

Perspective of Kinetic Plasma Modeling for Semiconductor Industry

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Online Low Temperature Plasma (OLTP) Seminar September 5, 2023



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Agenda

- Low-Temperature Plasmas in the Semiconductor Industry
- Particle-in-Cell Plasma Modeling
 - Capacitively Coupled Plasma with Non-sinusoidal Bias
 - Electron-Beam Generated Plasma
 - Magnetized Capacitively Coupled Plasma
 - Pulsed Dual Frequency Capacitively Coupled Plasmas
- Perspective on Kinetic Plasma Modeling
- Conclusions



Plasmas in the Semiconductor Industry



Plasmas and Microelectronics Fabrication

- The semiconductor industry is poised to grow to \$1T by the end of the decade.
- Plasmas are an essential technology used for fabricating microelectronics devices:
 - Etching
 - Deposition
 - Ion implantation
 - Clean
- Some widely used plasma sources in the semiconductor industry are:
 - Inductively coupled plasma (ICP)
 - Capacitively coupled plasma (CCP)
 - DC Magnetron

¹Agarwal *et al.*, J. Appl. Phys. 106, 103305 (2009). ²Georgieva *et al.*, Phys. Rev. E 69, 026406 (2004). ³Hopwood, Phys. Plasmas 5, 1624 (1998). Inductively Coupled Plasma¹



Capacitively Coupled Plasma²





Some Challenges in Plasma Processing Applications

- As microelectronics devices shrink to a few nm size and 3D microelectronics become prevalent, plasma processing technology is being pushed to its limits.
- It has become critical to control every aspect of the plasma:
 - Ion energy and angular distribution
 - Neutral radical composition
 - Plasma uniformity







Close-up image of V-NAND flash array



Kinetic Plasma Modeling

- Plasma modeling is critical for plasma product and process design in the semiconductor industry.
- To be useful, plasma models should be quantitatively accurate and capture experimental reality.



- Most plasma modeling in industry is done using fluid and hybrid models.
- However, many applications require kinetic plasma models:
 - Low-pressure RF CCP
 - Magnetrons and metal deposition plasmas
 - Low-pressure magnetized plasmas
- In addition, kinetic plasma models are important for testing and refining fluid and hybrid modeling methodologies.



Tailored Bias Voltage Waveform in CCPs - Plasma Dynamics



Introduction

- Dual frequency CCPs are being developed with non-sinusoidal low-frequency (LF) bias voltage.
- The primary motivation of using these nonsinusoidal waveforms is to control the IEDF.
- The LF voltage waveform might contribute less to plasma production directly but modulates plasma production by the high-frequency source.
- We explore a few implications of using nonsinusoidal LF voltages in the next sections.
- Detailed results are available in Rauf *et al.*, Plasma Sources Sci. Technol. **32**, 034002 (2023).



Hartmann *et al.*, Plasma Sources Sci. Technol. 31, 055017 (2022).



Close-up image of V-NAND flash array



Experimental Setup

- The CCP is powered by 2 RF sources:
 - ▶ 13.56 MHz
 - Tailored voltage waveform at 100s kHz
- A fast-gated ICCD camera (4 Picos, Stanford Computer Optics) is used to measure the spaceand time-resolved emission from the Ar 2p₁ → 1s₂ transition at a wavelength of 750.39 nm.



Tailored Voltage Waveform

 The low-frequency voltage waveform is generated using 20 harmonics:

$$\phi(t) = A \sum_{k=1}^{N} \frac{2}{k\pi} \sin(k\pi D) \cos(2k\pi t f_{\rm LF}) + V_{\rm HF} \sin(2\pi f_{\rm HF} t)$$

- The LF rectangular voltage waveform is generated using an arbitrary waveform generator (Keysight 33622A).
- An iterative feedback loop is applied to ensure the presence of the desired voltage waveform shape at the powered electrode.





Time-Averaged Plasma Properties vs. LF Voltage

- With increasing LF voltage, electron and Ar^{*} densities decrease due to:
 - enhanced loss and
 - thinner region of plasma production.



70 V (13.56 MHz), 271.2 kHz rectangular, 10% DC, 5 Pa, Ar



Plasma Dynamics – 150 V_{pp}, 10% DC Rectangular (1)

- Being lighter, electrons are strongly influenced by the applied voltage.
- Electrons move into and out of the sheath region in each 13.56 MHz cycle.
- When the LF voltage becomes positive, electrons are strongly pulled towards the top powered electrode (PE).
- Ion density doesn't change significantly during the LF cycle.



70 V (13.56 MHz), 150 V_{pp} (271.2 kHz rect., 10% DC), 5 Pa, Ar



Plasma Dynamics – 150 V_{pp}, 10% DC Rectangular (2)

SIMULATION

- Electrons and Ar^{*} are produced during the phase of the 13.56 MHz cycle when the electrons are pushed into the plasma by the expanding sheath → stochastic heating.
- Plasma and Ar* production significantly decrease when LF voltage at the powered electrode becomes positive.
- Plasma production remains weak even after the LF voltage returns to the pre-pulse voltage.



70 V (13.56 MHz), 150 V_{pp} (271.2 kHz rect., 10% DC), 5 Pa, Ar



Effect of LF Voltage of Optical Excitation Rate

- In experiments, the electron impact excitation rate is determined using the measured optical emission and the lifetime of the upper excited state.
- All figures are normalized separately.
- E-impact excitation occurs when the sheath expands at both sheaths.
- When LF voltage at the powered electrode becomes positive, e-impact excitation decreases and occurs asymmetrically.
- E-impact excitation remains suppressed for some time after the LF voltage returns to pre-pulse conditions.



Excitation Rate (a.u.)

• 70 V (13.56 MHz), 271.2 kHz rectangular, 10% DC, 5 Pa, Ar



EXPERIMEN

Effect of LF Voltage on Ar* Production Rate

- The model adequately captures most features observed in experiments:
 - Ar* are produced during the 13.56 MHz phase when the sheath expands
 - Ar* production occurs asymmetrically when the LF voltage at the powered electrode is positive
 - Ar* production decreases when the LF voltage on the powered electrode becomes positive
 - Ar* production remains suppressed even when LF voltage returns to pre-pulse conditions
 - This time of suppressed production is longer when the LF voltage is increased.
- Plasma production weakens as LF voltage is increased. In the simulations, plasma could not be sustained above $V_{LF} > 200$ V.





0.2

0.4

Production Rate[Ar*] (Max = $2.2 \times 10^{20} \text{ m}^{-3}\text{s}^{-1}$)

0.6



Effect of LF Voltage on Currents and Mid-Chamber Potential

- The total number of ions and electrons exiting at each electrode must be equal over an LF cycle.
- More electrons leave at the PE when the LF voltage is positive.
- At *V_{LF}* = 150 V:
 - Electron current during the short positive LF voltage phase is significantly higher
 - There are virtually no electrons exiting after the LF returns to prepulse conditions
 - Plasma potential in the chamber center remains raised for some time after the LF voltage returns to pre-pulse conditions.





70 V (13.56 MHz), 271.2 kHz rectangular, 10% DC, 5 Pa, Ar



SIMULATION

 $V_{1F} = 150 \text{ V}, 10\% \text{ DC}$

Effect of LF Voltage on Charge Density

- At 10% DC, electrons can only exit at the powered electrode during the positive voltage phase.
- This results in electron depletion in plasma bulk and in the opposite sheath region.
- After positive voltage pulse is turned off, it takes time for n[e] to be restored in plasma bulk and near opposite sheath.



70 V (13.56 MHz), 271.2 kHz rectangular, 10% DC, 5 Pa, Ar



Tailored Bias Voltage Waveform in CCPs - Influence on Plasma Uniformity



2D Modeling – Effect of Waveform on Plasma Uniformity

- We model a dual-frequency CCP (40 MHz + 800 kHz) in 2D cylindrical geometry.
- The LF voltage is either sinusoidal or rectangular.
- Details of these results are available in Rauf *et al.*, J. Vac. Sci. Technol. B 40, 032202 (2022).







Convergence of Important Plasma Quantities

- These are time-consuming simulations (up to 1 month with 16 cores) as plasma properties slowly evolve (ms) based on what's happening during the RF cycle (ns).
- We monitor many plasma properties including spatially averaged species densities and DC bias to ensure that simulation results have converged.
- All 2D simulations have been done for 10000 cycles of 40 MHz.





Electron Density vs. LF Voltage - Sinusoidal Waveform

- The electric field is highest at the edge of the powered electrode (PE). However, with a low LF voltage (500 V), n_e peaks at the chamber center due to ample diffusion at 20 mTorr.
- Sheath above the bottom electrode is thicker as a negative DC bias builds up at the blocking capacitor.
- As the LF voltage is increased:
 - The sheath above the bottom electrode becomes thicker
 - Plasma becomes more uniform as there is less diffusion in the thinner effective gap
 - n_e decreases as plasma production occurs in a narrower region and loss is enhanced



Electron Density vs. LF Voltage - Rectangular Waveform

- With rectangular LF waveform, n_e still peaks at the chamber center at low LF voltage.
- To get plasma with similar density, a higher 40 MHz voltage is needed.
- Sheath above the bottom electrode is thicker compared to similar sinusoidal LF voltage.
- As the LF voltage is increased:
 - The sheath above the bottom electrode becomes thicker
 - Plasma density peaks in 2 locations: chamber center and at the electrode edge
 - n_e decreases as plasma production occurs in a narrower region and loss is enhanced.



Plasma Production – Sinusoidal LF Voltage

- Despite a constant 40 MHz voltage, plasma is not produced continuously in time.
- Plasma is produced more strongly when the LF voltage is positive and the sheath above the bottom electrode is thinner.





250 V (40 MHz), 900 V (800 kHz sin.), 20 mTorr, Ar



Plasma Production – Rectangular LF Voltage

- Plasma is produced intensely for a short time when the LF voltage is positive and the sheath is thin.
- For most of the LF waveform:
 - The sheath is thick due to the large bias voltage
 - the plasma is produced at a slow pace, and plasma near the electrode edge can't diffuse inwards



400 V (40 MHz), 900 V (800 kHz rect.), 20 mTorr, Ar





Electron-Beam Generated Plasma



Introduction

- Plasmas generated using electron beams are known to have low electron temperature (T_e) and plasma potential,¹ which are particularly useful for atomic-precision plasma processing.
- Electron beam produced plasmas are typically confined using a magnetic field and operated at low gas pressures.
- Previous hybrid modeling of these plasmas² indicated that plasma transport is difficult to capture using classical models.
- A self-consistent 2-dimensional (2D) particle-in-cell (PIC) model of magnetized electron beam produced plasmas is described.
- Detailed results are available in Rauf *et al.*, Plasma Sources Sci. Technol. 32, 055009 (2023).

¹Lock, Fernsler and Walton, Plasma Sources Sci. Technol. 17, 025009 (2008). ²Rauf *et al.*, Plasma Sources Sci. Technol. 26, 065006 (2017).





PIC Modeling of Electron Beam Plasma

- The electron beam generated plasma is modeled in 2D Cartesian geometry with symmetry around x = 0.
- 2 keV electron beam is launched from a 2.8 mm half-width source at the bottom.
- A vertical spatially-uniform magnetic field is applied across the plasma region.
- Simulations are done for:
 - ▶ 10 40 mTorr gas pressure
 - ▶ 0 200 G magnetic field





Plasma Characteristics (1) – 20 mTorr, 100 G

- Energetic beam electrons cause ionization as they traverse the low-pressure gas.
- As the beam electrons are well confined by the magnetic field, ionization primarily occurs at the center of the chamber.
- Ions and electrons spread out through diffusion in the rest of the chamber.
- As explained in paper:
 - Ion behavior is well described by fluid transport equation
 - Electrons follow the Boltzmann relation along field lines in the plasma bulk
 - Electron flux to the top / bottom walls is athermal
 - Electron flux to sidewall is negligible.
- Ar, 20 mT, 100 G, 12.5 mA/m, 2 keV





Plasma Characteristics (2) – 20 mTorr, 100 G

- Electron temperature (T_e) and plasma potential are low in the plasma bulk, which make these plasmas attractive for atomic-scale plasma processing.
- *T_e* is quite uniform along magnetic field lines with ample energy diffusion in this direction.
- *T_e* decreases gradually perpendicular to the magnetic field, but less steeply than electron density (*n_e*).
- Most of the change in T_e occurs at the walls.



• Ar, 20 mT, 100 G, 12.5 mA/m, 2 keV



Effect of Magnetic Field on Electron Density – 20 mTorr

- As magnetic field is increased, n_e increases for otherwise identical conditions due to better confinement by the magnetic field.
- Plasma is better confined near the beam axis for stronger magnetic field.



Ar, 20 mT, xx G, 12.5 mA/m, 2 keV



Effect of Magnetic Field on Electron Temperature – 20 mTorr

- *T_e* is found to gradually increase with magnetic field due to better electron energy confinement.
- T_e is relatively uniform along magnetic field lines and T_e gradient in the x-direction is stronger at higher magnetic field.
- T_e decreases sharply near the walls.



Ar, 20 mT, xx G, 12.5 mA/m, 2 keV



Effect of Gas Pressure on Electron Density – 200 G

- As gas pressure is increased for a given magnetic field:
 - \blacktriangleright *n_e* increases due to more production and reduced loss
 - n_e falls off less rapidly in the x-direction with increasing pressure due to weaker magnetic confinement.







Ar, xx mT, 200 G, 6.25 mA/m, 2 keV

Effect of Gas Pressure on Electron Temperature – 200 G

- T_e remains reasonably uniform along the magnetic field lines from 10 40 mTorr.
- T_e is observed to increase with gas pressure. Most of this increase occurs at the sheath edge.



Ar, xx mT, 200 G, 6.25 mA/m, 2 keV



Magnetized Capacitively Coupled Plasma



PIC Modeling of Low-Pressure Magnetized Capacitive Plasmas

- Several etch and deposition applications are done in low-pressure magnetized capacitively coupled plasmas.
- PIC modeling is being done to understand plasma stability and uniformity issues.
- Detailed results are available at <u>https://doi.org/10.48550/arXiv.2305.15941</u>





Plasma with 10 G Magnetic Field

- A stable plasma is obtained at 10 G magnetic field.
- The plasma shifts towards the left at 10 G magnetic field due to the E×B drift.



Ar, 10 mT, 10 G, 100 V @ 40 MHz



Effect of Magnetic Field on Plasma Density

- As the magnetic field is increased, we observe:
 - Stable plasma when the magnetic field is small
 - Organized spokes at intermediate magnetic fields
 - Chaotic behavior at a high magnetic field



Ar, 10 mT, xx G, 100 V @ 40 MHz

Effect of Magnetic Field on Electron Density





Effect of Magnetic Field on Plasma Density – 75 and 100 G

- The spokes rotate in the anti-clockwise direction.
- The spokes are well-structured at 75 G but become chaotic at 100 G magnetic field.



75 G



100 G

Ar, 10 mT, xx G, 100 V @ 40 MHz



Pulsed Dual-Frequency Capacitively Coupled Plasma



Pulsed Capacitively Coupled Plasmas

- Pulsing offers unique benefits in plasma processing including ion / neutral flux and IAEDF control.
- We are using PIC modeling to look at advanced pulsing schemes, which provide even finer control over the plasma properties than the current state-of-the-art.
- Details can be found in <u>https://doi.org/10.48550/arXiv.2305.15482</u>





Ar, 10 mT, 200 V @ 50 MHz, 750 V @ 1 MHz, 10 kHz



Pulsed Plasma Characteristics – Synchronized Pulsing

- Both the LF and HF sources are turned off at 10 μ s.
- The electron temperature (T_e) drops quickly when the voltages are turned off.
- Due to the quasi-neutral plasma, electron and ion density decays at a slower pace.
- The LF and HF voltages are turned on at 50 μ s.
- T_e increases quickly and a spike in T_e can be observed.
- It takes 10s of μs for plasma density to build up.







What if LF Voltage is Turned Off Earlier than the HF Voltage?

- In the following results, the LF voltage is turned off a few μs earlier than the HF voltage.
- Without the LF voltage, plasma density increases rapidly when only the HF voltage is on.
- Plasma density during the off phase is significantly higher due to this delay.



Ar, 10 mT, 200 V @ 50 MHz, 750 V @ 1 MHz, 10 kHz



LF Turned on After the HF Voltage

- In the following results, the LF voltage is turned on a few μs later than the HF voltage.
- Without the LF voltage, plasma density increases rapidly when only the HF voltage is on.
- Plasma density during the off phase builds us significantly faster due to this delay.



Ar, 10 mT, 200 V @ 50 MHz, 750 V @ 1 MHz, 10 kHz



Time (µs)



Perspective on Kinetic Plasma Modeling in Semiconductor Industry



Experimental Validation

- Plasma models need to be quantitatively accurate for product and process design.
- More emphasis is needed on validating plasma models and testing against experiments.
- Vigorous testing should be done against a set of complimentary experimental measurements.



Figure 7. IEDFs from simulation and RFEA measurements $(V_{\rm HF} = 100 \pm 10 \text{ V}, V_{\rm LH} = 280 \pm 5 \text{ V})$ at 2.25 mTorr, 10.5 mTorr and 19.5 mTorr.

Wang et al., Plasma Source Sci. Technol. 30, 075031 (2021)



Derzsi et al., Plasma Source Sci. Technol. 25, 015004 (2016)



Computational Speed

- Kinetic plasma models are computationally demanding.
- Besides understanding kinetic plasma physics, fundamental research is needed to develop highfidelity and computationally efficient fully kinetic computational methodologies.
- The semiconductor industry particularly needs computationally efficient particle techniques in 2D axisymmetric cylindrical geometry.



Figure 4. Time-averaged plasma profile for 25 mTorr over a range of the α values. Initial number of MPs is $N_{p,init} = 10$ for all cases. (a) Electron density for $\alpha = 0.5$; (b) electron density for $\alpha = 0.025$; (c) electron density at z = 5 cm; (d) electron energy at z = 5 cm.

Hara et al., Plasma Source Sci. Technol. 32, 015008 (2023)



Figure 7: Time averaged plots for the RF-CCP with non-uniform grids with different maximum cell sizes for the energy-conserving (EC)-PIC algorithm. Plots of (a) electron density, (b) ion density, (c) charge density, (d) potential, (e) electric field (f) power deposition, (g) x-component of electron temperature, (h) x-component of ion temperature, (i) EDF at center of discharge, (j) ion impact energy distribution function and (k) ion impact angular distribution function. All cases accurately reproduce the results from the high resolution fully resolved case.

Powis & Kaganovich, https://doi.org/10.48550/arXiv.2308.13092



Chemistry

- Kinetic plasma simulations are often done with simple chemistries (e.g., Ar, He) and often without neutral species and the full plasma chemistry.
- These models are sufficient for basic plasma physics studies but are not adequate for modeling applications in the semiconductor industry.
- All plasma processing applications use complicated chemistries, and chemistry is often critically important for the end results.



 $\begin{array}{c} (i) \\ (i)$

FIG. 2. Time averaged (a) electron density, (b) ionization source by bulk electrons, (c) ionization source by secondary electrons, and (d) electron temperature in a TF-CCP sustained in an $Ar/C_4F_8/O_2$ mixture. (Operating conditions: $Ar/C_4F_8/O_2$ = 75/15/10, 25 mTorr, 500 sccm, 80/10/5 MHz power = 0.4/2.5/5 kW.)

Georgieva et al., J. Appl. Phys. 94, 3478 (2003)

Huang et al., J. Vac. Sci. Technol. A 37, 031304 (2019)



Hybrid Plasma Models and Testing

- While fully kinetic models are important, it is equally essential to develop and refine hybrid schemes that:
 - Include the dominant phenomena identified in fully kinetic simulations, but
 - Allow modeling to be done in a reasonable time with full chemistry.
- Hybrid schemes should be tested against experiments, but also against fully kinetic models.
- One option might be to:
 - Use kinetic simulations to develop quasi-analytical models for charged and neutral species transport and boundary conditions, and
 - ► Use these quasi-analytical modules in hybrid plasma models.
- Machine learning can help with the development of low-pressure species transport models.



High Density Plasmas

- The computational cost of explicit PIC models increases considerably with:
 - Increasing plasma density Debye length constraint
 - Increasing voltage Courant condition
- PIC models are impractically slow to be useful as an LTP system design tool for real powers and voltages used in plasma processing applications in the semiconductor industry.
- Semi-implicit and implicit PIC schemes have been developed,¹ but they have not found widespread usage for LTP applications.
 - ► Could these techniques be refined so the resulting models are numerically accurate and robust?
 - Could one develop hybrid schemes that capture important aspects of the kinetic behavior of electrons and ions, while retaining some of the attractive features of fluid plasma models?

¹See references in <u>https://doi.org/10.48550/arXiv.2308.13092</u>



Magnetrons + Magnetized Plasmas

- Another set of problems where kinetic models are not adequate for use in the semiconductor industry are magnetrons and metal deposition plasmas.
- Typically, these plasmas are 3D, operate at low pressure with strong B, and have high plasma density.
- Hybrid models of magnetized plasmas should be developed with adequate treatment of charged and neutral species.
- There are still not many validated modeling studies in the literature for ionized PVD.

Kolev & Bogaerts, Plasma Process. Polym. 3, 127 (2006)



Figure 7. Calculated density distribution of the Cu^+ ions at p = 10 mTorr.

Figure 8. Calculated density distribution of the Cu atoms at p = 10 mTorr.

20 Height (cm) 0.8 Thermal Cu⁰ (10¹⁰ cm⁻³) (cm) 봄 10 (b) Thermal Cu^{*} (10¹⁰ cm⁻³) 20 łeight (cm) 01 10

Inflight Cu⁰ (10¹¹ cm⁻³)

FIG. 2. Predicted Cu species with IEIE at 2 mTorr. (a) Inflight Cu⁰ density, (b) thermal Cu⁰ density, and (c) thermal Cu^{*} density. The majority of the Cu species are inflight.

Lu & Kushner, J. Appl. Phys. 89, 878 (2001)



Concluding Remarks



Conclusions

- Plasmas are an essential technology used for fabricating microelectronics devices.
- Many widely used plasma sources in the semiconductor industry operate under conditions where kinetic effects are important.
- A few examples of kinetic plasma modeling were discussed where semiconductor industry relevant problems were explored:
 - CCP with non-sinusoidal bias,
 - Electron-beam generated plasma,
 - Magnetized CCP,
 - Pulsed dual-frequency CCP.
- In our opinion, important kinetic plasma modeling research problems include:
 - Model validation,
 - Development of computationally efficient kinetic modeling methodologies,
 - Kinetic plasma modeling with chemistry,
 - Using kinetic modeling to develop accurate hybrid modeling techniques.



