PIC-MCC/Fluid Hybrid Model for Low Pressure Capacitively Coupled O₂ Plasma

Kallol Bera\textsuperscript{a}, Shahid Rauf\textsuperscript{a} and Ken Collins\textsuperscript{a}

\textsuperscript{a}Applied Materials, Inc.
974 E. Arques Ave., M/S 81517, Sunnyvale, CA 94085, USA

Abstract. Low pressure capacitive coupled plasmas are extensively used for advanced micro-electronic device fabrication. Due to long electron mean free path and large bias voltages in this regime, kinetic effects play an important role in the dynamics of low pressure discharges. To take into account the kinetic effects, a one-dimensional hybrid plasma model has been developed that couples particle in cell (PIC) technique for charged species and fluid method for neutral species. The PIC model uses the Monte Carlo Collision (MCC) method to account for collision processes. The fluid model for neutral species takes into account species transport in the plasma, chemical reactions, and surface processes. An electronegative O₂ plasma is simulated for a range of pressures (10-300 mTorr), rf voltages (200-800 V) and excitation frequencies (30-120 MHz). Our model for the O₂ plasma considers electrons, O₂⁺, O⁺, O, and O*. The reaction mechanism includes electron impact dissociation, ionization, dissociative attachment and ion-ion recombination. Computational results are compared to our previous simulations for an electropositive Ar discharge. The electrons primarily absorb power from the external power supply at the sheath edge during sheath expansion. Energetic electron beams are generated at the sheath edge during electron heating, which are responsible for plasma production and sustenance through collisions. The negative ions are found to be confined in the bulk plasma due to the potential well. The ratio of negative ions to electrons increases with increase in pressure, and decrease in rf voltage and rf frequency. Secondary electron emission is found critical for plasma sustenance at low frequency. The spatial profiles of charged and neutral species in the plasma are found to primarily depend on species sources due to collisional processes.

Keywords: PIC/MCC, hybrid model, capacitive plasma, electronegative, oxygen plasma.

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INTRODUCTION

Capacitively coupled plasma (CCP) discharges are widely used for plasma etching and deposition in the semiconductor industry. As feature sizes shrink in microelectronics devices, many plasma etching applications have transitioned to low pressures (< 30 mTorr) to reduce collision induced broadening of the ion angular distribution. Compared to medium/high pressure, CCP operation remains relatively less well-understood at low pressure as kinetic effects start playing an important role in the plasma dynamics. In the past, Turner and colleagues used PIC models to illustrate electron heating mechanisms in low pressure CCPs [1,2]. Pressure effects and collisional drag forces on electrons were found to influence ohmic and non-collisional electron heating at the sheath edge. Kawamura et al. used a PIC-MC model to investigate the dynamics of combined rf/dc sources [3]. Using PIC/MCC, Georgieva et al. showed that CF₄ plasma behaves like an electronegative discharge, and that CF₃⁺ is the major positive ion [4]. Rauf et al. demonstrated that for Ar plasma, the electrons absorb power at the sheath edge during sheath expansion, and the beam electrons are primarily responsible for plasma production and sustenance [5].

COMPUTATIONAL MODEL

A 1D hybrid plasma model has been developed that couples particle in cell (PIC) technique for charged species and fluid method for neutral species at each time step. Our PIC model for charged species generally follows the methodology outlined in [6,7]. The PIC model includes Monte Carlo Collision (MCC) method to calculate collision
frequencies for various processes [8]. A database of collision cross-sections for various processes allows us to model both electropositive and electronegative plasmas [9]. The fluid model for neutral species takes into account species transport in the plasma, chemical reactions, and surface processes.

The program starts by initializing the location of all charged particles, velocities of all charged particles, and neutral species densities distribution. Probability arrays are set up for all particle collisions using the specified set of reaction cross-sections and initial species densities. When a particle of species k collides with another species j with density n_j in reaction j, the collision frequency for this reaction is determined using

$$v_{k,j}(y,\varepsilon) = \sigma_{ij}(\varepsilon)n_j(y)\sqrt{\frac{2\varepsilon}{m_k}}$$

where \(\sigma_i\) is the collision cross-section for reaction i and \(m_k\) is mass of species k. y is the distance from the ground electrode and \(\varepsilon\) is the particle kinetic energy. Starting with the initial conditions, the electrode voltage is updated and particle positions are used to determine specie densities \(n_k(y,t)\) for all charged species k, which are used to calculate the charge density \(\rho(y,t)\). The Poisson equation is solved to compute the electrical potential, \(\phi(y,t)\), that yields the electric field, \(E(y,t)\). Using this electric field, all charged particles velocities are updated and the particles are moved. Particle velocity and location are staggered by half time-step and the leap-frog scheme is used for integrating the equations of motion [6]. The updated particle velocities and positions are used to gather statistics for the energy distribution functions. The power absorbed by each particle i of charged species k is determined as

$$P_{i,k} = q_k\omega_k v_{i,k} E(x_{i,k})$$

where \(\omega_k\) is the weight of the particle. The particle power absorption is then used to determine the spatial power distribution \(P_{R}(y,t)\). Statistics of particles leaving the surfaces are collected and surface processes such as secondary electron emission are considered. Based on the probability arrays, particle collisions with each other and with the neutral fluid are next considered. These collisions adjust the particle velocities, can destroy the particles or introduce new particles. Statistics of these collisions are used to determine how electron energy is dissipated in the plasma, \(P_{e,loss}\). Neutral species densities are modified by solving the continuity equations for all neutral species explicitly in time. In order to evolve the neutral species at a fast pace, an acceleration factor is used.

**COMPUTATIONAL RESULTS**

Simulations are performed for O_2 plasmas for 5400 rf cycles at 60 MHz to ensure convergence of plasma properties. The inter-electrode gap is 0.05 m. The secondary electron emission coefficient is set to be 0.3. Results for statistical average of last 36 cycles are reported. The simulation starts with 100000 particles and the time step for particle simulation is 50 ps. The O_2 plasma simulation results are compared with Ar plasma [5].

For the baseline condition of O_2 plasma at 200 V, 60 MHz, the simulation results for electric potential, electron, O\(^+\) and O\(_2\)\(^+\) densities are presented in Fig. 1 as a function of distance from the grounded electrode (y) and phase during one rf cycle. The rf voltage is applied to the right electrode. The positive ions (O\(_2\)\(^+\)) are formed through ionization and negative ions (O\(^-\)) by electron attachment. During the first half of the rf cycle, the applied voltage is positive, and this voltage primarily drops at the left electrode. The sheath collapses at the right electrode, and electrons are pulled to the right electrode. The situation reverses in the second half of the rf cycle. Both positive and negative ions having large masses, their densities do not change significantly during the rf cycle.

![FIGURE 1. Electrical potential, and electron, O\(^-\) and O\(_2\)\(^+\) densities at 20 mT, 200V, 60 MHz](image-url)
The $O^-$ density is confined in the bulk plasma due to the potential well, and has a peak near the center of the discharge. The $O^-$ density being larger than electron density, the $O_2$ plasma is highly electronegative. To maintain charge neutrality in the bulk region, $O_2^+$ density is the sum of electron and $O^-$ densities. The peak electron density for Ar plasma under the same condition is $1.61 \times 10^{16} \text{ m}^{-3}$ [5]. The electron density is lower for $O_2$ plasma as power is used for dissociation and attachment in addition to ionization and excitation.

The power absorbed by $O_2^+$ and electrons from electric field, power lost by electrons during collision and electron source due to ionization are shown in Fig. 2. The plasma potential being positive compared to the electrodes, positive ions gain energy during acceleration to the electrodes. The electrons gain energy from the electric field at the sheath edge when the sheath expands into the plasma, and pushes electrons into the plasma. When the sheath contracts, electrons return some of the power back to the electric field, and decelerate in the sheath. The $O^-$ ions are pushed by the electric field as well, however, due to ion inertia there is a time delay in ion motion. The $O^-$ power deposition occurs later in time compared to the electrons. The electron gains energy during sheath expansion, and the energetic electron beams shoot into the bulk plasma. The beam electrons travel considerable distance into the bulk, and dissipate their energy through collisions. Apart from beam electrons, secondary electrons emerging from the electrodes due to ion bombardment carry energy that is dissipated in the bulk plasma. Most of the energy lost by electrons is through ionization and dissociation of $O_2$. There is small amount of energy lost due to excitation of O. These inelastic processes occur mainly due to high energy beam electrons. The electron energy loss in elastic collision is small and spread over the discharge region.

**Pressure Effect**

The effect of pressure on electron density is shown in Fig. 3 for $O_2$ plasma at 200 V, 60 MHz. For constant rf voltage, electron density increases with pressure as neutral density increases which is similar to what observed in Ar plasma [5]. The sheath thickness decreases as electron density increases. The peak electron power deposition increases from $4.7 \times 10^5 \text{ W/m}^3$ at 10 mT to $3.4 \times 10^6 \text{ W/m}^3$ at 300 mT. As shown in Fig. 4, the negative ion density increases with pressure due to more electron attachment at higher neutral density. The ratio of $O^-$/electron density increases with pressure as electron attachment increases faster than electron impact ionization.

Electron power loss during collision is shown in Fig. 5 for gas pressure ranging 10 to 300 mT. At lower pressure electron beams are stronger, and retain their beam character for a long distance even after another electron beam is launched from the other sheath. At 10 mT, the electron beams entering the opposite sheath during sheath contraction causes ripple effect as shown in Fig. 3. At higher pressure electron beams originating from one sheath stops before electron beam launched from the opposite sheath.
The electron energy distribution (EED) in the bulk plasma is shown in Fig. 6 at different pressures. At higher pressure electron temperature is lower compared to that at lower pressure. Lower temperature reduces ionization, diminishing the effectiveness in increase in electron density due to higher neutral density as shown in Fig. 3. Negative ions also play a role in determining electron density at different pressures. At 10 mT, electron energy is enhanced near 20 eV. This is due to beam electrons that reach further into the bulk plasma. As the beam electron effect diminishes at higher pressure, this peak in EED reduces.
The effect of rf voltage on electron density is shown in Fig. 7 for O$_2$ plasma at 20 mT, 60 MHz. The electrons are more energetic at higher rf voltage leading to better ionization, and electron source. With increases in voltage electron density increases, and sheath thickness decreases. Also, the ratio of O- to electron density decreases. The peak electron power deposition increases from 1.0 x 10$^6$ W/m$^3$ at 200 V to 7.0 x 10$^6$ W/m$^3$ at 600 V. At higher voltage, beam electrons penetrate further into the bulk plasma leading to higher collisional loss in the bulk plasma as shown in Fig. 8. The electron energy distribution (not shown) exhibits energy enhancement near 20 eV at 600 V due to the beam electrons.

The frequency of rf source has significant effect on plasma characteristics. For this study, we have simulated plasma in the frequency range of 30 to 120 MHz. The rf voltage is 800 V at 30 MHz, 400 V at 60 MHz and 200 V at 120 MHz. The discharge pressure is 50 mT and secondary electron emission coefficient is set to 0.3. The Secondary electron emission coefficient is found important to sustain the plasma at 30 MHz. With increase in
frequency electron density increases, and sheath thickness decreases as shown in Fig. 9. The simulation results are similar to our previous findings for Ar plasma [5]. The electron power deposition during sheath expansion increases significantly with frequency due to shorter time for energy gain per electron. The peak electron power deposition increases from \(1.4 \times 10^8 \text{ W/m}^3\) at 30 MHz to \(1.9 \times 10^8 \text{ W/m}^3\) at 120 MHz. The power deposition to \(\text{O}_2^+\) and \(\text{O}^-\) ions also increases with frequency. The electron beam launched from one sheath stops before the beam launched from opposite sheath at 30 MHz as shown in Fig. 10. At 120 MHz, the electron beams intersect as the time difference between the launching of the beams reduces. The more frequent propagation of the electron beams in the bulk plasma where the beam electrons engage in collisions lead to more efficient power coupling, and higher plasma density. The ratio of power dissipated in electron collision to electron power deposition increases from 18.9 \% at 30 MHz to 72.1 \% at 120 MHz. The ratio of \(\text{O}/\text{electron}\) density decreases with increase in frequency.

![FIGURE 9. Electron density at different frequencies (30-120 MHz) at 50 mT](image1)

![FIGURE 10. Electron energy loss at different frequencies (30-120 MHz) at 50 mT](image2)

**CONCLUSIONS**

For low pressure rf capacitively coupled plasma, electrons primarily absorb power from at the sheath edge during sheath expansion. Energetic electron beams, generated at the sheath edge during electron heating, are responsible for plasma production and sustenance through collisions. For \(\text{O}_2\) plasma, electron density is lower compared to Ar plasma due to dissociation and attachment processes. The ratio of \(\text{O}/\text{electron}\) density increases with increase in pressure, and decrease in rf voltage and rf frequency where effectiveness of beam electrons diminishes.

**REFERENCES**