x_i, y_i) = N_S q . \sum_{p=1,k=1}^{N_x, N_y} W[(x_i, y_j) - (x_p, y_k)].E_y(x_p, y_k)$$

5. SIMULATION

The plasma modeling was done using the SCILAB software, a scientific program for numeric computation [3]. Plasma analyses were carried out in one and two dimensions. For the following plots, the following simulation parameters were used: $N_p = 1000$ (total number of superparticles), $N_g = 15$ (number of mesh points), $\omega_p DT = 0,25$ (stable) and $H = 5\lambda_D$.

In Figure 2, it can be observed that the energy of the system is being preserved, as expected for a system with charge conservation, periodic boundary conditions and that is not submitted to external forces, that is, the energy of the particles depend solely on the initial conditions and their interaction within the system. Actually there is an energy fluctuation. Such fluctuation is expected and caused by the software's numeric approximation. From the phase space plots of the one-dimensional system it is possible to analyze the spreading of the particles and the plasma oscillation.

From Figures 3 and 4 it can be observed that the behavior of the superparticles inside the computational mesh is in concordance with the expected for classic plasma model.

From the bidimensional model one can analyze the movement of the particles considering the moment conservation, that is, the particles are subject to elastic reflection when they collide with the walls of the computational mesh. Thus, with the moment and charge conservation and with the system isolated from interference of external sources, the energy of the system has to be conserved.

The plasma simulated in two dimensions has the following parameters: $N_p = 1920$, $N_x = N_y = 8$, $\omega_p DT = 0,01$ and $H_x = H_y = 5\lambda_D$. The initial distribution of the superparticles positions is uniform and the normalized velocities have a normal distribution, where half of the superparticles have velocity 0,05 and the other half -0,05 with variance of 0,01.

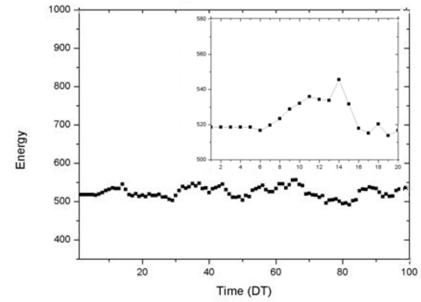

Figure 2: Plot of the total system energy for the unidimensional plasma model, showing the energy fluctuation.

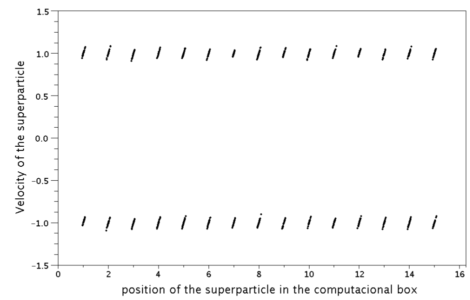

Figure 3: Phase space plot of the initial system state, with the initial distribution uniform in the position and normal velocity distribution, where half of the superparticles have normalized velocity 1 and the other half -1 with a variance of 0,03.

From Figure 5 it can be observed that the energy is conserved, displaying a minor fluctuation, as in the unidimensional case.

The bidimensional model was done considering the system to be adiabatic, so that the displacement of the particles in short periods of time is almost undetectable. From Figures 6 and 7, the movement of the particles is close to the expected for an adiabatic system. However their displacement should only be perceivable for a larger DT interval. Such fact needs to be better analyzed and reducing even more the discrete time parameter (DT) it is expected a better evolution of the displacement of the particles in an adiabatic system.

The bidimensional model implemented can be used to model the applications that happen with the aid of plasma, such as plasma etching. Using the proposed idea for numeric simulation of plasma etching, the following results were obtained using 1740 superparticles, 6 forbidden regions, $N_x = N_y = 8$, $\omega_p DT = 0,01$, $H_x = H_y = 5\lambda_D$.

From Figure 8 it can be observed that the total energy of the system is practically constant while anyone of the superparticles collides with the forbidden regions. The part of the plot where the energy is descending correspond to the lost of superparticle´s energy due the inelastic collision with the forbidden regions when the energy is higher than a minimum energy, that is, the forbidden regions are being allowed. Finally, when the total energy stabilize in a value lesser than the initial energy of the system means that all six forbidden regions are now allowed and the system look like the bidimensional case explained previously. Due to this descent that happens with the energy of the system, an external source is needed so that the energy is kept constant, as is the case with real plasma. Such model of plasma etching is being studied and implemented for the analysis of this application so important to microelectronics.

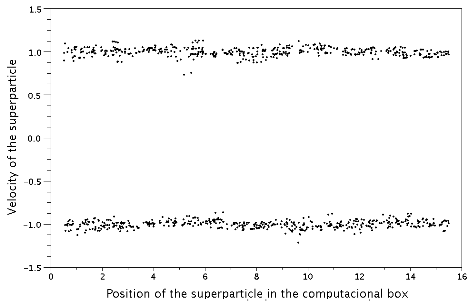

Figure 4: Phase space plot of the system at DT=100, illustrating the spreading of the superparticles within the plasma.

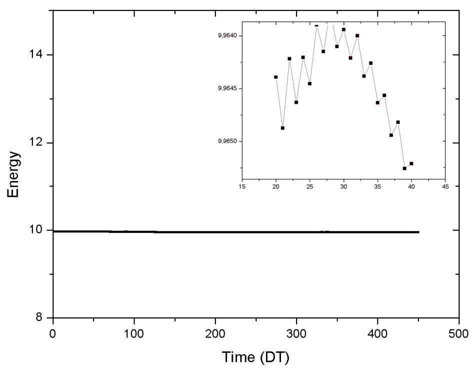

Figure 5: Plot of the total system energy of the bidimensional plasma model, showing the fluctuation of the energy.

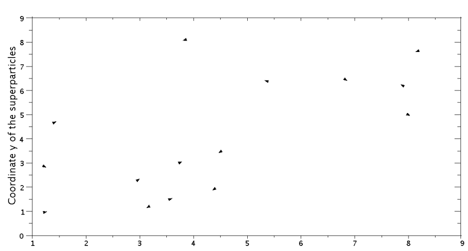

Figure 6: Plot illustrating the positions and the velocity vectors in a sample of the superparticles at DT=200 within the computational mesh.

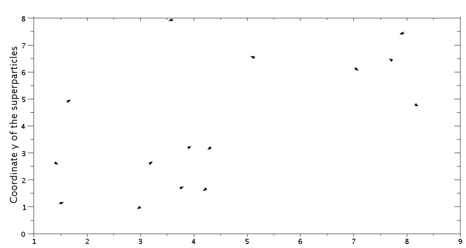

Figure 7: Plot illustrating the positions and the velocity vectors in a sample of the superparticles at DT=208 within the computational mesh.

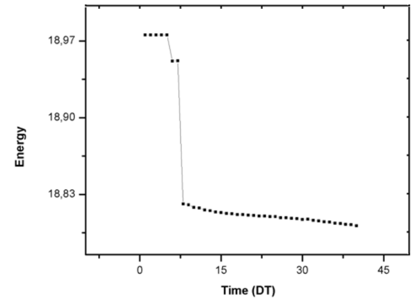

Figura 8: Plot of the total energy of the numeric simulation of plasma etching, showing the descending of the energy due the collision of the superparticles with the forbidden regions.

6. CONCLUSION

One and two-dimensional plasma models were studied and implemented using the Vlasov equation. The computation model was obtained from the discretization of the equations admitted in the physical analysis of the system and implemented on SCILAB. Although the model is simplified, with classical interactions and with the particles not being subject to collision between them, the results could capture the behavior of the particles, their spreading as a function of time and the analysis of phenomena that occur within the plasma. Besides, computationally, it is done faster and with greater versatility, for it suffices to adjust the system to the desired parameters.

For the proposed system in which the charge was totally preserved and had no external sources, both the unidimensional model with periodic boundary conditions or the bidimensional model with elastic collisions between the particles and the walls of the mesh obtained energy practically constant, with a minor fluctuation due to the software's numeric approximations. Therefore, the energy obtained is in concordance with the expected results for a conservative system.

The energy obtained in the proposed model for numeric simulation of plasma etching is in concordance with the expected too, with the total energy of the system descending due the collision of the particles with the matter which want to etch.

The possibility of extending this model, adjusting the needed particularities to the application that one desires to simulate, makes it a great instrument for the study of plasma and its applications.

7. REFERENCES

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