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High-Fidelity Particle-in-Cell Simulations of Thermionic Converters

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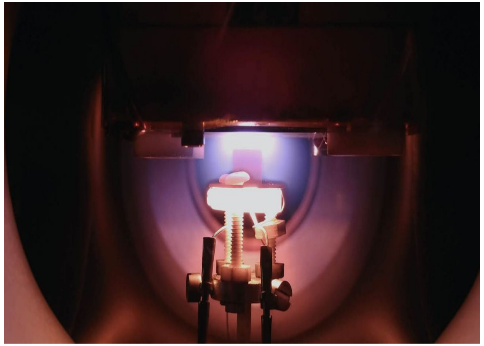
Modern Electron: Thermionic convertors for residential heating

- Integrate electricity-producing thermionics into natural gas furnaces and boilers
- Silent converters with no moving parts
- Compact and high power density
- All “waste” heat is still used
  - 100% marginal efficiency electricity production
- Enables blackout-proof furnaces



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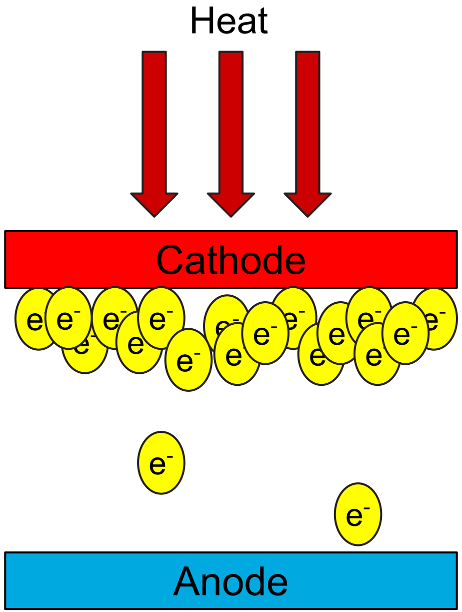
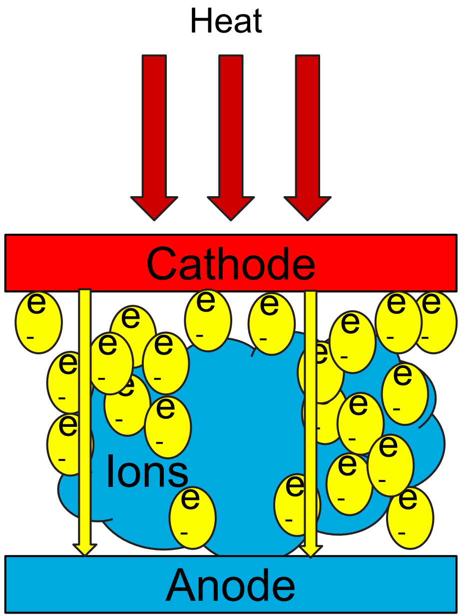
Plasma-based Thermionic Converters

- Heat is converted to electricity due to an electric current from a hot cathode to a cold anode
- With a plasma, the ion background allows movement of electrons in a net-neutral medium

Basic thermionic diode
Space-charge limited; little current



Plasma
Desired situation; significant current



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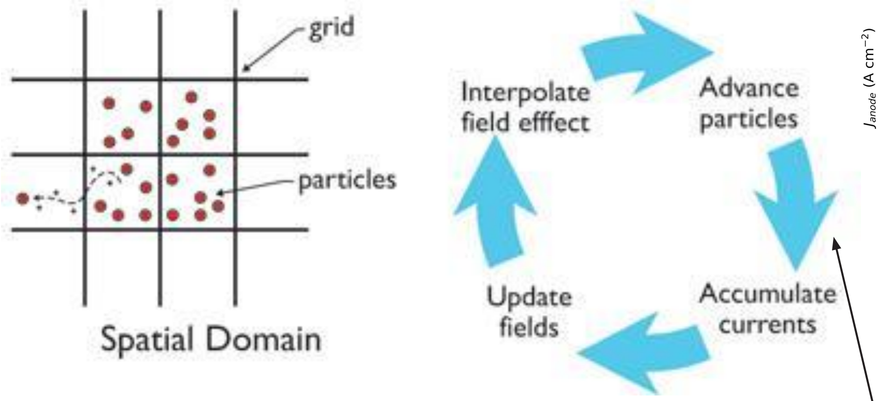
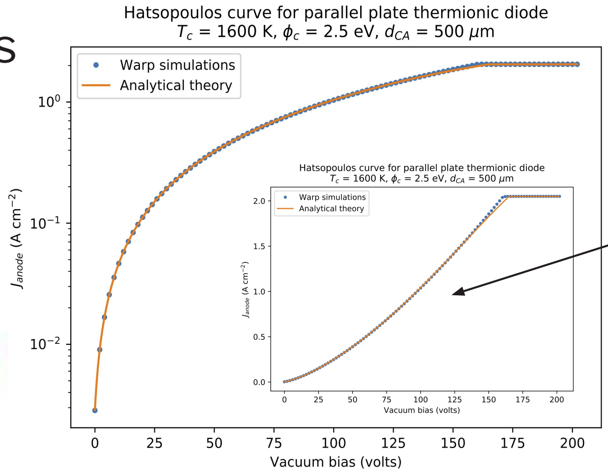
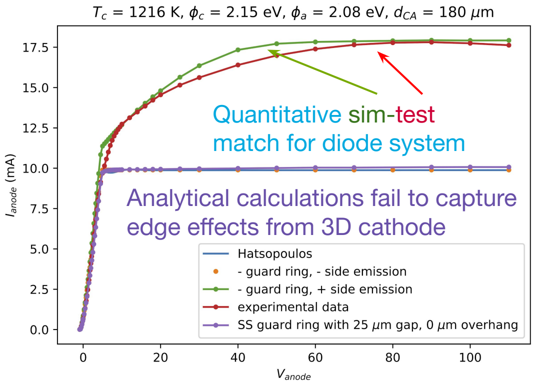
Simulations of Particle Dynamics in Thermionic Converters

Particle-in-cell method for simulations of dense charged particle systems





Thermionic emission models were developed and validated against both analytical theory and experimental data



Add physics unique to plasmas and boundaries:

- Remove particles that passed boundaries
- Handle particle collisions
  - Create new particles
  - Adjust particle velocities
- Inject new particles

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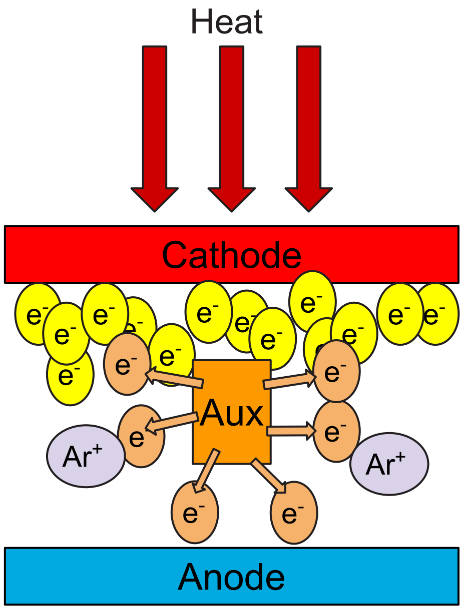
Triode Converter

- Take advantage of argon's low e^--neutral cross-section
- Inject high-energy electrons from a third "aux" electrode that ionize Ar
- Simulations establish I_{diode} possible for a given plasma density, and plasma density possible for a given I_{aux}

Auxiliary electrode emits high-energy electrons to ionize Ar



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Triode Converter - “Plasmatron”

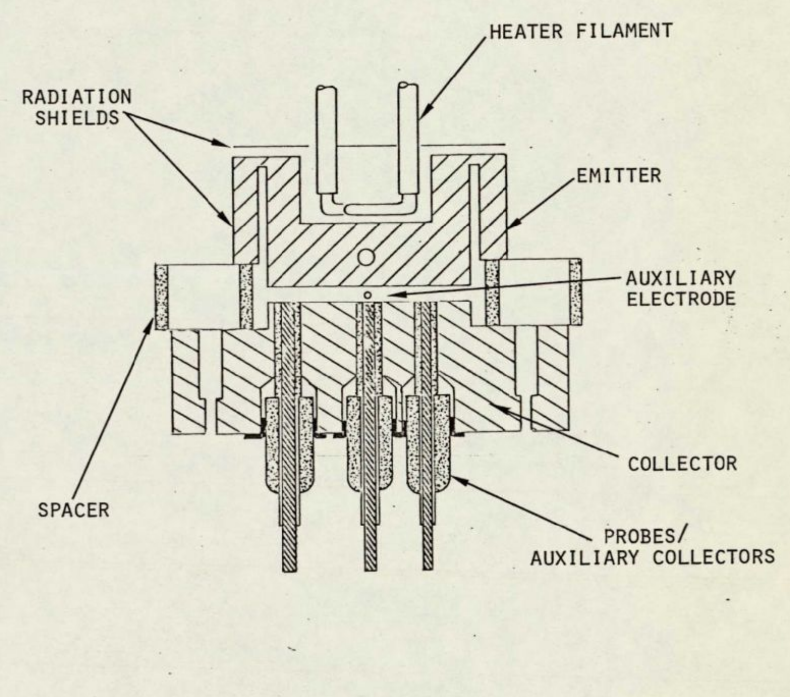

Fig. 2 Demountable Plasmatron Converter With Plane Parallel Electrodes

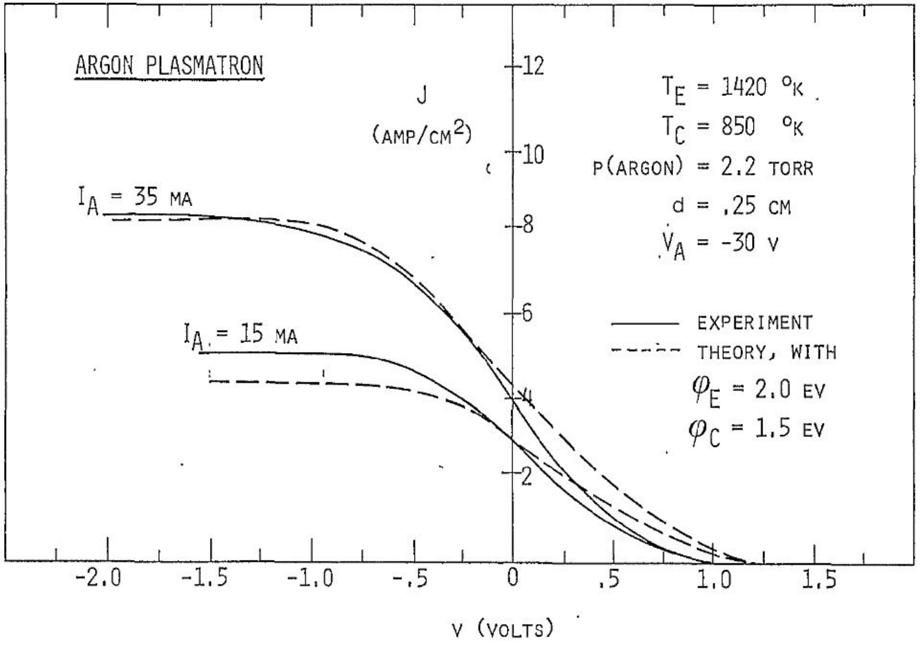

Fig. 8 Theoretical and Experimental I-V Characteristics for an Argon Plasmatron

Thermo Electron. Hansen, B Y L K, G L Hatch, and N S Rasor. “THE PLASMATRON.” Rasor Associates, Inc., Sunnyvale, CA (USA), 1976
See also Knechtli, R. C., and Marvin Fox. “Theory and Performance of Auxiliary Discharge Thermionic Energy Converters.” Advanced Energy Conversion, Thermionic Power Conversion, 3, no. 1 (January 1, 1963): 333–49. https://doi.org/10.1016/0365-1789(63)90104-8.

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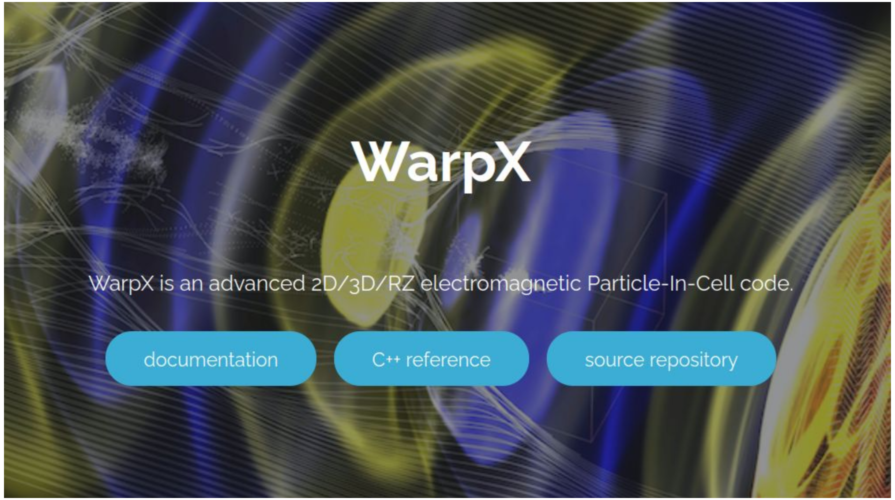
WarpX

- Developed at Lawrence Berkeley National Lab
    - Part of the Exascale Computing Project
- Uses the AMReX adaptive mesh refinement library
    - Allows platform-portable code
    - Shares functionality with other software packages
- Modern Electron maintains a fork with thermionic-specific functionality
    - We also contribute to the primary WarpX code base



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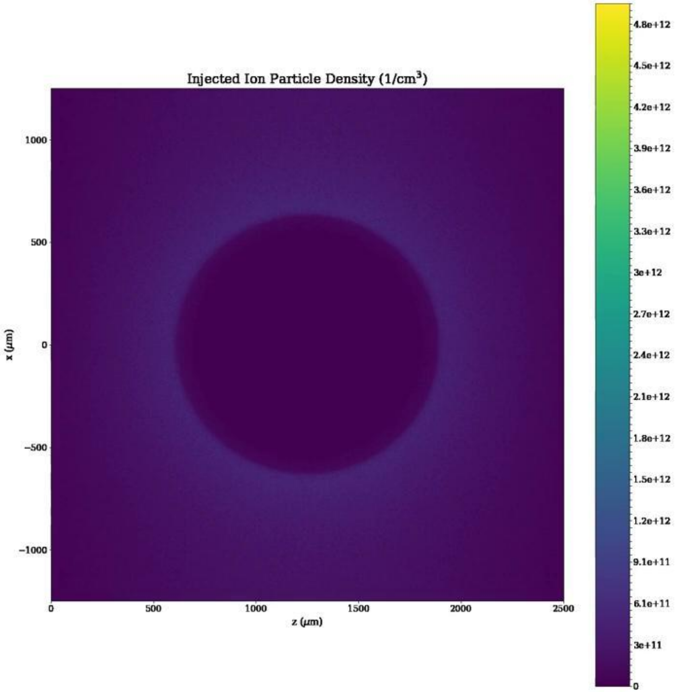
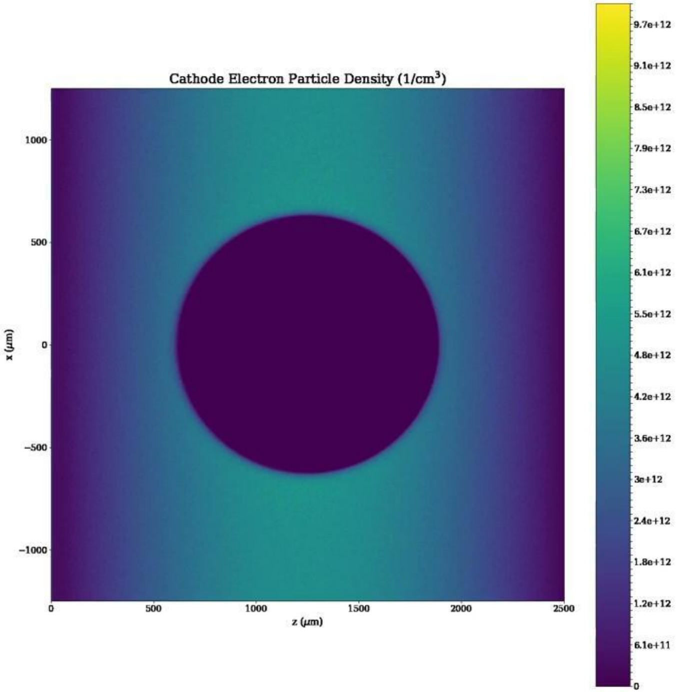
Example Plasmatron Simulation

- 1664x1664 grid
- $4*10^{-13}$ s timestep
- ~160M particles
- 4.5M timesteps
  - 1.8 μs
- 950 M particle* steps/second
  - 4 A100 GPUs





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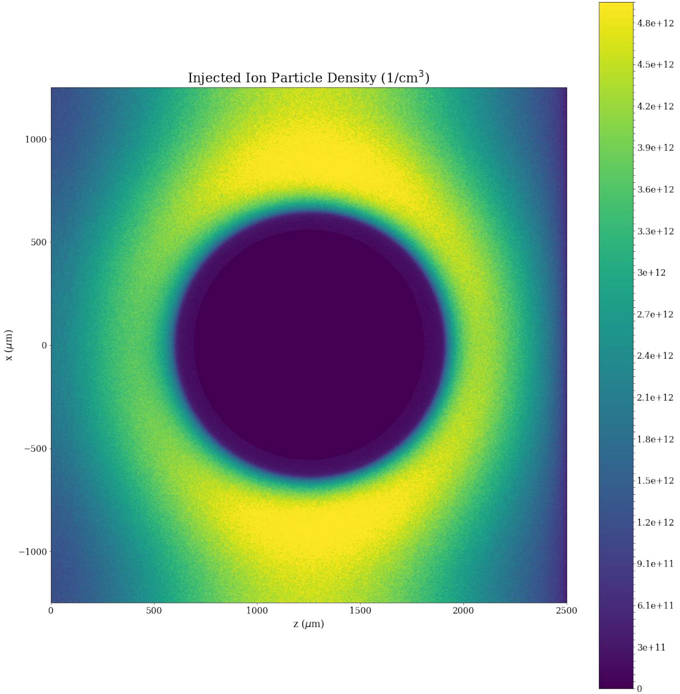

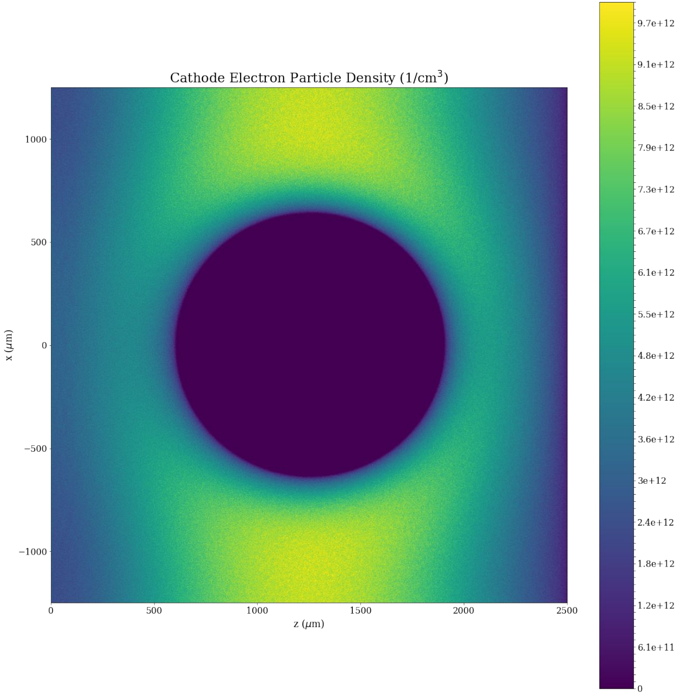

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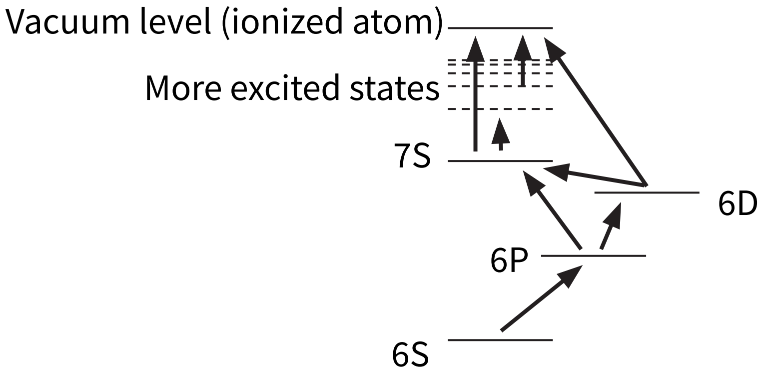
Simulations of ignited Cs plasmas

- Cs plasmas are sustained by "multi-step ionization", where electron impacts first excite, then ionize, Cs atoms
- We work with collaborators at Sandia National Labs to track electrons, neutral Cs atoms, 52 excited Cs states, and Cs ions and the reactions between them
- Obtain much higher fidelity than any previous model



Reactions	Cs* = 52 excited states
Inelastic	*Radiative*
$e^- + Cs \rightarrow e^- + Cs^+ + e^-$	$Cs^* \rightarrow Cs^{**}$
$e^- + Cs^* \rightarrow e^- + Cs^+ + e^-$	*Elastic*
$e^- + Cs \leftrightarrow e^- + Cs^*$	$e^- + Cs \rightarrow e^- + Cs$
$e^- + Cs^* \leftrightarrow e^- + Cs^{**}$	$e^- + Cs^* \rightarrow e^- + Cs^*$
	$Cs^+ + Cs \rightarrow Cs^+ + Cs$

Cs* = 52 excited states

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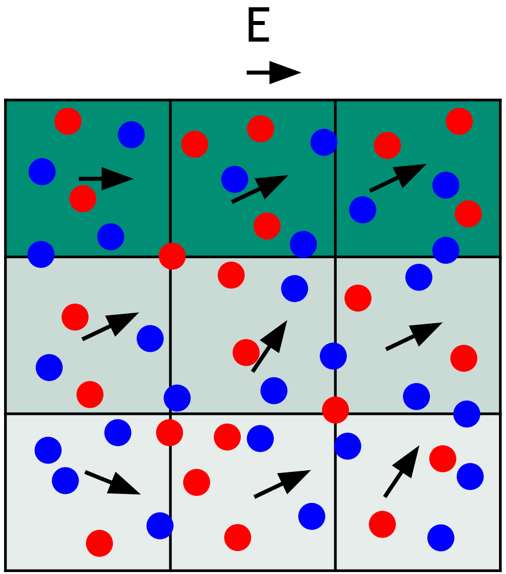
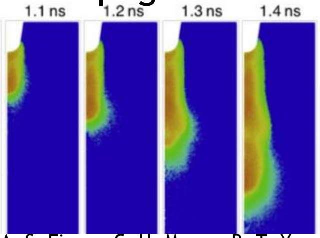
Simulations with Aleph at Sandia National Laboratories

- 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.
- 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.

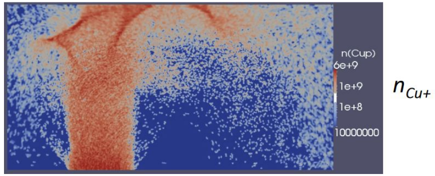


Streamer Propagation



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. Crozie International Conf. on Numerical Simulation of Plasma Beijing, China (2013).

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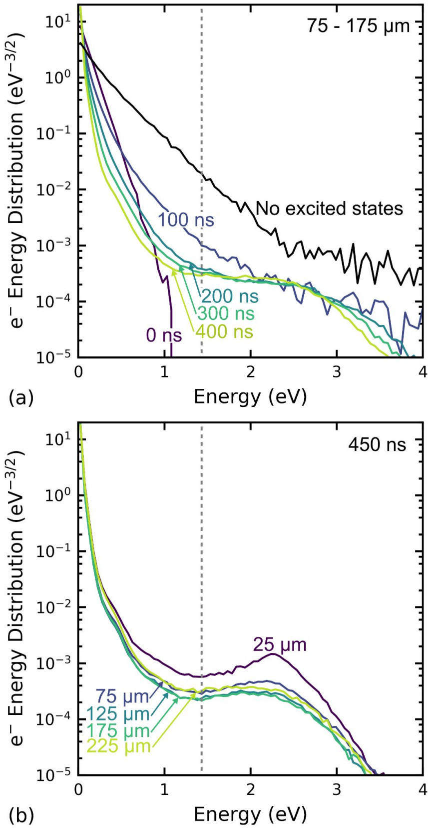
Results - Electron Energies

- Electron energy distribution functions (EEDFs) reflect electron evolution in the presence of excitation and ionization events
- As plotted, Maxwellian distributions are linear
- The strong nonlinearity observed is a result of multistep ionization processes
- All previous models have assumed Maxwellian energy distributions, a clear shortcoming of their models



Parameters: 1.82 V, p_{Cs}=113 mTorr, 10 A/cm^2 emission

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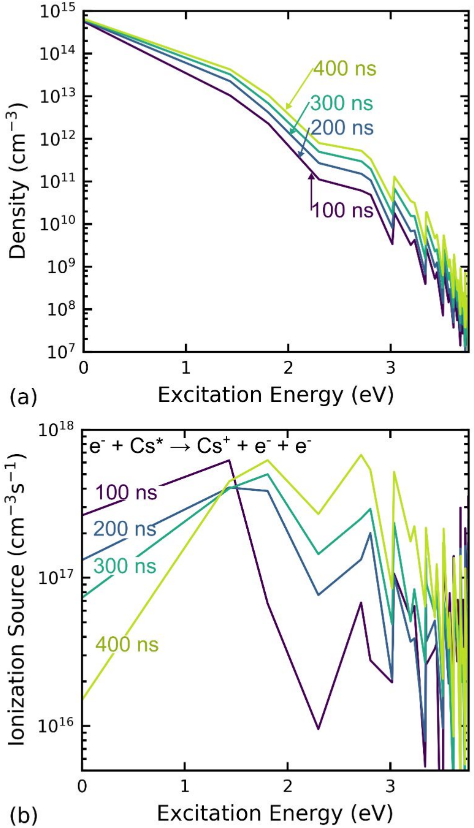
Results - Level Populations

- The network of electron-collision and radiative reactions among Cs excited states creates complex density variations per state
- Electron impact ionization occurs from a variety of levels, with the majority of ionization from levels above the first excited state
- These ionization rates impact whether a given voltage and pressure will remain ignited
  - We find no evidence of a “double sheath” where $J < J_{sat}$ systems remain ignited
  - In these cases spatial inhomogeneity is likely dominant



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Conclusions

- Particle-in-cell simulations are a powerful, high-fidelity tool for simulations of plasma (and vacuum) thermionic converters
- Modern supercomputers and GPUs have sufficient power to simulate experimental systems
- Modern Electron has demonstrated Thermo Electron’s plasmatron device operation in simulation
- Sandia National Laboratories and Modern Electron have demonstrated an ignited Cs-plasma converter in simulation

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Questions?

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- National Energy Research Scientific Computing Center
  - U.S. Department of Energy Office of Science User Facility at Lawrence Berkeley National Laboratory
  - NERSC award FES-ERCAP0022235

- Modern Electron:
  - Founded 2015, Seattle area
  - Backed by Bill Gates and others
  - Team of 50
- We're hiring!
  - modernelectron.com/careers/
  - peter.scherpelz@modernelectron.com

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