2-DIMENSIONAL MODELING OF PULSED PLASMAS
WITH AND WITHOUT SUBSTRATE BIAS
USING MODERATE PARALLELISM*

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• Introduction

• Description of the moderately parallel model

• Validation

• Properties of Pulsed Cl$_2$ Plasmas
  • With and without rf substrate bias
  • Bias voltage
  • Feedstock composition

• Conclusions
PULSED ICP PLASMAS

- Pulsed plasmas
  - Damage free plasma etching with better uniformity and anisotropy
  - Improved etch selectivity by modifying the ratio of chemical species
  - Additional controllable degrees of freedom: Duty cycle and modulation frequency
  - Reduce charge buildup on wafers and suppress notching
  - Reduced particle generation in the plasma

- Current models for investigating pulsed operation are typically global or 1-dimensional

- Difficult to resolve long-term transients in multi-dimensional plasma equipment models

- Moderately parallel algorithms for 2-dimensional hybrid models were developed to investigate long term transients.
DESCRIPTION OF THE PARALLEL HYBRID MODEL

• The HPEM, a modular simulator, was parallelized by employing a shared memory programming paradigm on a Symmetric Multi-Processor (SMP) machine.

• The Electromagnetics, Electron Monte Carlo and Fluid-kinetics Modules are simultaneously executed on three processors.

• The variables updated in different modules are immediately made available through shared memory for use by other modules.

• Dynamic load balancing is implemented to equal the tasks on different processors.
GOVERNING EQUATIONS IN HPEM

- Continuity (heavy species):
  \[ \frac{\partial N_i}{\partial t} = \nabla \cdot (N_i \vec{v}_i) + S_i \]

- Momentum (heavy species):
  \[ \frac{\partial (N_i \vec{v}_i)}{\partial t} = \frac{q_i}{m_i} N_i \left( \vec{E}_s + \vec{v}_i \times \vec{B}_s \right) - \frac{1}{m_i} \nabla P_i - \nabla \cdot (N_i \vec{v}_i \vec{v}_i) - \nabla \cdot \vec{\tau}_i + \sum_j N_i N_j k_{ij} (\vec{v}_j - \vec{v}_i) \]

- Energy (heavy species):
  \[ \frac{\partial}{\partial t} \left( \frac{3}{2} N_i k_B T_i \right) = \frac{N_i q_i^2 \vec{v}_i}{m_i (\vec{v}_i^2 + \omega_i^2)} E_s^2 + \frac{N_i q_i^2}{m_i \vec{v}_i} E_s^2 - \nabla \cdot \left( \frac{5}{2} k_B T_i \vec{\phi}_i - \lambda_i \nabla T_i \right) \]

  \[ + \sum_i 3 \frac{m_{ij}}{m_i + m_j} N_i N_j \vec{v}_{ij} k_B (T_j - T_i) \pm \sum_i 3N_i N_j R_{ij} k_B T_j \]

- Drift-diffusion (electron):
  \[ \frac{\partial n_e}{\partial t} = \nabla \cdot \left( n_e \vec{\mu}_e E_s + \vec{D}_e \nabla n_e \right) + S_e \]
GOVERNING EQUATIONS IN HPEM (continued)

• Electrons:
  • Energy
    \[ \nabla \cdot k \nabla T_e + \nabla \cdot (\Gamma T_e) = P_{\text{heating}} - P_{\text{loss}} \]

  • Monte Carlo Simulation
    \[
    \frac{d\vec{v}}{dt} = \frac{q_e}{m_e} \left(\vec{E} + \vec{v} \times \vec{B}\right) \\
    \frac{d\vec{r}}{dt} = \vec{v} \\
    v_i = \left(\frac{2\varepsilon_i}{m_e}\right)^{1/2} \sum_{j,k} \sigma_{ijk} N_j
    \]

• Poisson's equation:
  \[ \nabla \cdot \varepsilon \nabla \Phi(t + \Delta t) = \rho(t) + \frac{dp(t)}{dt} \cdot \Delta t = \rho(t) + \sum q_i \Delta t \left[-\nabla \cdot \Phi_i + S_i\right] \]

• Wave equation:
  \[ \nabla \cdot \frac{1}{\mu} \nabla E = \frac{\partial^2 (\varepsilon_0 E)}{\partial t^2} + \frac{\partial (\sigma E + J_0)}{\partial t} \]

• Vector potential:
  \[ \nabla \times \frac{1}{\mu} \nabla \times A = j_B \]
  \[ B_s = \nabla \times A \]
• Reactor geometry taken from Malyshev et. al.*

• Base case conditions:
  • Peak ICP power: 600 W
  • rf bias: 250 V, 10 MHz
  • PRF: 10 kHz
  • Pressure: 10 mTorr
  • Gas flow rate: 100 sccm
  • Cl₂, Ar/Cl₂

• ICP power at 10 MHz (rf) is pulsed at PRF of 10 kHz.

• Several pulses are required to attain periodic steady state

• \([e]\) attains steady state value in the late active glow corresponding to cw operation

• \([e]\) decays several orders of magnitude, as the electrons are lost due to dissociative attachment

• With substrate bias, \([e]\) attains a steady state value in the late after glow corresponding to capacitive mode

• \(\text{Cl}_2, 10 \text{ mTorr}, 600 \text{ W}, 10 \text{ MHz}, 10 \text{ kHz/50\%}\)
DYNAMICS OF PULSED PLASMAS: ELECTRON TEMPERATURE

• \(T_e\) peaks at the leading edge, as the power deposition occurs into a smaller inventory of electrons

• No substrate bias results in higher peak \(T_e\), as the electrons decay away several orders of magnitude lower in the late afterglow

• \(T_e\) is similar during late active glow and early afterglow period

• With substrate bias, \(T_e\) increases in the late afterglow due to sheath heating

• Electrons thermalize to gas temperature without substrate bias

Electron Temperature

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VALIDATION OF THE MODEL: PHYSICS

- Model results compare well with experiments*
- With substrate bias, $T_e$ rises to values above the steady state value

- Without rf bias
  - $\text{Cl}_2$, 10 mTorr, 600 W, 10 MHz, 10 kHz/50%

- With rf bias (250 V, 10 MHz)

• Sheath heating scales with the square of the sheath speed, $v_s$

• Sheath thickness $\lambda$ scales as $n_e^{-1/2}$

• Sheath speed $v_s \approx \omega \lambda$

• Total sheath heating $H$, therefore scales as $H \sim v_s^2 n_e$ and is not a function of electron density

• Specific heating rate (per electron), $h$, scales as $H/n_e \sim 1/n_e$

• As the electron density decays, primarily by dissociative attachment to $\text{Cl}_2$, the sheath thickness $\lambda$ increases

• Oscillating sheath produces a net increase in specific heating rate $h$ and hence an increase in (or slowing in rate of decrease in) $T_e$
• The peak \([e]\) migrates to below the coils during "power-on" where the source is maximum.

• \([e]\) is similar with and without substrate bias during the activeglow and early afterglow phase.

• As the power is turned off, in the early afterglow ambipolar losses dominate over generation of electrons.

• In the late afterglow, sheath heating dominates and the plasma transitions from inductively coupled to capacitively coupled mode with substrate bias.
The peak in $T_e$ at the leading edge is due to power deposition into smaller inventory of electrons.

Sheath heating prevails, even after 10 $\mu$s into the power-on period, owing to low $n_e$.

At 45 $\mu$s, the $T_e$ profile looks similar to no substrate bias case

After 25 $\mu$s into the power-off period, sheath heating begins

$T_e$ increases in the late afterglow, as power is deposited into electrons near the substrate by oscillating sheath.
EFFECT OF BIAS VOLTAGE AND ICP POWER ON ONSET TIME

- As the bias voltage is increased, the onset time to the capacitive coupling mode, $\tau_c$, decreases.

- This is attributed to the greater sheath heating at higher bias voltages.

- As the ICP power is varied from 450 W to 600 W, $\tau_c$ increases as the peak electron density in the late active glow is higher (thinner sheath).

- At higher ICP powers, the plasma is more dissociating and less attaching, which increases the [e] in the late active glow and increases $\tau_c$.

- Cl$_2$ pulsed plasma
- 10 mTorr, 100 sccm
- PRF: 10 kHz
- Duty cycle: 50%
- Bias: 250 V

![Graph showing the effect of bias voltage and ICP power on onset time.](attachment:image.png)
EFFECT OF GAS MIXTURES ON ONSET TIME

- As the Ar fraction is increased, $\tau_c$ increases significantly.

- For $\text{Ar/Cl}_2 = 40/60$, $\tau_c$ is longer than the pulse off time, due to the higher [e] in afterglow (thinner sheath).

- As sheath heating is reduced, negative ions can be extracted during the pulse off period.

- Bias voltage, frequency and feedstock composition need to be optimized to investigate the possibility of negative ion extraction with substrate bias.

- Ar/Cl$_2$ pulsed plasma
- 450 W, 10 mTorr
- 100 sccm
- PRF: 10 kHz
- Duty cycle: 50%
- Bias: 250 V

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CONCLUSIONS

• A new 2-D hybrid model was developed to address transients based on moderate computational parallelism.

• Computational studies were performed for pulsed operation of Cl\textsubscript{2} and Ar/Cl\textsubscript{2} ICPs.

• $T_e$ at the leading edge is nearly twice the steady state value.

• In electronegative plasmas, electron-ion plasma in the activeglow becomes ion-ion plasma in the afterglow.

• For pulsed Cl\textsubscript{2} plasmas with continuous substrate bias, sheath heating was observed to be predominant in the late afterglow.

• The $\tau_c$ increases with ICP power as the plasma is more dissociated in the late activeglow and it takes more time for electron density to decay away.

• The extraction of negative ions in the afterglow is difficult with a continuous substrate bias as the sheaths typically do not collapse.

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