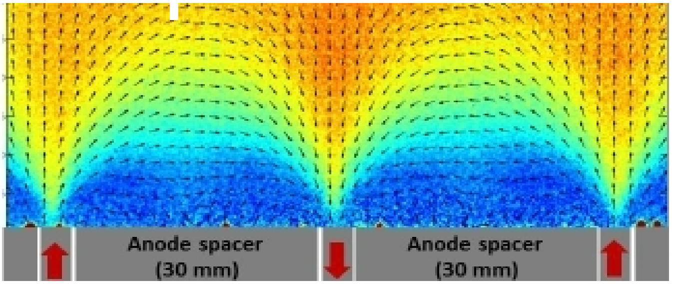
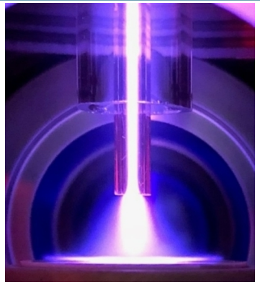
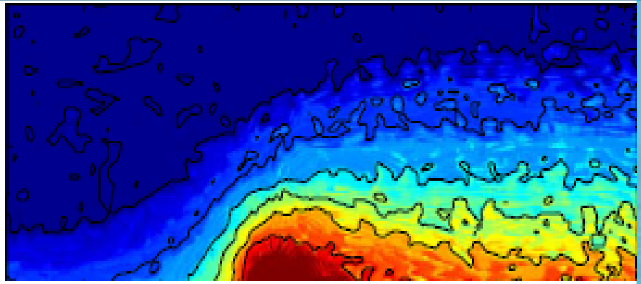
SAND2021-12980C

Sandia National Laboratories

Particle-in-cell modeling of low pressure, high voltage capacitively coupled Ar plasmas







AVS 67th International Symposium & Exhibition

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U.S. Department of Energy

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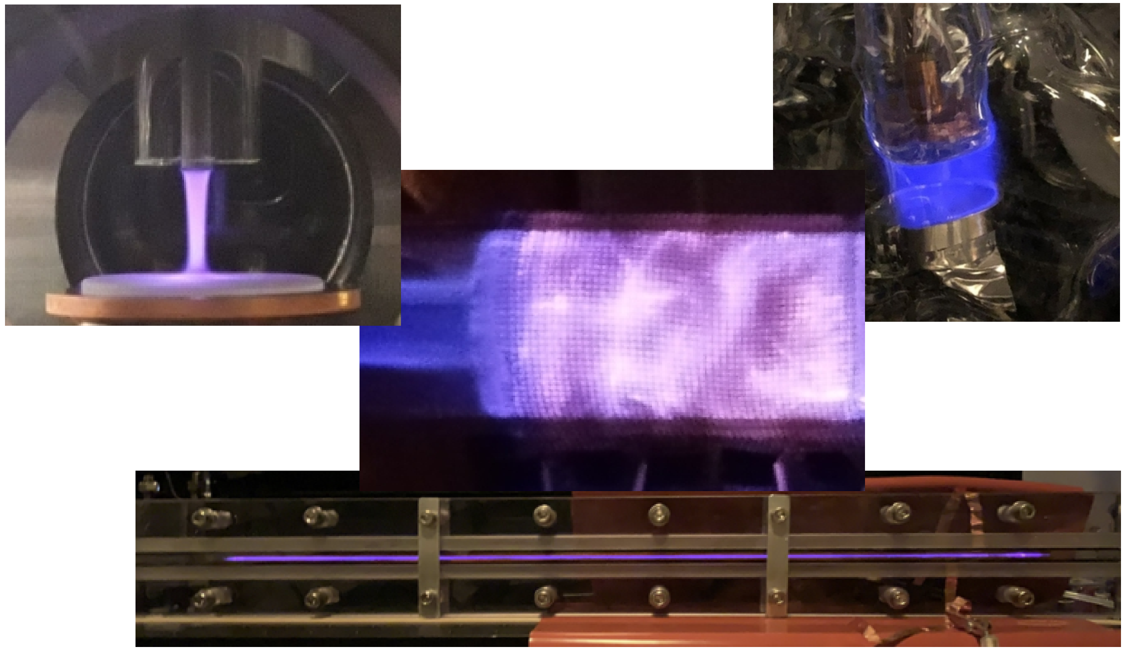
Agenda

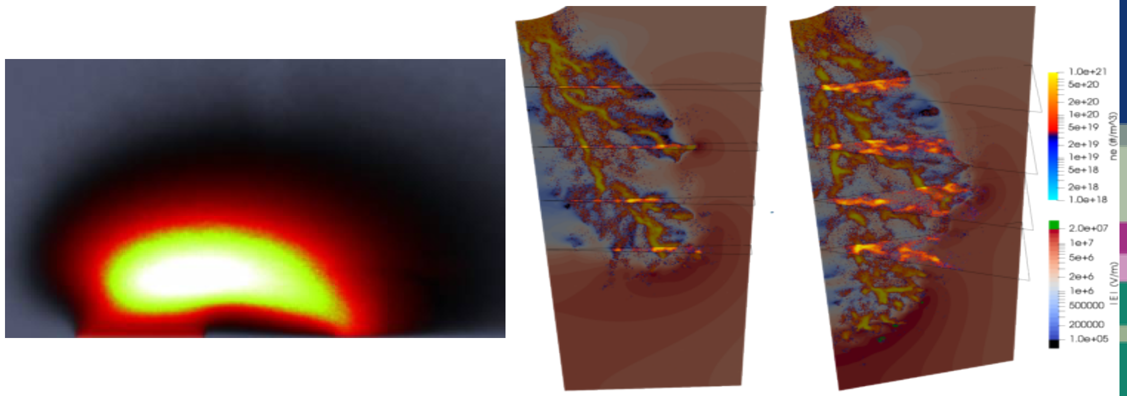
- Ion Energy and Angular Distributions for High Aspect Ratio Etching
- Model Description
- Plasma Dynamics
- Ion Energy Distributions
- Vary Low Frequency Voltage

Sandia Low-Temperature Plasma Research Facility (PRF)

- **Experimental Capabilities:**
  - Femtosecond, picosecond, nanosecond and CW lasers.
  - Diagnostics for measuring various neutral species densities (MBMS, LIF, PF-LIF), electric fields (LIF-Dip, EFISH), electron densities (LCIF), and temperatures (CARS).
  - High speed detectors for imaging and spectroscopy
  - Plasma generating capabilities from vacuum to atmospheric pressure.



- **Computational Capabilities:**
  - Aleph and EMPIRE: Massively parallel PIC-DSMC, extensive chemistry and photonic processes
  - Aria: multiphase fluid simulation capability being extended to highly collisional plasmas
  - 0D global modeling

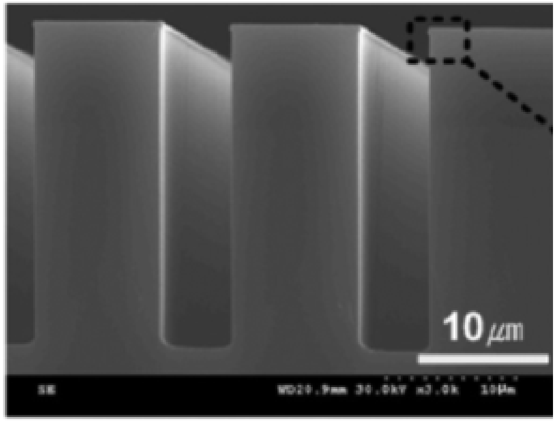


Propose a collaboration at: www.sandia.gov/prf

Sandia National Laboratories' Plasma Research Facility is funded by the U.S. Department of Energy's Office of Science, Fusion Energy Sciences.

Ion Energy and Angular Distributions (IEAD)

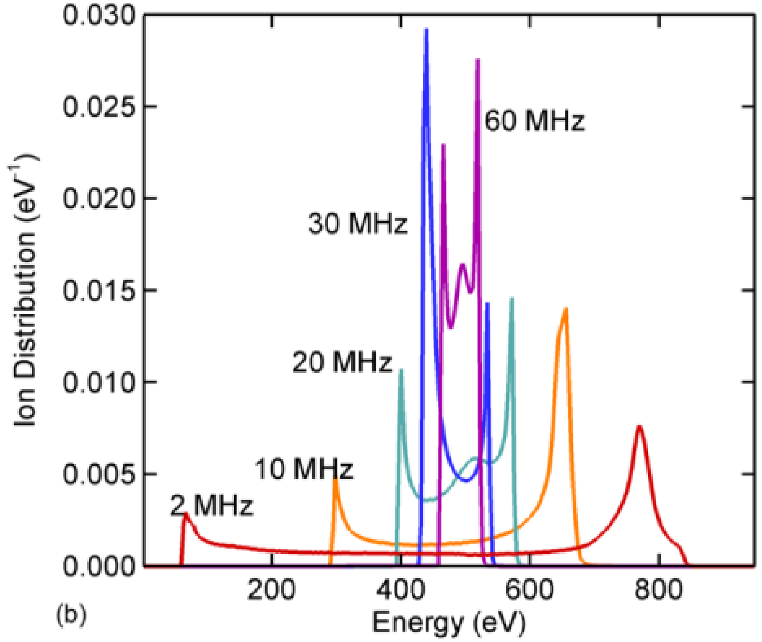
- Energetic ions enable anisotropic etching which is critical for semiconductor processing.



Wu et al., J. of Appl. Phys. 108, 051101 (2010).

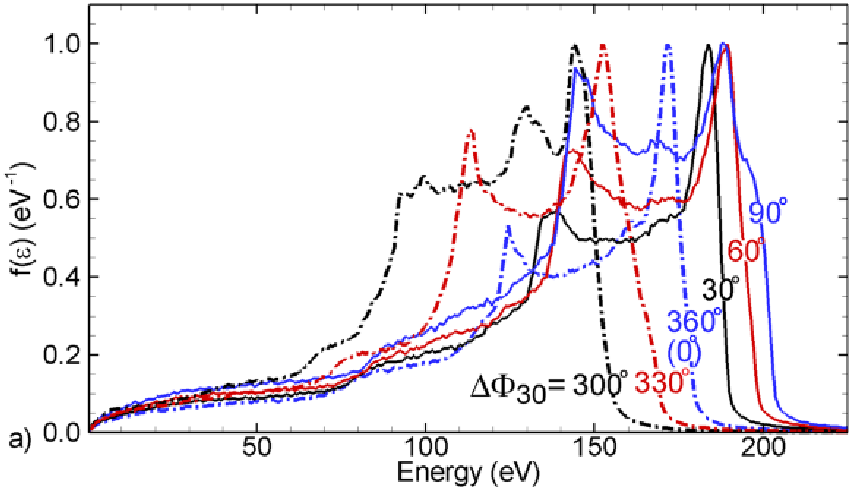
- Low frequency ($\omega < \omega_{pi}$):
  - Ion experiences instantaneous field
  - Double peak
- High frequency ($\omega > \omega_{pi}$):
  - Ion experiences average field
  - Single peak
- < 2° angular distribution is required
- 2-3 frequencies are often used to provide more independent control of flux and energy.

Single Frequency



Y. Zhang, J. Vac. Sci. Technol. A. 31, 061311 (2013).

Three Frequency

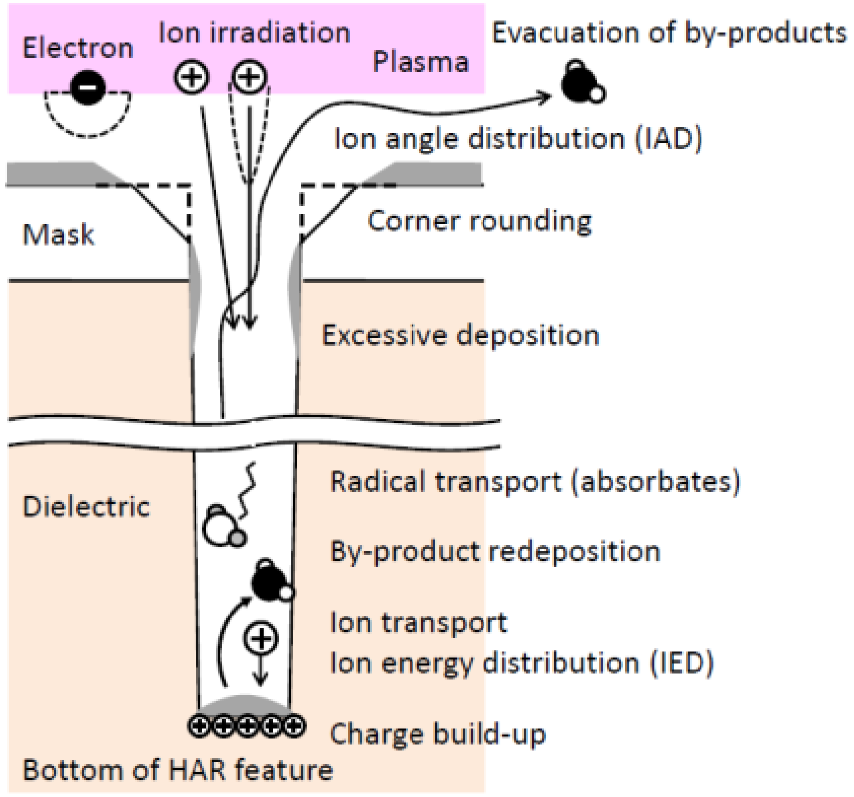


Y. Zhang, J. Appl. Phys. 117, 233302 (2015).

High Aspect Ratio Etching

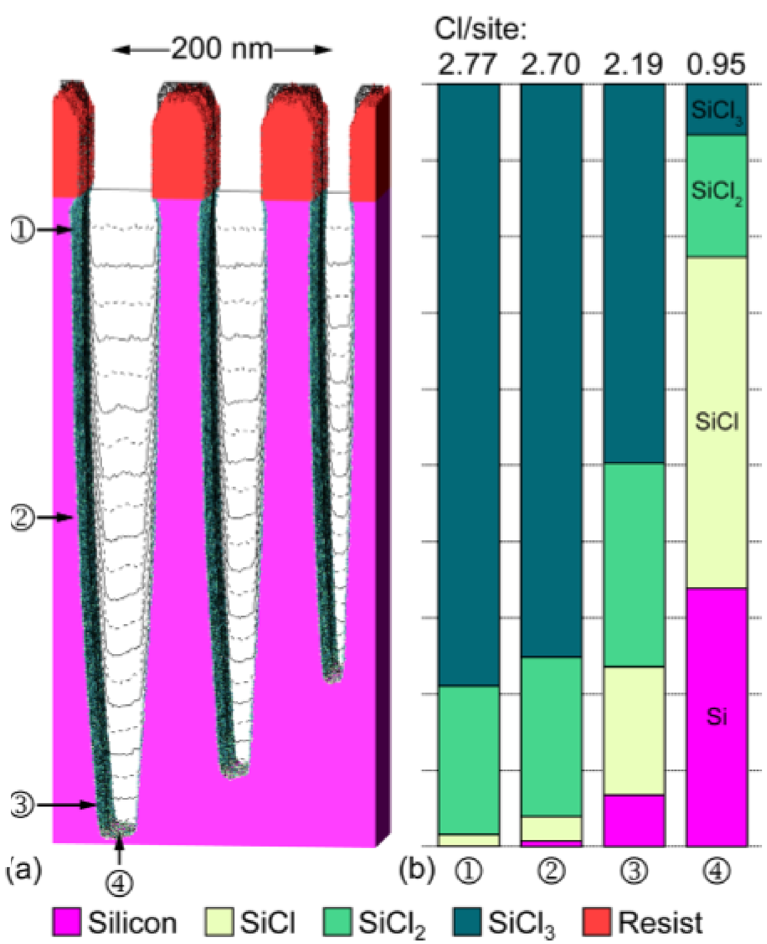
- Many non-idealities are exacerbated at high aspect ratios (HARs) of 50-100.
  - Higher ion energies are required.
- Few electrons reach the bottom of the feature.
- Etch rate is often limited by the ion flux, but for HAR few neutrals reach the bottom of the feature.
- Etch rate can be dependent on aspect ratio.
- Polymer growth is often used to protect the sidewalls.

Considerations at High Aspect Ratio



K. Ishikawa et al., Jap. J. Appl. Phys. 57, 06JA01 (2018).

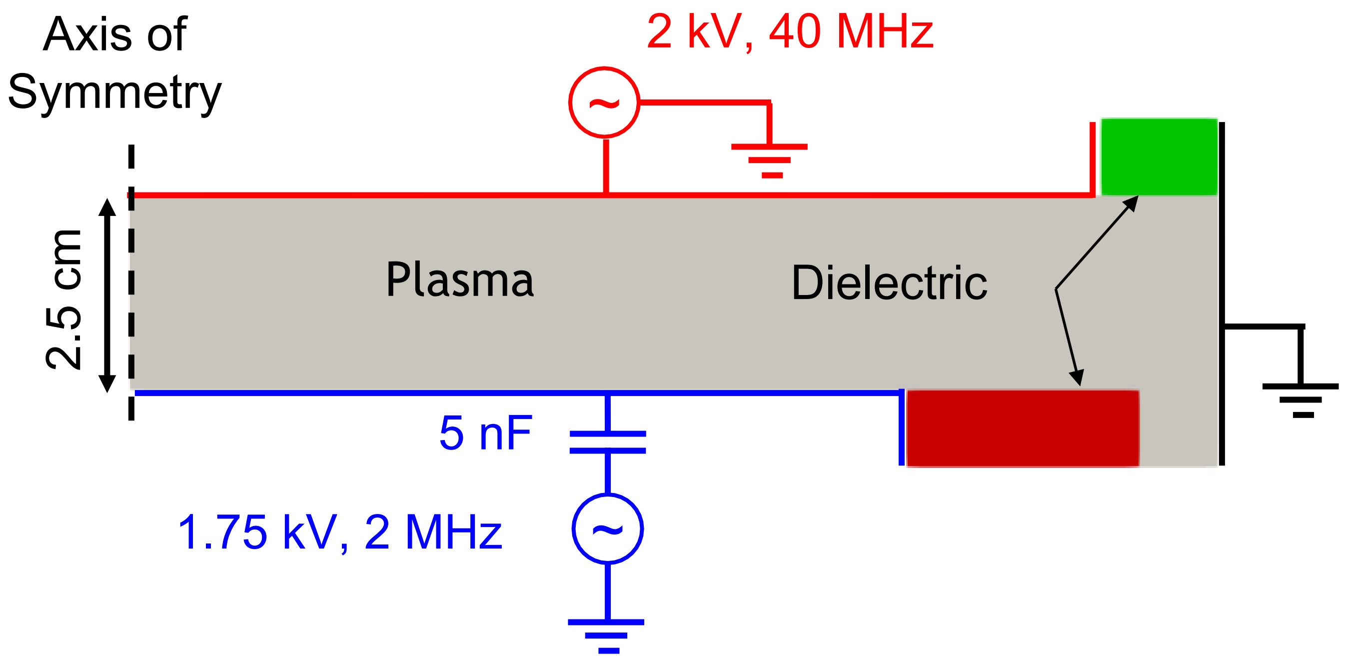
Aspect Ratio Dependent Etching



Huard et al., J. Vac. Sci. Tecnol. A,35, 05C301 (2017)

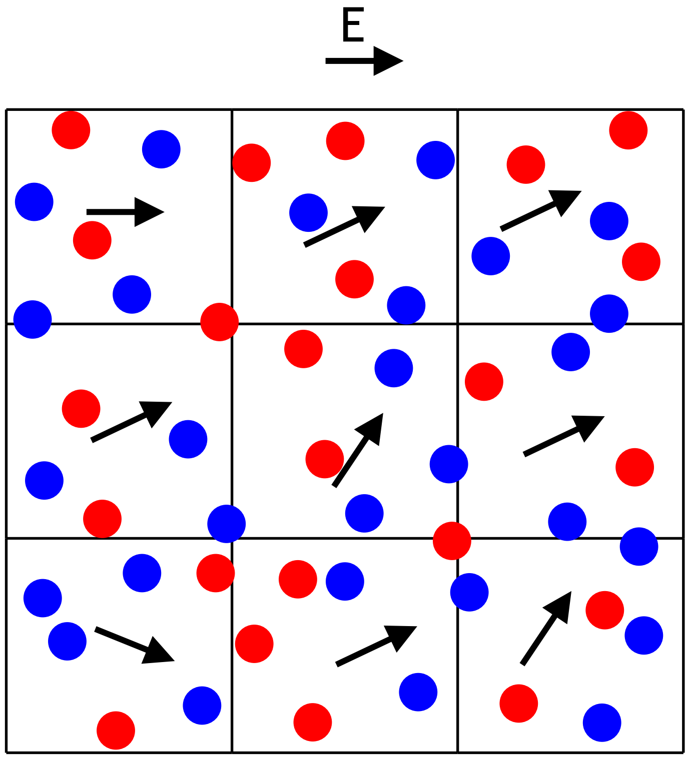
Model Setup

- Goal: Study low pressure, 2-frequency capacitively coupled plasmas (CCPs) for high aspect ratio etching.
  - Evaluate/understand the limits of simplified models.
- Conditions:
  - 8 mTorr Ar
  - 2.5 cm gap
  - Upper electrode: V_{hf} = 2 kV, 40 MHz
  - Lower electrode: V_{lf} = 1.75 kV, 2 MHz
  - Currently 1-D
- Massively parallel PIC enables investigation of lower pressures + higher voltages than would be possible otherwise.
- Primarily interested in
  - Basic plasma dynamics
  - IEADs.

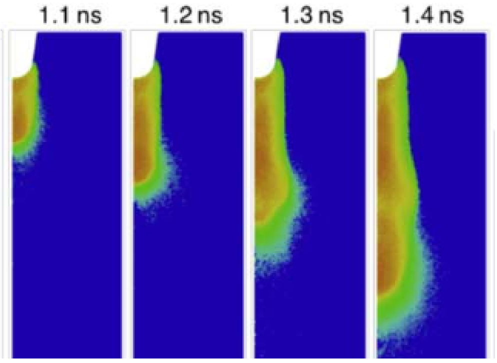


Aleph Model Description

- 0D, 1D, 2D, or 3D
- Particle-in-cell direct simulation Monte Carlo model (PIC-DSMC)
  - Treating electrons, ions, and neutrals as particles means there are no assumptions about the distribution functions.
  - This is a more expensive, but higher-fidelity method than is commonly used in the semiconductor industry (fluid or hybrid)
- Unstructured finite element mesh.
- Electrostatic.
- Used to study development of arcs in vacuums, streamer propagation in air, glow discharges, etc.
- Particle merging algorithms keep the counts of computational particles in check with minimal disruptions to distribution functions.

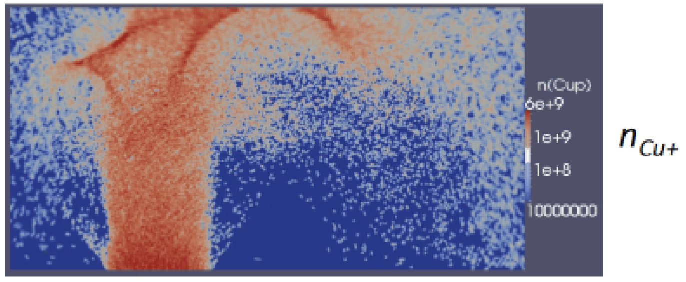


Streamer Propagation



A. S. Fierro, C. H. Moore, B. T. Yee, and M. M. Hopkins, Plasma Sources Sci. Technol. 27, 105008 (2018).

Vacuum Arc

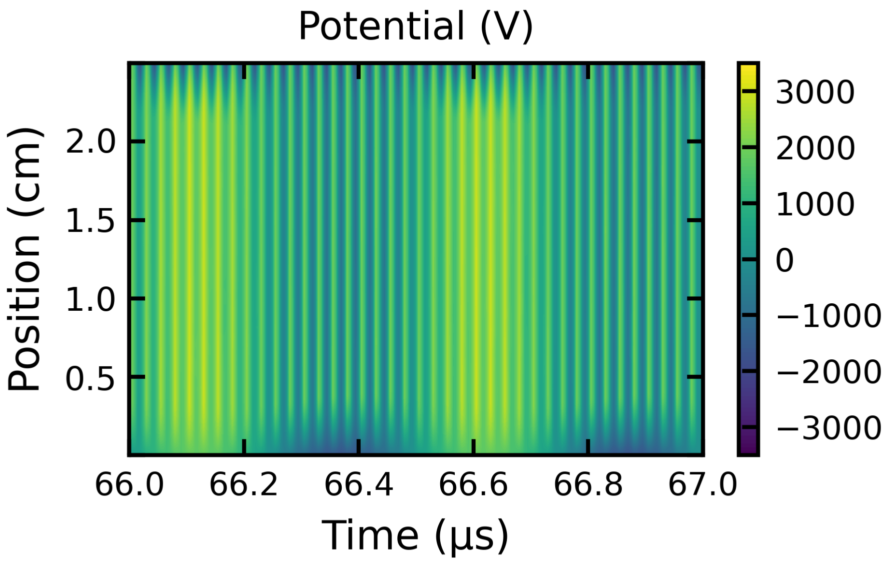


M. M. Hopkins, J. J. Boerner, C. H. Moore, P. S. Crozier, International Conf. on Numerical Simulation of Plasmas, Beijing, China (2013).

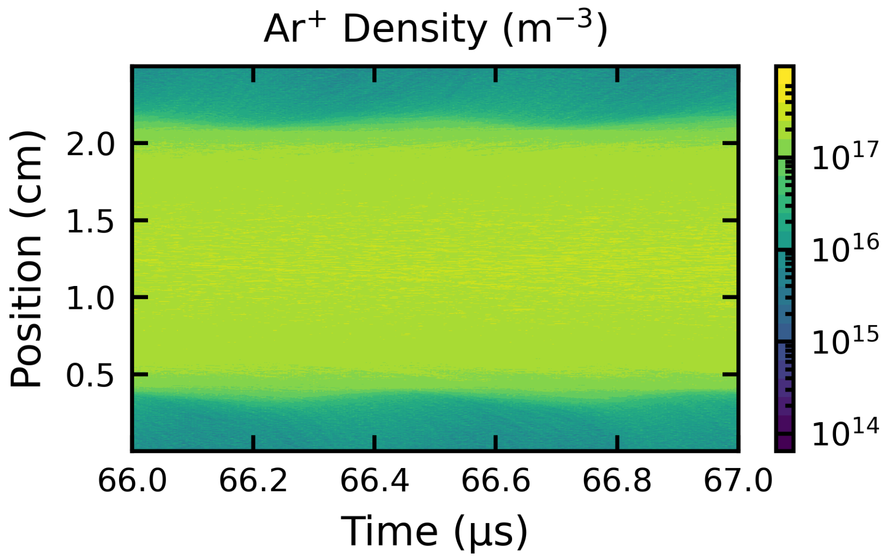
Plasma Dynamics

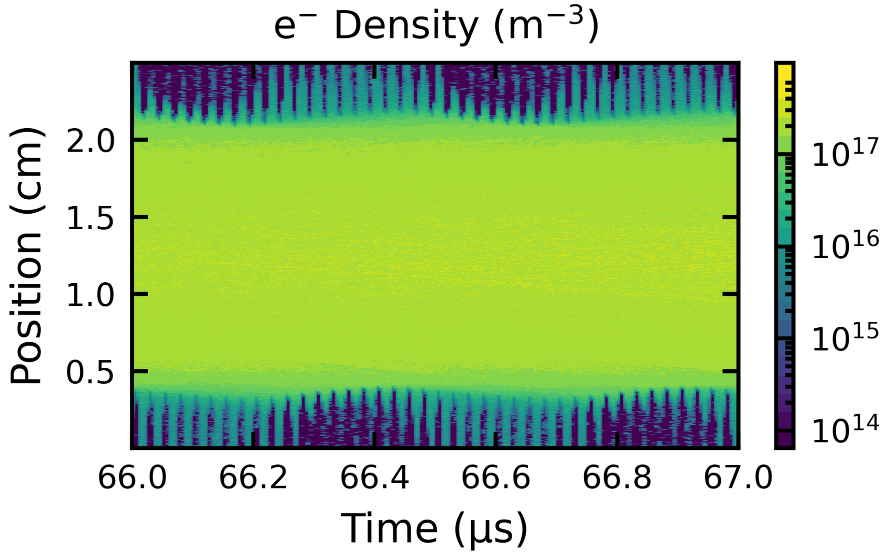
2 Cycles Shown

- 8 mTorr Ar
- 2 kV at 40 MHz
- 1.75 kV at 2 MHz
- Numerical parameters:
  - $\Delta x = 10\ \mu m \approx 0.4\lambda_D$
  - $\Delta t = 400$ fs $\approx 0.3CFL_e$
  - Targeted particles per cell: 150 e^-, 100 Ar^+, 30 Ar, 5 Ar*
- 5 excited states of Ar
- 27 interactions
- $n_e \approx 2 \times 10^{17}\ m^{-3}$
- Average bulk e^- energy = 5-10 eV



- $\omega_{pe} \approx 2 \times 10^{15}$ Hz
- $\omega_{pi} \approx 15$ MHz
- Plasma is always positive with respect to electrodes.
- Not yet to steady state.



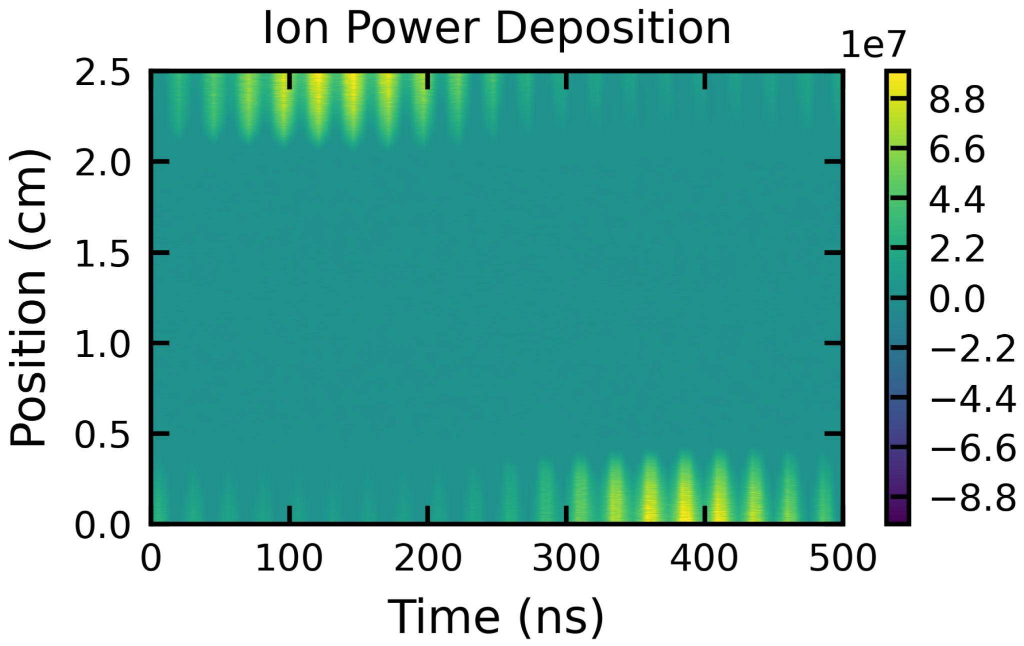


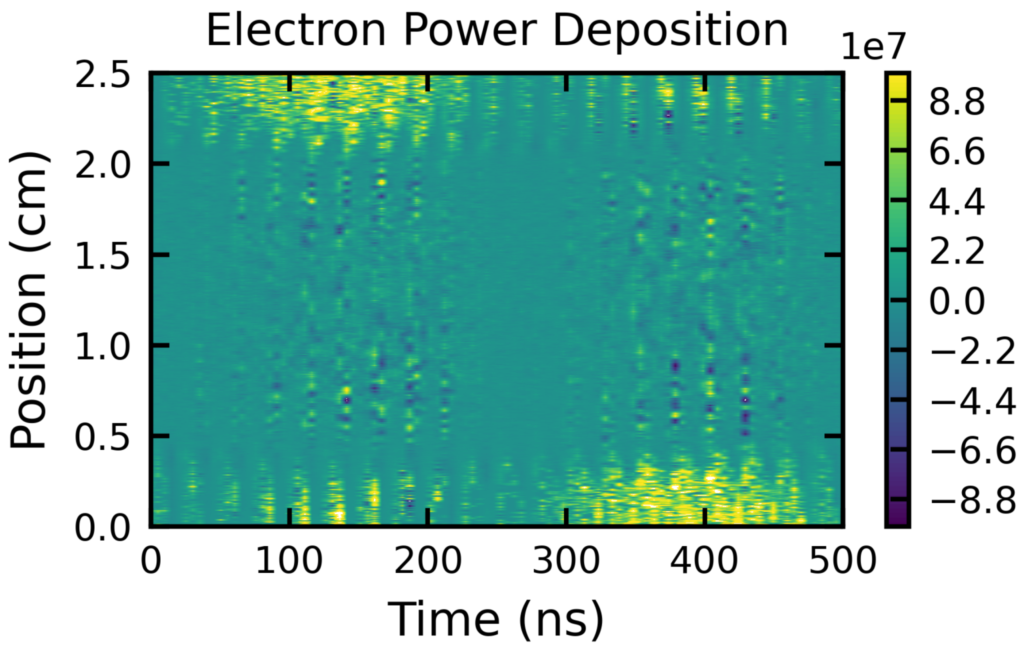
Power Deposition

- Power deposited into the electrons/ions in the plasma:

$$P_e = \vec{J}_e \cdot \vec{E}$$
$$P_i = \vec{J}_i \cdot \vec{E}$$

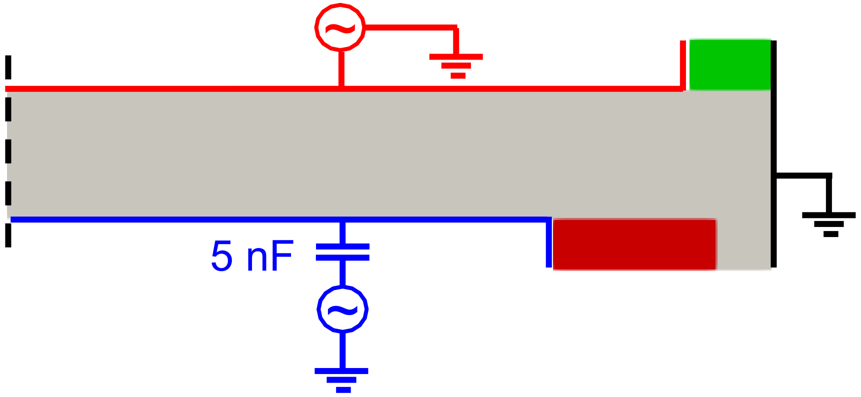
  - $\vec{E}$ = electric field
  - $\vec{J}_e$ = electron current density
  - $\vec{J}_i$ = ion current density
- Averaged over cycles 56 – 67 μs
- Negative power deposition can be physical:
  - Plasma transfers energy back to the circuit.
  - Current flows against the electric field.
- Ion energy deposition is always positive.
- Ion power deposition is limited to the sheath, especially near negative electrodes.

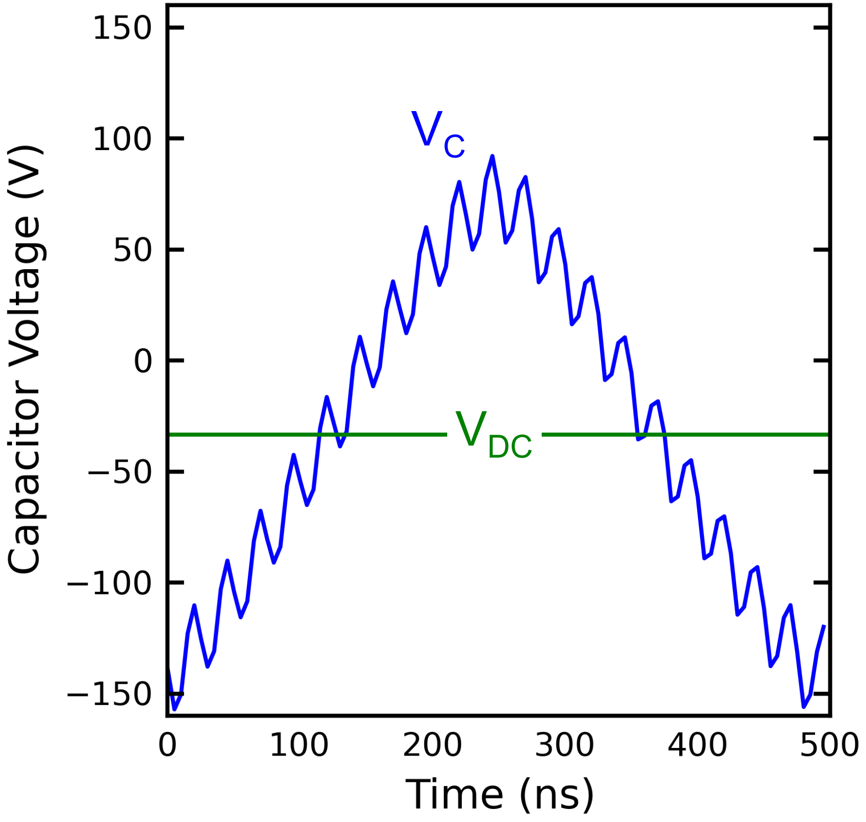




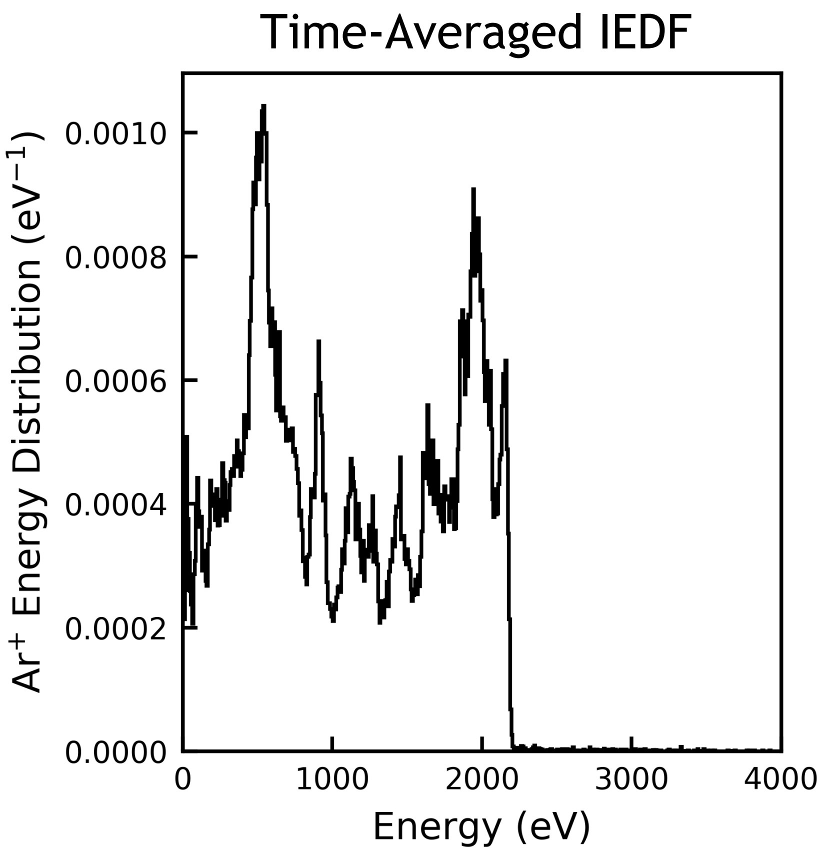
DC self-bias

- ‘Blocking capacitor’ allows AC current to flow, but not DC current.
- This allows a DC bias to form as a result of the plasma dynamics.
- Geometric asymmetry in the electrodes.
  - In 1-D, this is applied in the area used to convert fluxes to currents.
- V_{DC} = -33 V
- DC bias further increases the ion energy.

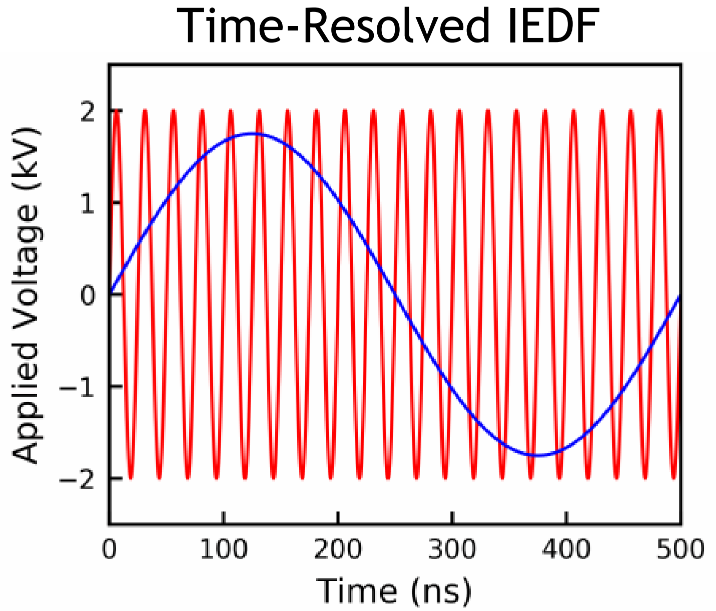


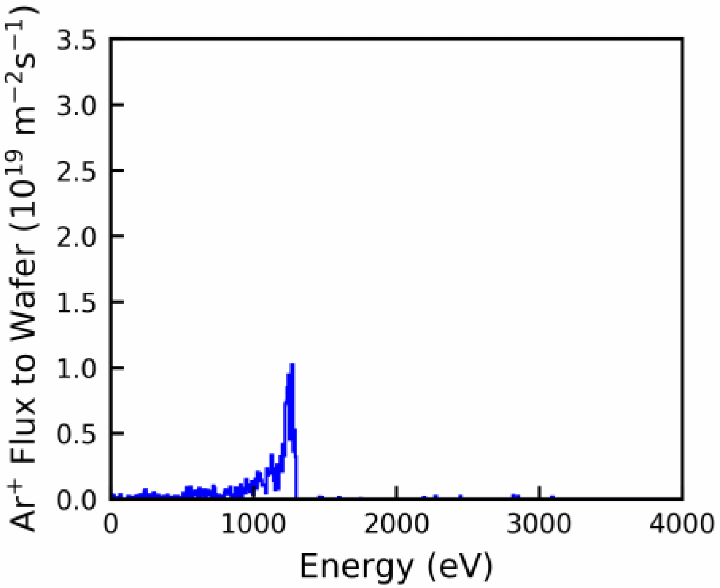


Ion energy distributions



- V_{lf} = 1.75 kV
- Finer structure is generally due to high-frequency component.
- Maximum energy occurs at the rising portion of the low-frequency cycle.
- Most ions reach the surface at the positive polarity part of the low-frequency cycle.

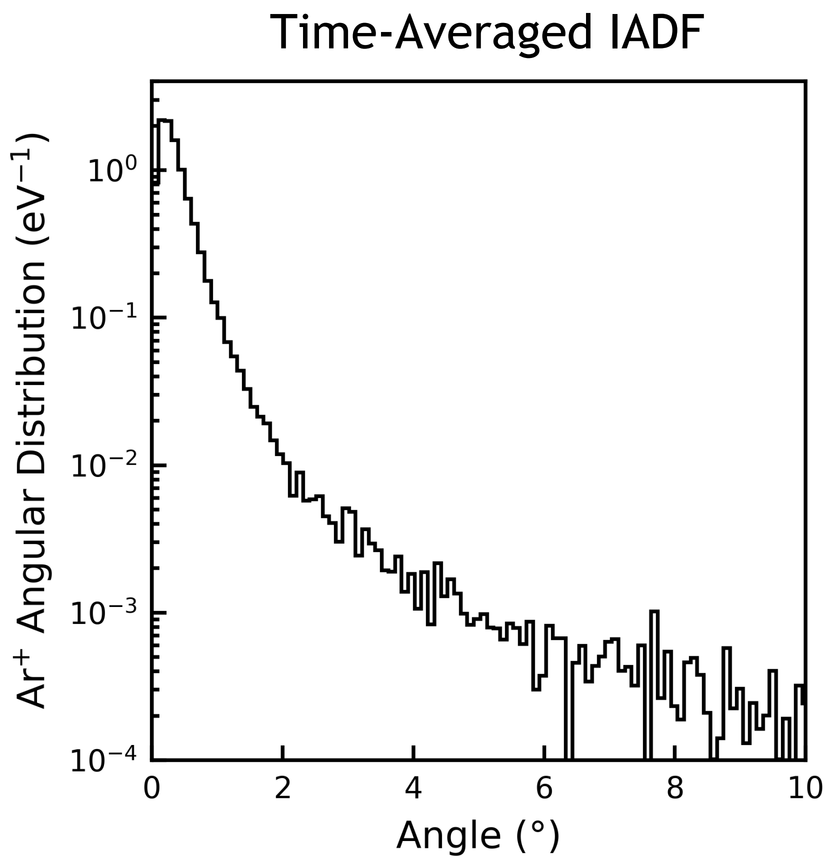




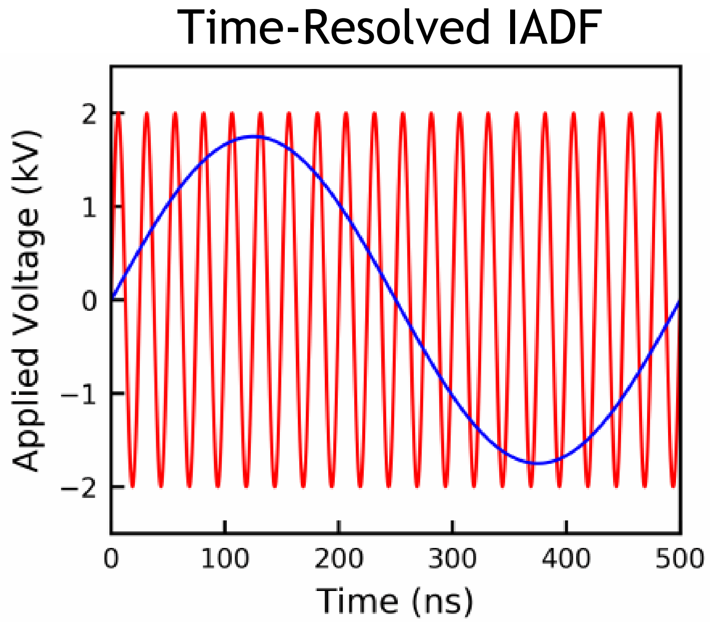
- 10^5 particles total, averaged over 23 cycles

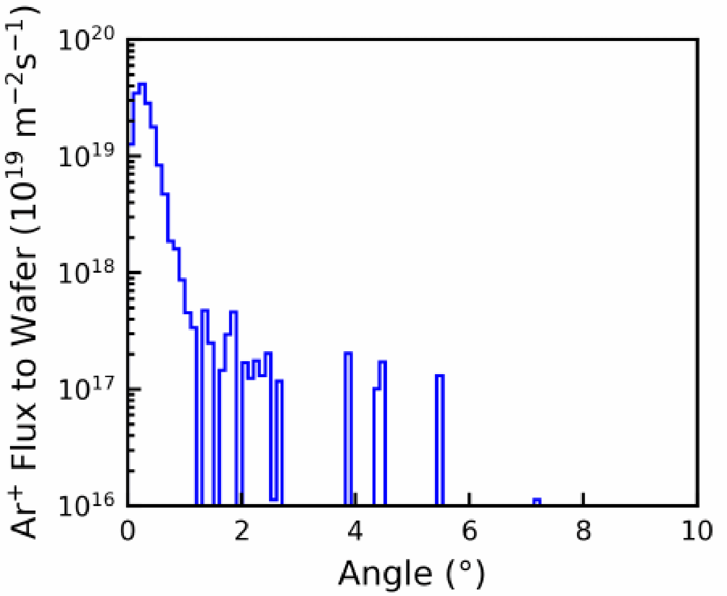
Animation Slide

Ion angular distributions



- V_{lf} = 1.75 kV
- In order to avoid distorting features, the angular distribution must be less than a few °.
- Most ions reach the surface at the positive part of the low-frequency cycle.
  - The distribution is narrower at this time due to a greater $v_\perp$.
  - $\theta = \tan^{-1}(v_{||}/v_\perp)$

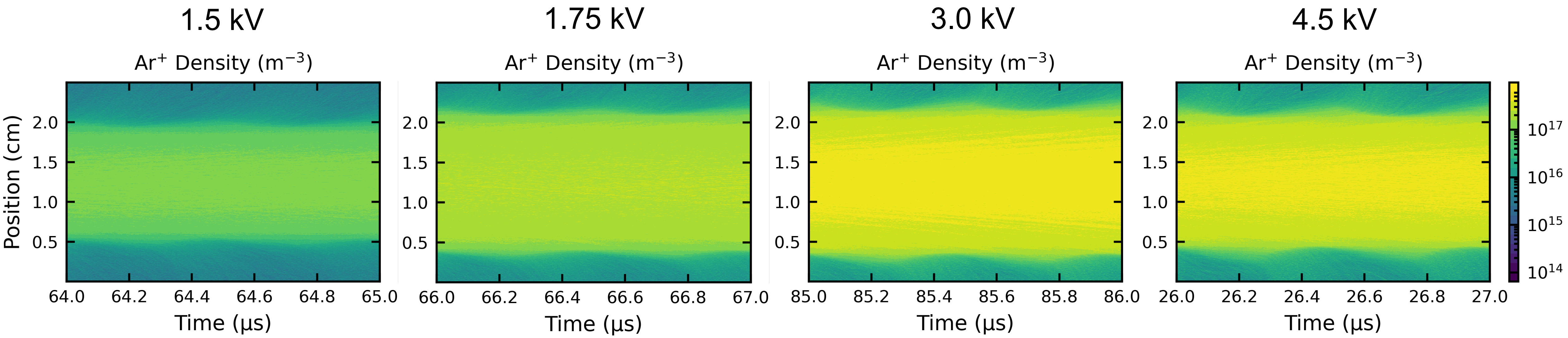




- Particles with an angle > 2° are generally due to collisions within the sheath.
- In HAR, even rare broadening of the IAD can cause feature distortion. This is why we look at 4 orders of magnitude.

Animation Slide

Vary V_{lf}: Sheaths

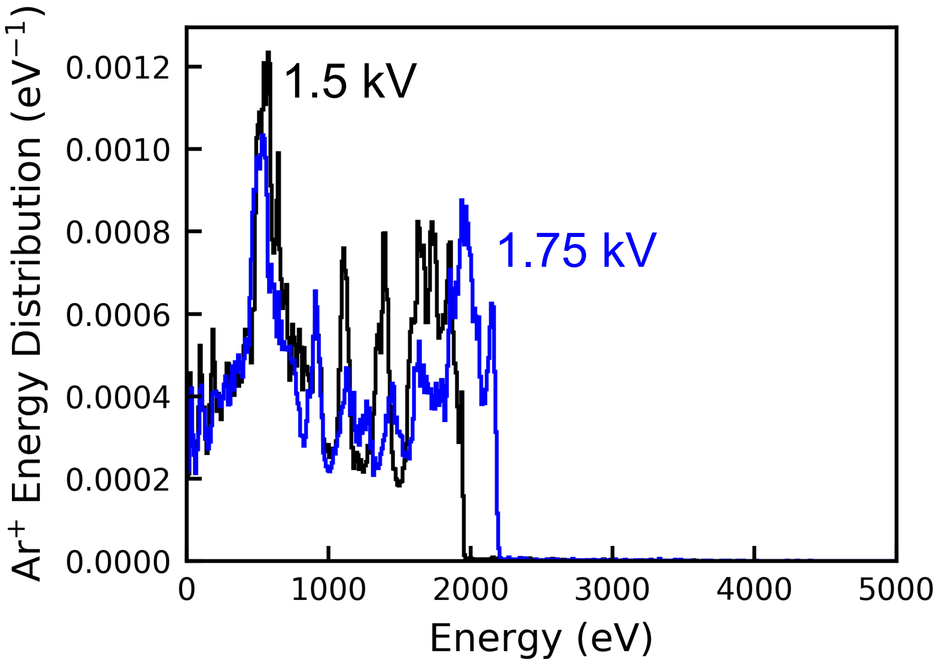


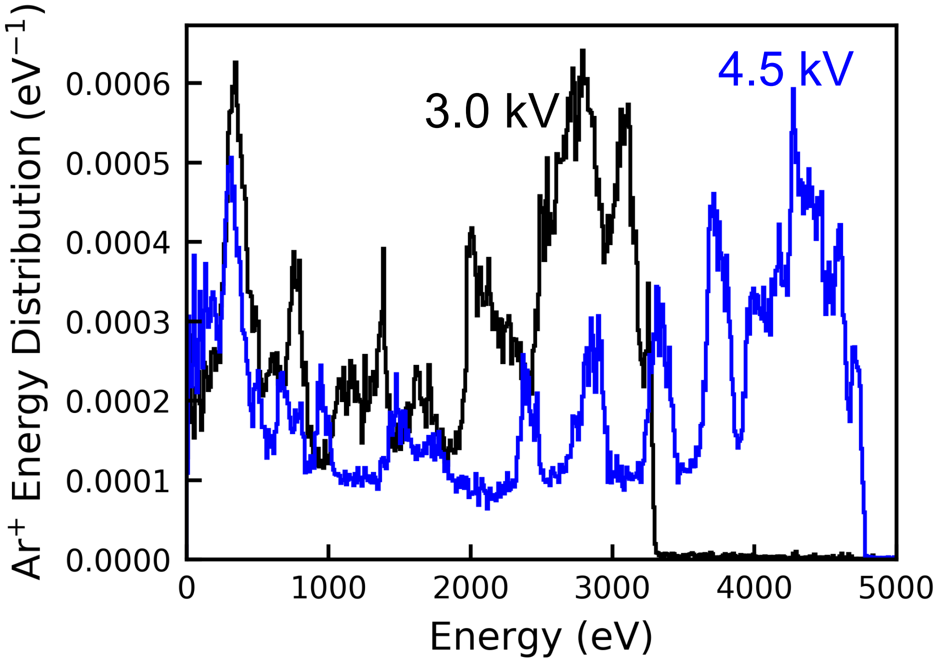
- V_{hf} = 2 kV, 40 MHz
- 8 mTorr Ar, 2.5 cm gap
- 2 cycles shown
- For constant n_e, the sheath size should increase with V_{lf}.

- Because these simulations are not at the steady state, the n_e is still increasing.
- Generally n_e increases more rapidly when V_{lf} is closer to 2.5 kV.

Vary V_{lf}: IED

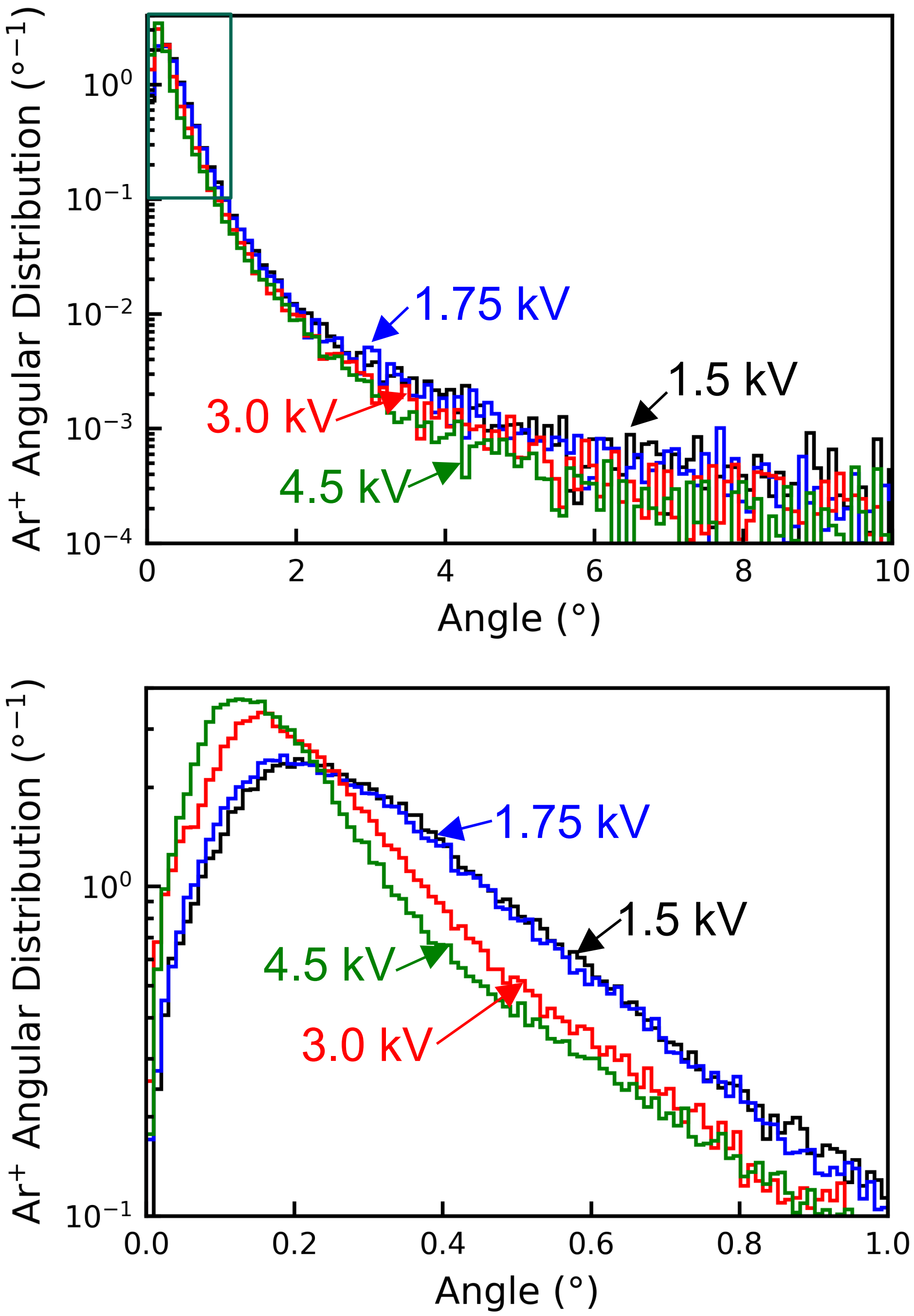
- V_{hf} = 2 kV, 40 MHz
- 8 mTorr Ar, 2.5 cm gap
- Increasing the low frequency voltage results in a much broader distribution of ion energies.
- Even when $V_{hf} < V_{lf}$, the high frequency features are still visible in the IEDF.
- The lower energy peak tends to be shifted left at higher V_{lf}.





Vary V_{lf}: IAD

- V_{hf} = 2 kV, 40 MHz
- 8 mTorr Ar, 2.5 cm gap
- Higher V_{lf} narrows the distribution, especially at small angles.
- This may be highly pressure dependent:
  - Larger V_{lf} produces larger sheath
  - Ion collisions within sheath more likely
- Majority of broadening is likely due to thermal distribution of ions in bulk plasma:
  - $v_{||} \approx v_{thermal}$
  - $\theta = \tan^{-1}(v_{||}/v_{\perp})$



Conclusions

- High frequency component adds structure to the ion energy distribution between the main peaks.
- The angular distribution is broader for lower energy ions.
- Increasing the low frequency voltage results in a much broader distribution of ion energies.
- Future work:
  - Run simulations to steady state
  - Effect of gap sizes and pressure
  - 2-dimensional simulations
    - Wafer-scale uniformity is critical

Work with us: 3rd Plasma Research Facility Proposal Call

Propose a collaboration at: www.sandia.gov/prf

Open of PRF Proposal Call	October 12, 2021
Close of PRF proposal Call	December 17, 2021
External Reviews	~ 1 month
Notification of Principal Investigators	February 4, 2022

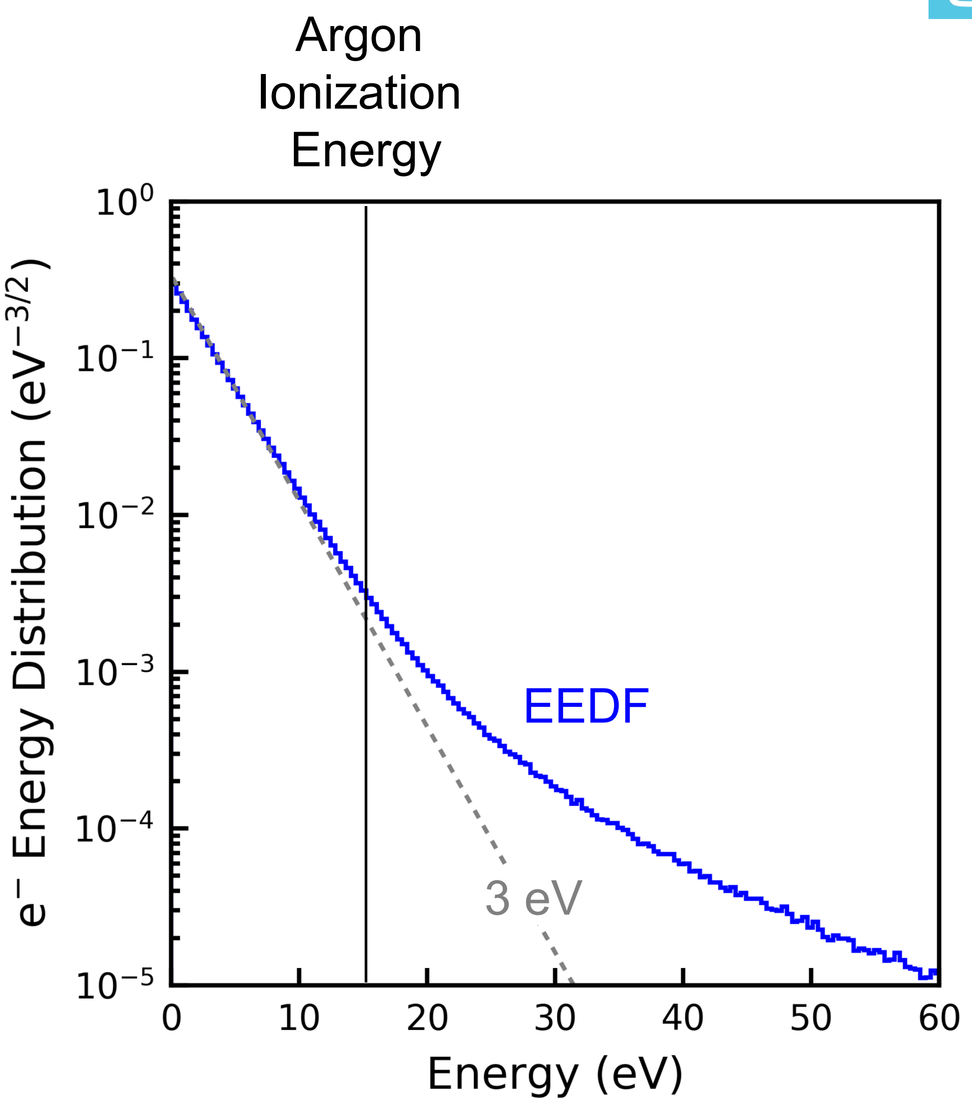
Contact us to ensure projects are well-aligned with our capabilities:

- Brian Bentz (bzbentz@sandia.gov)
- Jonathan Frank (jhfrank@sandia.gov)
- Nils Hansen (nhansen@sandia.gov)
- Matthew Hopkins (mmhopki@sandia.gov)
- Christopher Kliewer (cjkliew@sandia.gov)
- Shane Sickafoose (smsicka@sandia.gov)

BACKUP

Electron Generation

- A bi-Maxwellian electron energy distribution is common in CCPs.



8mTorr, Higher voltage

- Increased initial n_e for $V_{lf} \geq$ 3kV