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THE UNIVERSITY OF NEW MEXICO

Photoionization and photoemission in helium and helium/nitrogen mixtures

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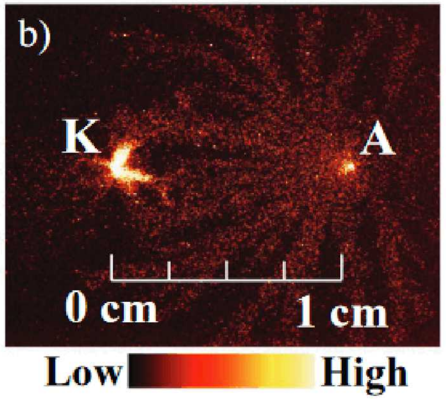
Light emission in gas discharges

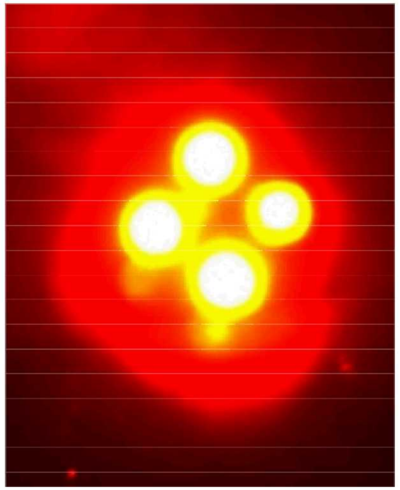
Light emission is a defining characteristic of plasma discharges

In spectroscopy, used to determine discharge gas participants, species densities, and charged particle densities

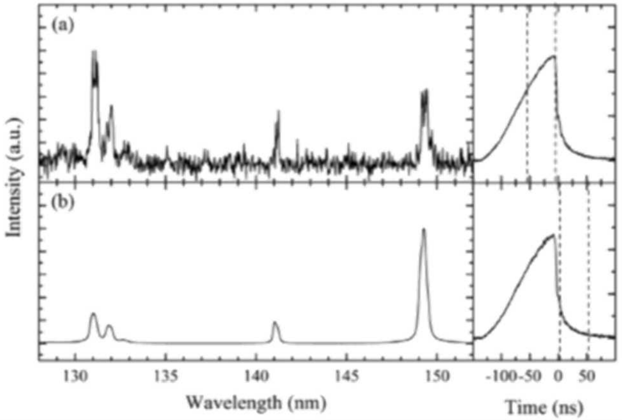
Some discharges, such as positive streamers in air, are influenced by energetic photons in the plasma.

High speed imaging of streamer formation





Four channel microdischarge array



Vacuum ultraviolet emission spectra in a nitrogen discharge

M. Hopkins, *et al.*, 7th Annual Plasma Science Center Annual Meeting, 2016.
J. Stephens, *et al.*, Plasma Sources Sci. Technol., **25**, 025024, 2016.
A. Fierro, *et al.*, J. Phys. D: Appl. Phys., **45**, 495202, 2012.

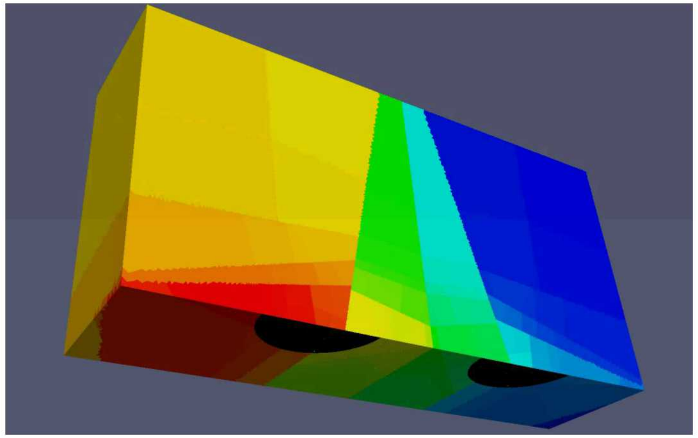
ALEPH
Advanced Plasma Transport & Kinetics

Unstructured FEM ES Particle-In-Cell model for non-equilibrium plasmas

- Trilinos used to solve Poisson eqn. (w/ML multigrid preconditioner)
- Massively parallel (scales to >50K cores) w/dynamic load balancing and reweighting of particles

Surface physics models:

- Fowler-Nordheim, thermionic, and Murphy-Good e^- emission models
- Sputtering, surface charging, Auger-neutralization, SEE, photoemission, sublimation/vaporization
- Can use time-varying flux files (e.g., from data or pre-computed)



Direct Simulation Monte Carlo collision physics:

- Elastic, charge exchange, chemistry (dissociation, charge exchange, etc.), excited states (w/ radiative decay & self-absorption), ionization, Coulomb collisions (Nanbu)

Slide courtesy C. Moore and M. Hopkins, Sandia National Laboratories

Discrete photon method with line broadening

- For each excited particle in the simulation, evaluate

$$R_1 < 1 - e^{-\Delta t/\tau}$$

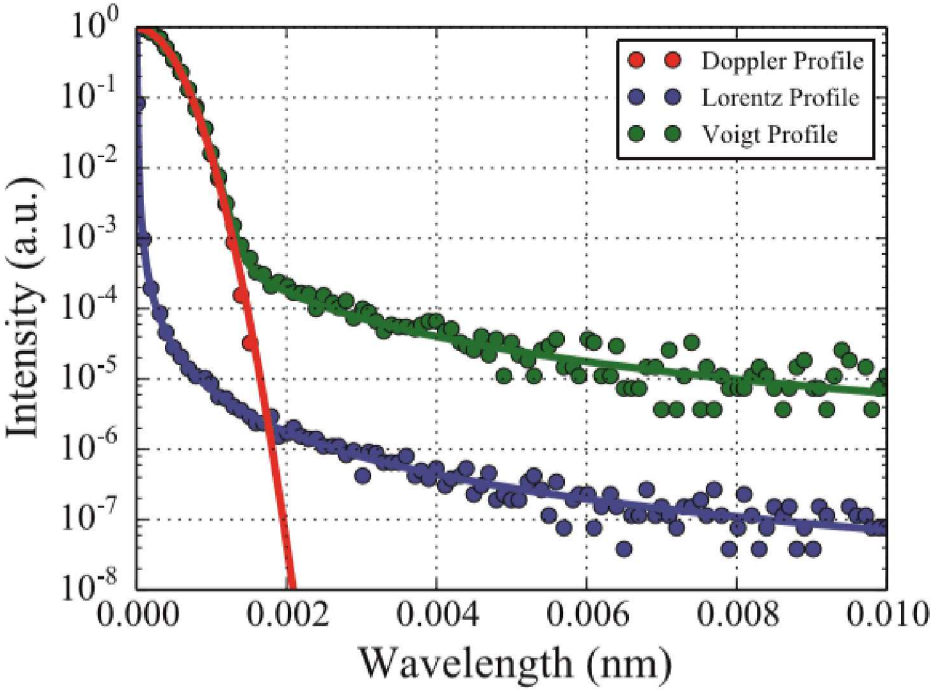
- Compute the natural line width using

$$\lambda_s = \tan[(R_2 - 0.5)\pi]\Delta\lambda_L + \lambda_0$$

with $\Delta\lambda_L = \lambda_0^2 \frac{1}{2\pi c\tau}$ to account for natural line broadening

- Final wavelength accounting for doppler shift

$$\lambda_f = \frac{(c + \hat{\boldsymbol{v}}_{\boldsymbol{ph}} \cdot \boldsymbol{v}_{\boldsymbol{p}})\lambda_s}{c}$$

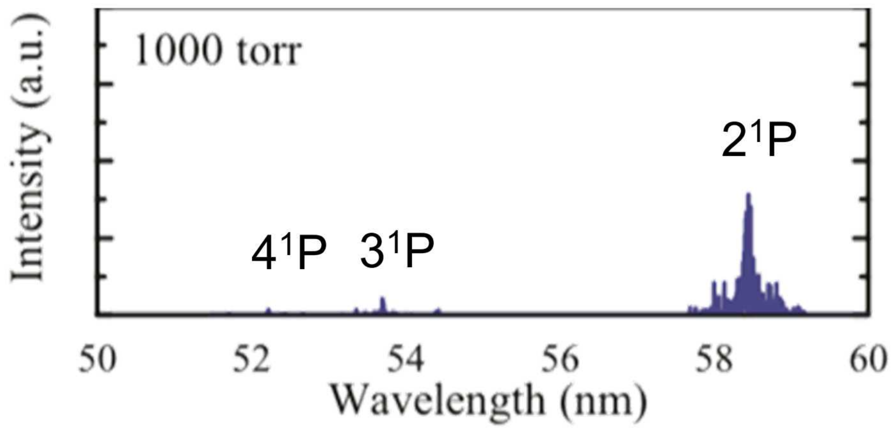


A. Fierro, *et al.*, *J. Phys. D.: Appl. Phys.*, **50**, 065202, 2017

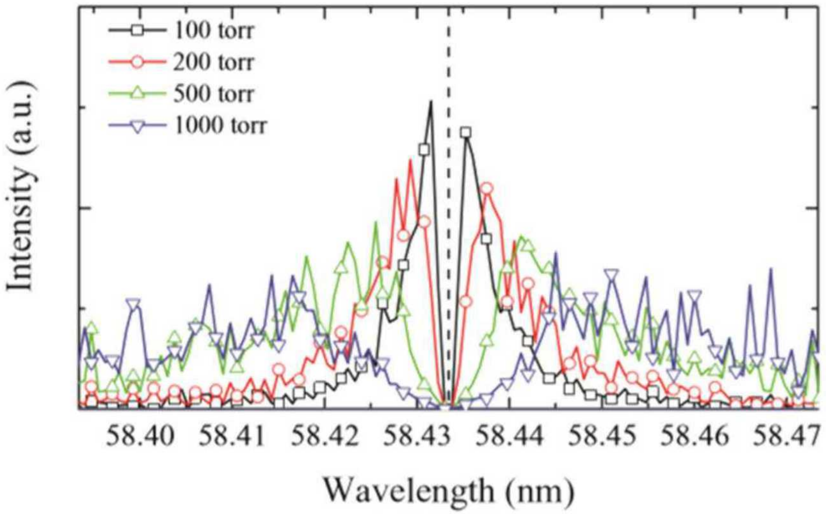
Self-absorption in helium

A key physics mechanism to include is self-absorption for the resonance states of the helium atom

- $He(2^1P)$, $He(3^1P)$, and $He(4^1P)$
- These excited states exhibit short lifetimes (~ 1 ns) and emit energetic photons (E > 19 eV)
- However, they suffer from self-absorption that effectively increases their lifetime and only photons with wavelengths in the wings of the emission profile escape

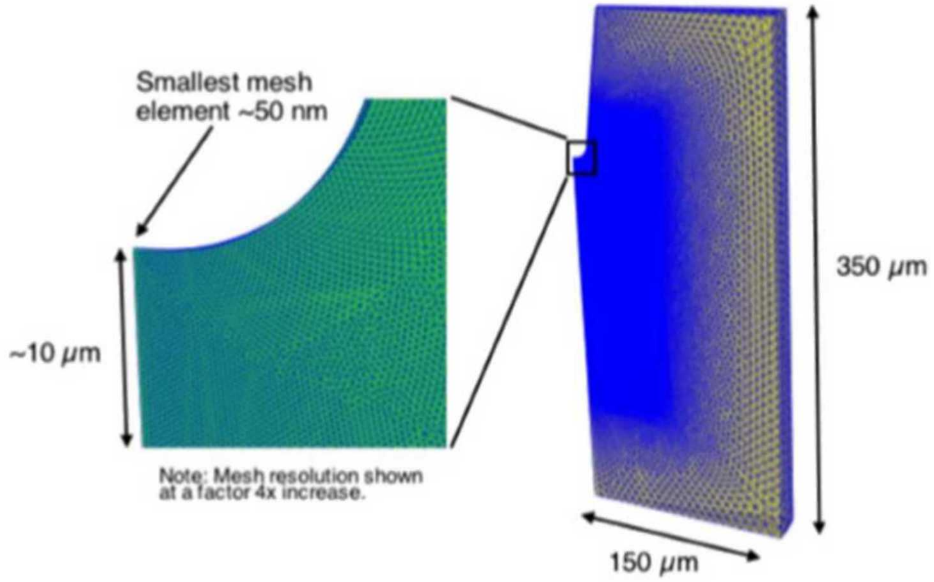


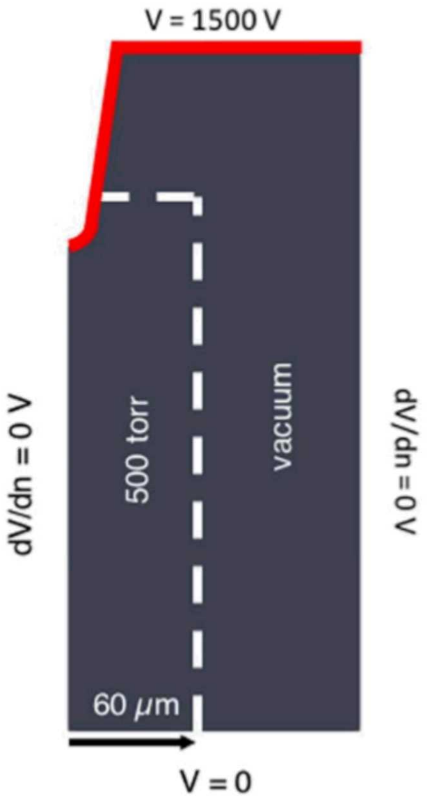
A. Fierro, *et al.*, *J. Phys. D.: Appl. Phys.*, **50**, 065202, 2017



Photoionization in He/N_2

Studied photoionization in He/N_2 mixtures in a fully-resolved three-dimensional simulation. Contained over 160 million elements and ran on 5000 processors for 8 days. Total operating pressure of 500 torr.





A. Fierro, *et al.*, *Plasma Sources Sci. Technol.*, **27**, 105008, 2018

Discharge evolution

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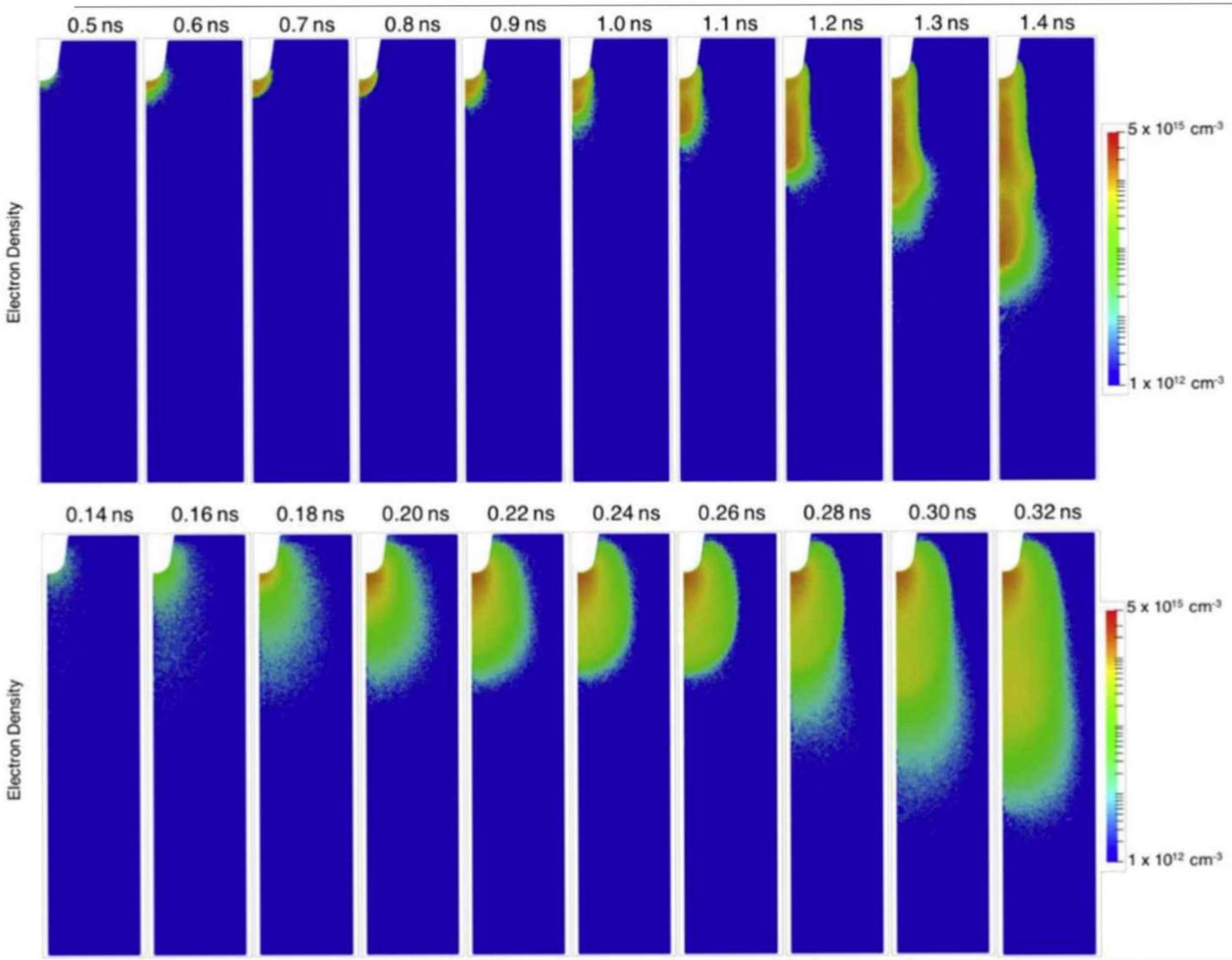
90% N_2, 10% He

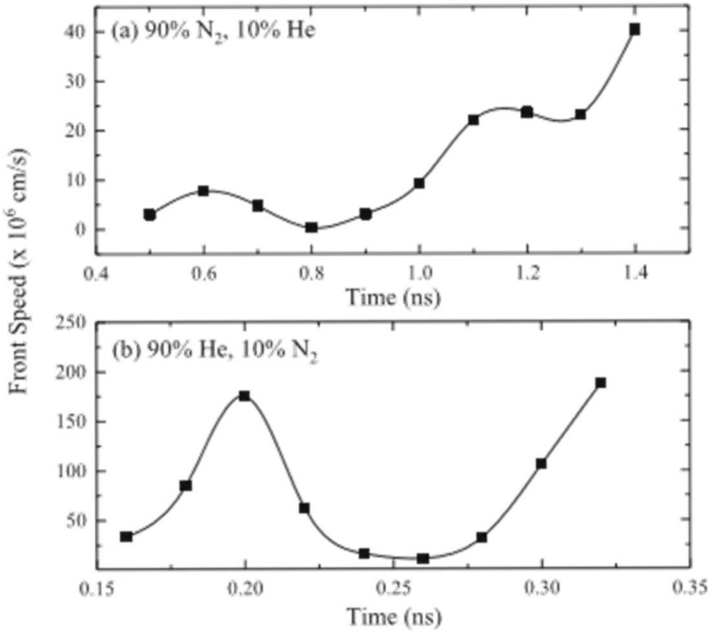
90% He, 10% N_2



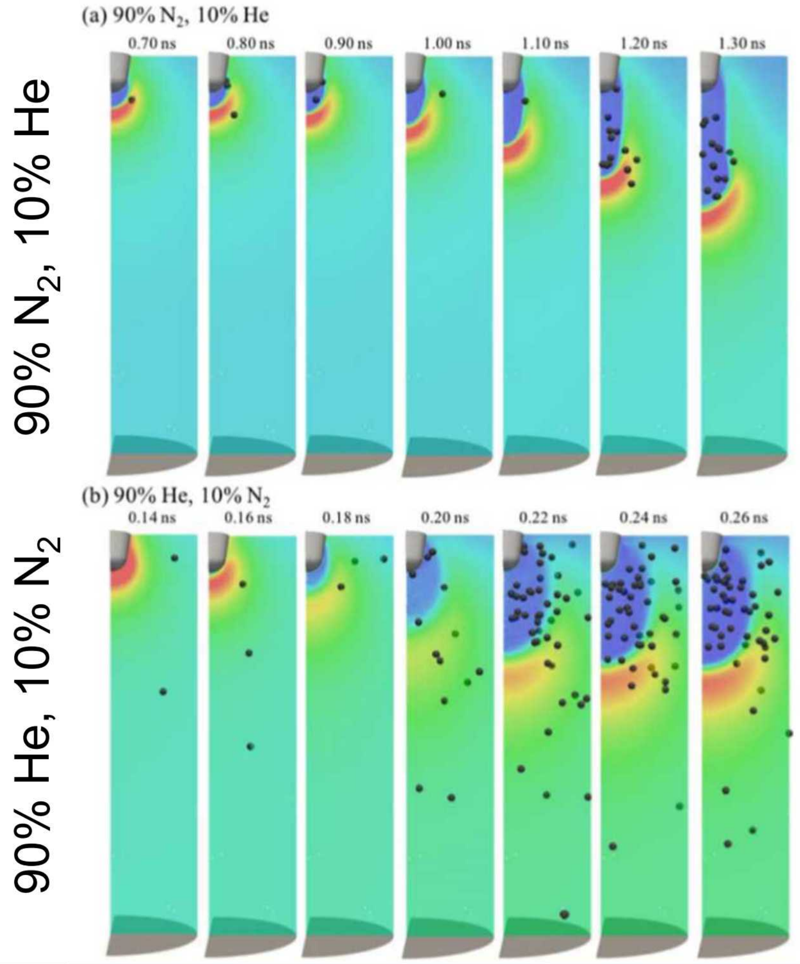
Discharge evolution is shown for 2 He/N_2 mixture cases:

- 90% N_2, 10% He
- 90% He, 10% N_2

Speed is faster in the mostly helium case



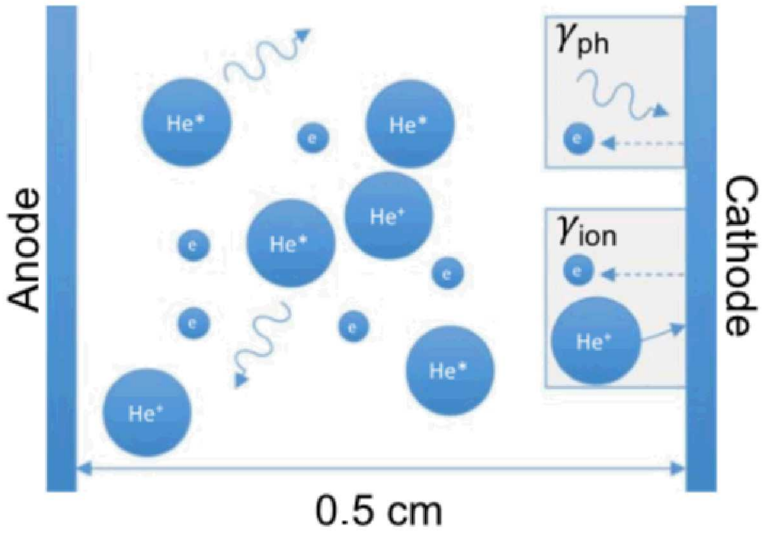
Location of photoionization events



- The location of the photoionization events at different times is shown by the black spheres relative to the magnitude of the electric field (the colormap).
- Changing the gas mixture changes among other things, ionization rates, electron mobilities, production of excited species.
- From the location of photoionization events, however, it appears that photoionization is more non-local in the higher helium partial pressure.

A. Fierro, *et al.*, *Plasma Sources Sci. Technol.*, **27**, 105008, 2018

Influence of photoemission

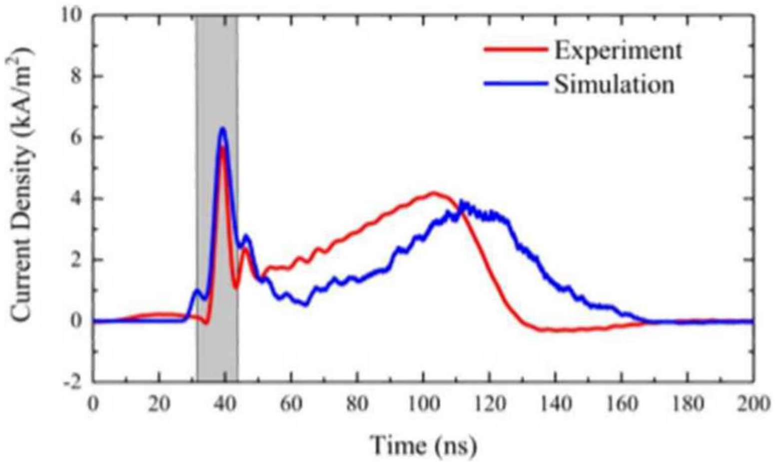


A. Fierro, *et al.*, *Plasma Sources Sci. Technol.*, **28**, 055012, 2019

1D simulation in pure helium at 75 torr that includes two important surface mechanisms:

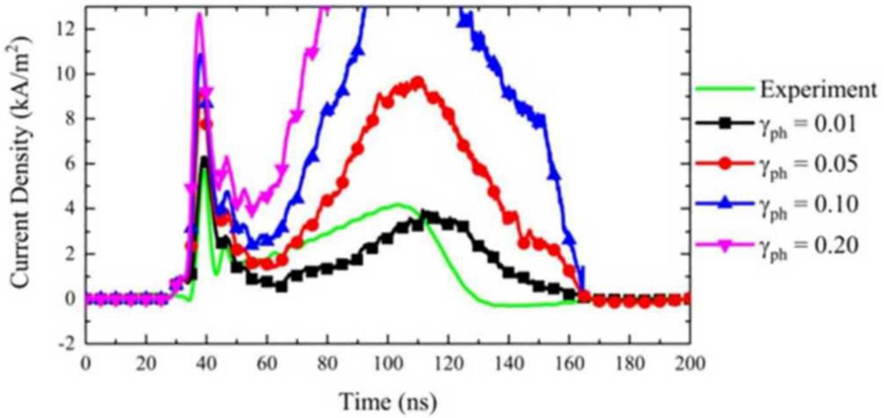
- Photoemission from the surface
  - $\gamma_{ph} = Const$ for $\lambda < 100$ nm
- Secondary emission due to ion impact
  - $\gamma_{ion} = Const$ for all ions

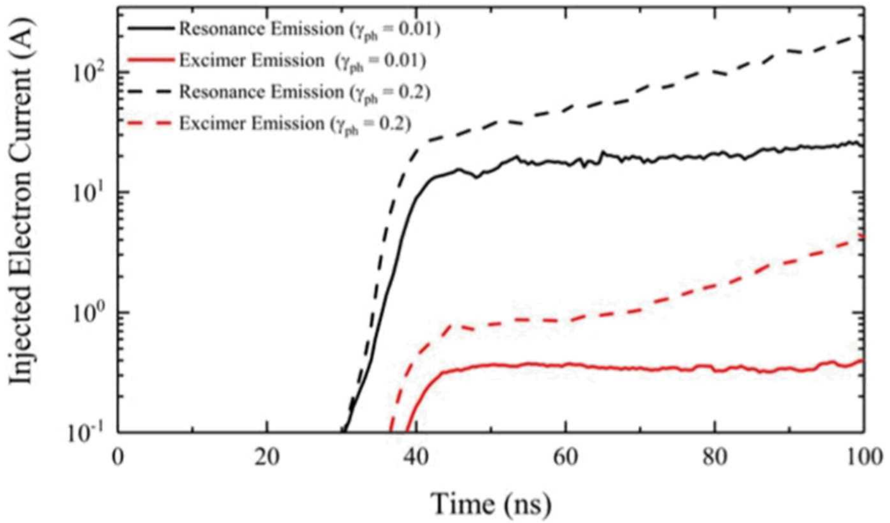
Compared the simulation with an experiment to find best fit parameters for the photoemission and secondary yield from ion impact.



Influence of photoemission

- Varying the photoemission yield coefficient from 0.01 to 0.2 demonstrated different current waveforms with a best fit parameter using $\gamma_{ph} = 0.01$
- The photoemission yield has a large impact in both early and late stages of the discharge.





- Also examined the influence of the helium excimer (He_2*) versus the atomic resonance emission.
- While radiation trapped, the resonance emission is still more responsible for injected electron current at the cathode than the helium excimer.

Conclusions

A model has been developed that can discretely track photons in the simulation volume and accounts for photon-gas interactions and photon-surface interactions. However, this comes with a large computational price – Fully 3D simulations are even more expensive!

Photoionization studies in different He/N_2 mixtures showed that the location of photoionization events in the mostly helium case were more non-local than in the more nitrogen case.

A one-dimensional pulsed discharge simulation in pure helium showed the large influence of photoemission from the surface on the discharge current. Furthermore, the resonance emission accounted for more injected electron current due to photoemission than the helium excimer state.

Future

Comparison of fundamental photoionization simulations with experimental data

Incorporation of highly Doppler shifted emission from fast excited species