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

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AGENDA

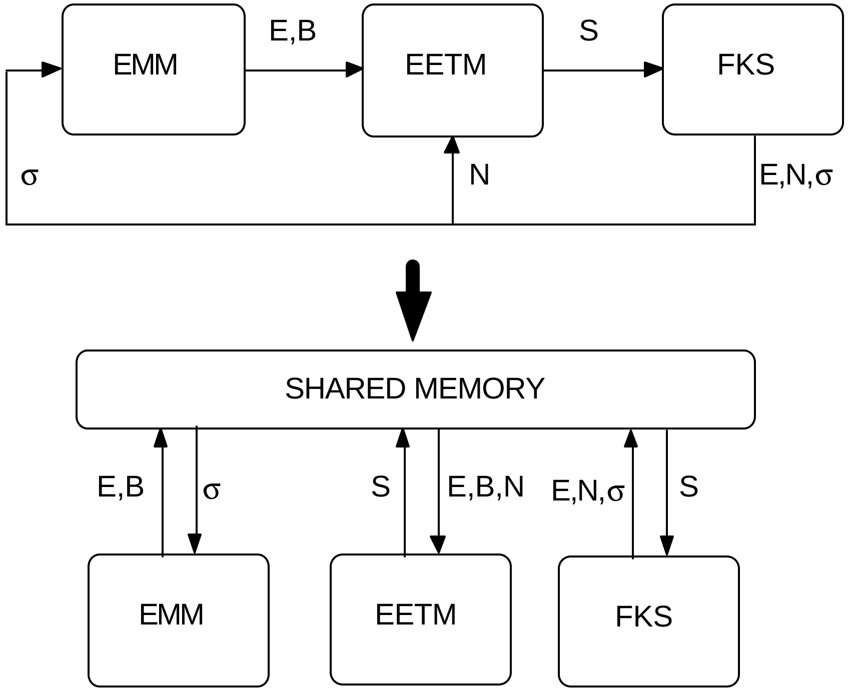
- Introduction
- Description of the moderately parallel model
- Validation
- Properties of Pulsed Cl_2 Plasmas
    - With and without rf substrate bias
    - Bias voltage
    - Feedstock composition
- Conclusions

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) :

$$\frac{\partial N_i}{\partial t} = \nabla \cdot \left(N_i \vec{v}_i \right) + S_i$$

- Momentum (heavy species) :

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

- Energy (heavy species) :

$$\frac{\partial}{\partial t} \left(\frac{3}{2} N_i k_B T_i \right) = \frac{N_i q_i^2 \boldsymbol{n}_i}{m_i \left(\boldsymbol{n}_i^2 + \boldsymbol{w}^2 \right)} E^2 + \frac{N_i q_i^2}{m_i \boldsymbol{n}_i} E_s^2 - \nabla \cdot \left(\frac{5}{2} k_B T_i \vec{\boldsymbol{j}}_i - \boldsymbol{l}_i \nabla T_i \right)$$

$$+ \sum_i 3 \frac{m_{ij}}{m_i + m_j} N_i N_j \boldsymbol{n}_{ij} k_B (T_j - T_i) \pm \sum_i 3 N_i N_j R_{ij} k_B T_j$$

- Drift-diffusion (electron) :

$$\frac{\partial n_e}{\partial t} = \nabla \cdot \left(n_e \bar{\bar{\mu}}_e E_s + \bar{\bar{D}}_e \nabla n_e \right) + S_e$$

GOVERNING EQUATIONS IN HPEM (continued)

- Electrons:
  - Energy $\nabla \cdot k\nabla T_e + \nabla \cdot (\Gamma T_e) = P_{heating} - P_{loss}$
  - Monte Carlo Simulation

$$\frac{d\vec{v}}{dt} = \frac{q_e}{m_e}\left(\vec{E} + \vec{v} \text{ x } \vec{B}\right) \qquad \frac{d\vec{r}}{dt} = \vec{v} \qquad \nu_i = \left(\frac{2\varepsilon_i}{m_e}\right)^{\frac{1}{2}} \sum_{j,k} \sigma_{ijk} N_j$$

- Poisson's equation:

$$\nabla \cdot \varepsilon\nabla\Phi(t+\Delta t) = \rho(t) + \frac{d\rho(t)}{t} \cdot \Delta t = \rho(t) + \sum_i q_i \Delta t[-\nabla.\vec{\varphi}_i + S_i]$$

- Wave equation:

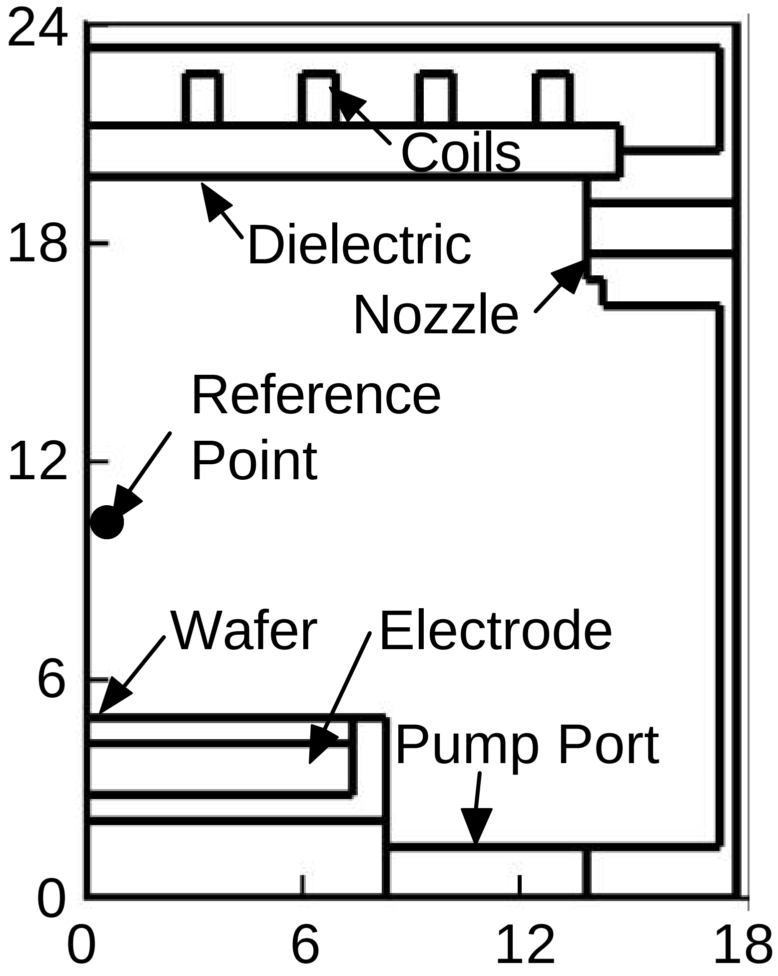
$$\nabla \cdot \frac{1}{m}\nabla E = \frac{\partial^2 (e_0 E)}{\partial t^2} + \frac{\partial\left(\bar{\bar{s}} E + J_0\right)}{\partial t}$$

- Vector potential:

$$\nabla \times \frac{1}{m}\nabla \times A = j_B \qquad B_s = \nabla \times A$$

REACTOR GEOMETRY AND SIMULATION CONDITIONS

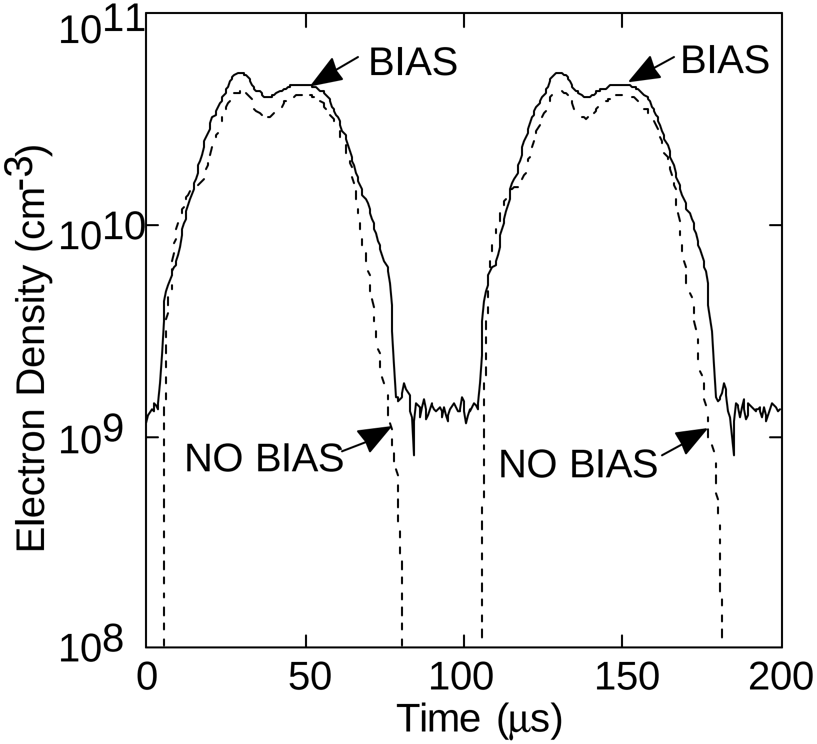
- **Reactor geometry taken from Malyshev et. al.***
- **Base case conditions:**
  - **Peak ICP power: 600 W**
  - **rf bias: 250 V, 10 MHz**
  - **PRF: 10 kHz**
  - **Pressure: 10 mTorr**
  - **Gas flow rate: 100 sccm**
  - **Cl_2, Ar/Cl_2**



***M. V. Malyshev, V. M. Donnelly, Plasma Sources Sci. Technol. 9, 353 (2000)**

DYNAMICS OF PULSED PLASMAS: ELECTRON DENSITY

- **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 activeglow 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**

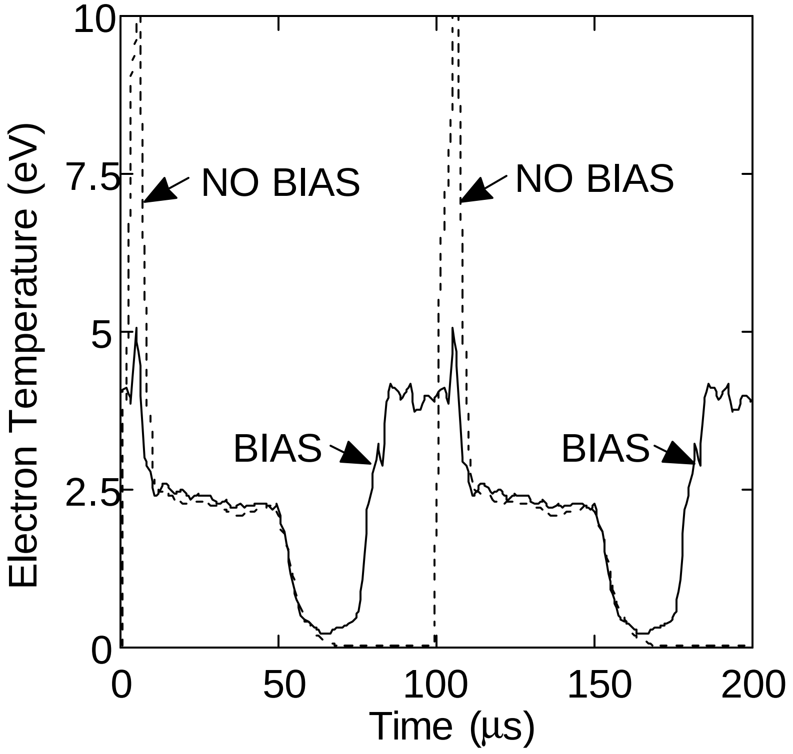


- **Electron Density**

- **Cl_2, 10 mTorr, 600 W, 10 MHz, 10 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 activeglow 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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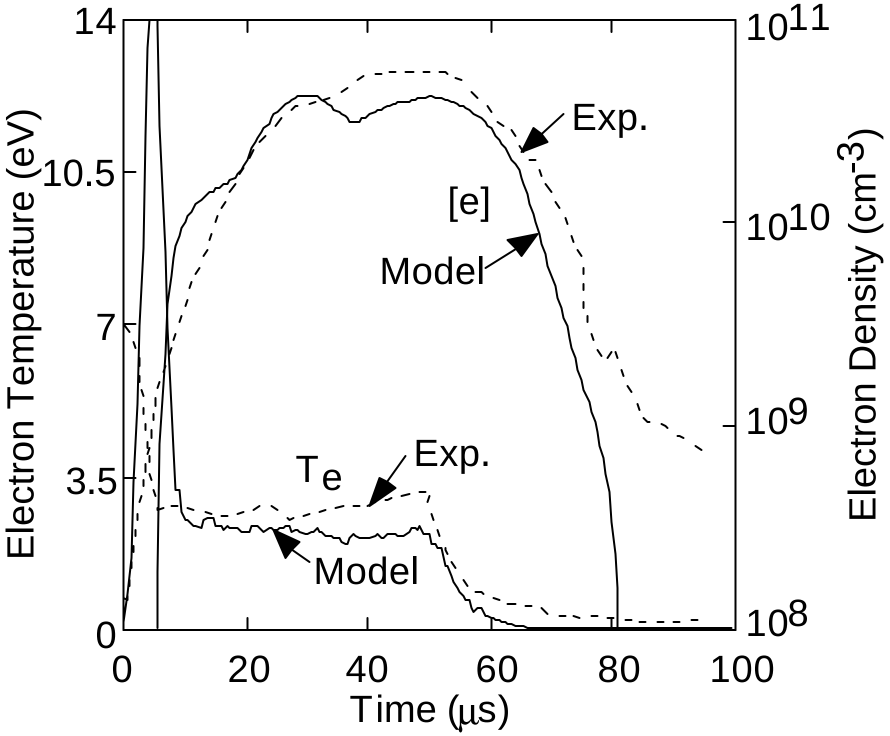
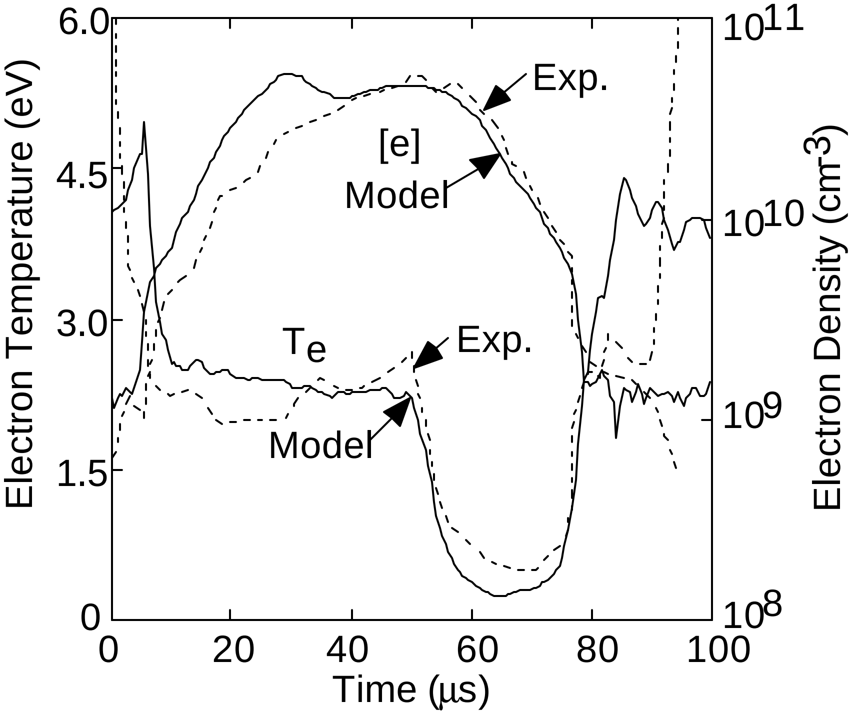
VALIDATION OF THE MODEL: PHYSICS

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





- **Without rf bias**
- **With rf bias (250 V, 10 MHz)**
- **Cl_2, 10 mTorr, 600 W, 10 MHz, 10 kHz/50%**

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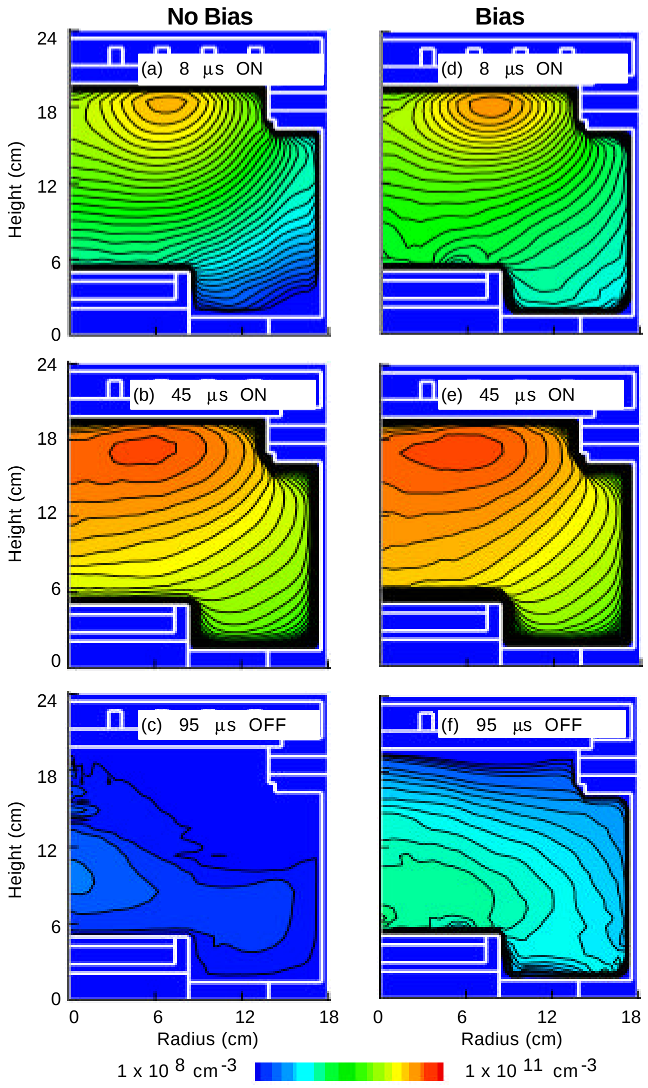
SHEATH HEATING IN PULSED PLASMAS WITH SUBSTRATE BIAS

- **Sheath heating scales with the square of the sheath speed, v_s**
- **Sheath thickness l scales as $n_e^{-1/2}$**
- **Sheath speed v_s » w l**
- **Total sheath heating H, therefore scales as H ~ $v_s^2 n_e$ and is not a function of electron density**
- **Specific heating rate (per electron), h, scales as H/n_e ~ $1/n_e$**
- **As the electron density decays, primarily by dissociative attachment to Cl_2, the sheath thickness l 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**

Cl_2 PULSED PLASMAS WITH AND WITHOUT RF BIAS: ELECTRON DENSITY

- **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.**



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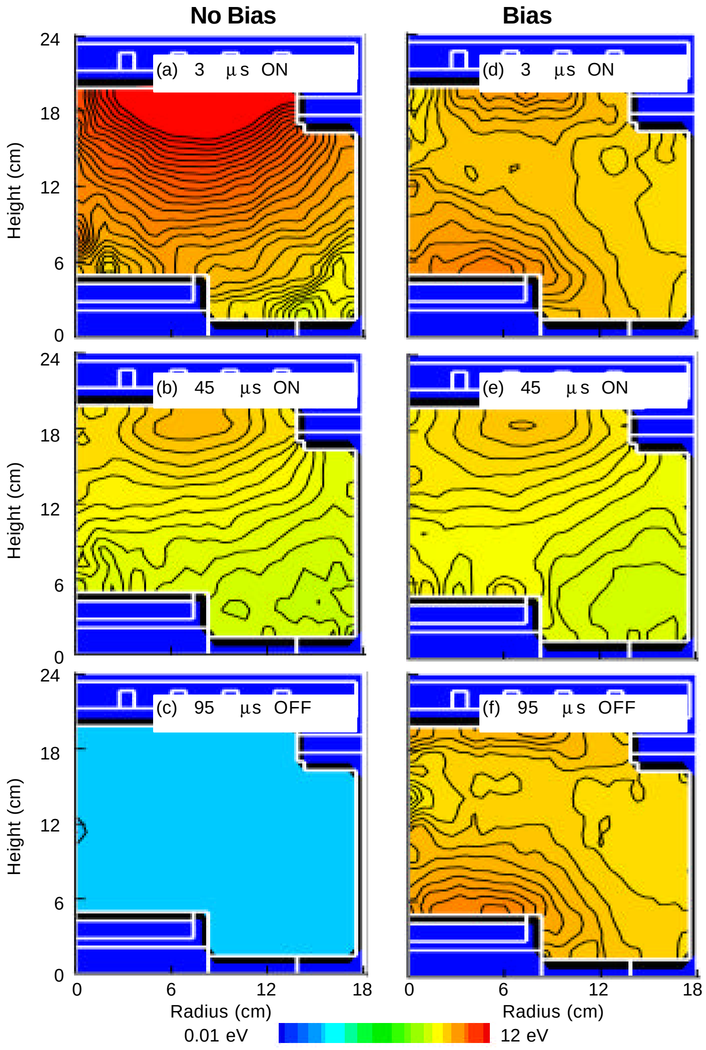
Cl_2 PULSED PLASMAS WITH AND WITHOUT RF BIAS: ELECTRON TEMPERATURE

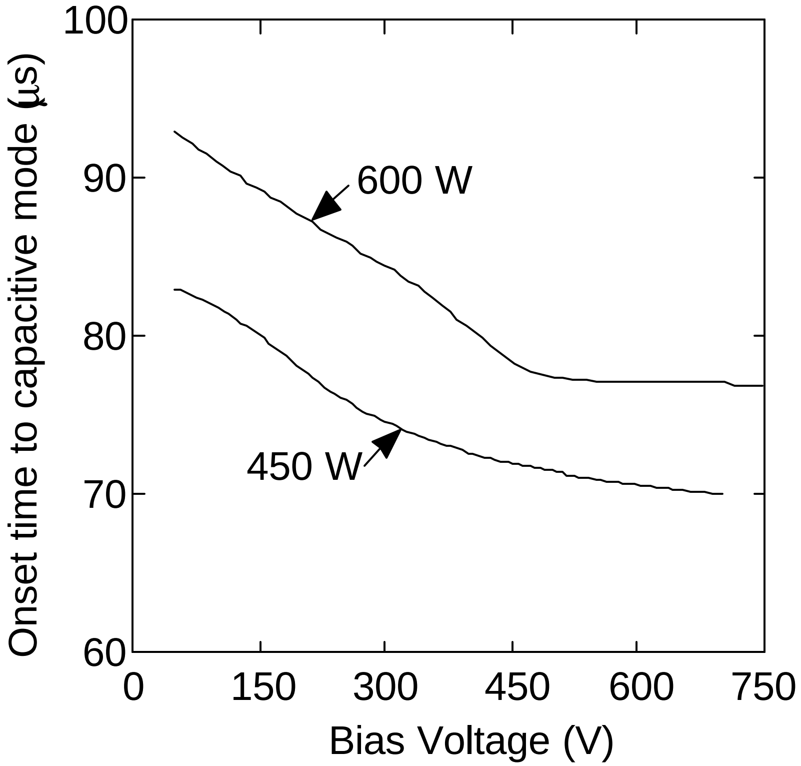
- **The peak in T_e at the leading edge is due to power deposition into smaller inventory of electrons.**
- **Sheath heating prevails, even after 10 ms into the power-on period, owing to low n_e.**
- **At 45 ms, the T_e profile looks similar to no substrate bias case**
- **After 25 ms into the power-off 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, τ_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, τ_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 τ_c.**

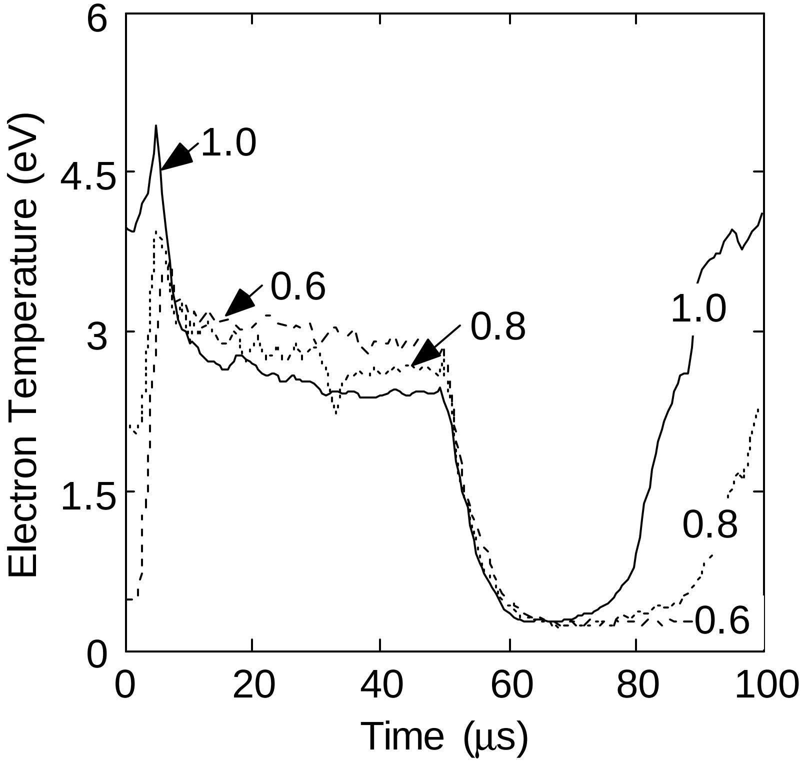
- **Cl_2 pulsed plasma**
- **10 mTorr, 100 sccm**
- **PRF: 10 kHz**
- **Duty cycle: 50%**
- **Bias: 250 V**



EFFECT OF GAS MIXTURES ON ONSET TIME

- **Ar/Cl_2 pulsed plasma**
- **450 W, 10 mTorr**
- **100 sccm**
- **PRF: 10 kHz**
- **Duty cycle: 50%**
- **Bias: 250 V**

- **As the Ar fraction is increased, t_c increases significantly.**
- **For Ar/Cl_2 =40/60, t_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.**



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_2 and Ar/Cl_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_2 plasmas with continuous substrate bias, sheath heating was observed to be predominant in the late afterglow.**

- **The t_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.**