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Striations in PIC Simulations of Atmospheric Pressure Narrow Gap He/H_2O rf Capacitive Discharges

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Narrow gap, atmospheric pressure capacitive discharges (APCDs) have wide bio-medical and materials processing applications. A common feedstock is helium with a small molecular gas admixture. He/H_2O discharges are of particular interest. Most APCDs have been studied using fluid simulations which neglect kinetic effects that may be important. We therefore conducted kinetic 1D3v particle-in-cell (PIC) simulations of a narrow gap APCD sustained in helium with 2% H_2O, the saturation level of water vapor in air at 300 K. We observed stationary striations in the bulk region not observed in our previous He/N_2 PIC simulations of comparable discharges [1].

The base He/H_2O chemistry was modified to make it more similar to the He/N_2 chemistry to determine the source of the striations. The e-H_2O scattering, attachment, vibrational and rotational excitation rates were set to zero and negative ions were eliminated, but this did not suppress the striations. However, reducing the electron-ion recombination rate coefficient by a factor C_{rec}<<1 did suppress the striations. We conducted PIC simulations of a 1 mm gap APCD sustained at 27 MHz with a current density of 0.23 A/cm^2 using the modified He/H_2O chemistry in which C_{rec} was varied from 0.05 to 5. Striations occured for $C_{rec} \geq 0.5$ but not for $C_{rec} < 0.5$. The results are interpreted in terms of a system in which the balance between direct ionization and recombination loss determines the bulk plasma equilibrium. Perturbing the equilibrium, the striations are consistent with an ionization instability induced by non-local electron kinetics that form a spatially-varying high energy tail of the electron energy distribution. This causes the ionization rate coefficient, K_{iz}, to decrease with increasing electron temperature T_e and reduced electric field E/N in the instability regime. (See Fig. 1). A theoretical instability criterion was developed that showed excellent agreement with the PIC results. We found that discharges with large volume losses (compared to surface losses) tend to be unstable while those with small volume losses tend to be stable.

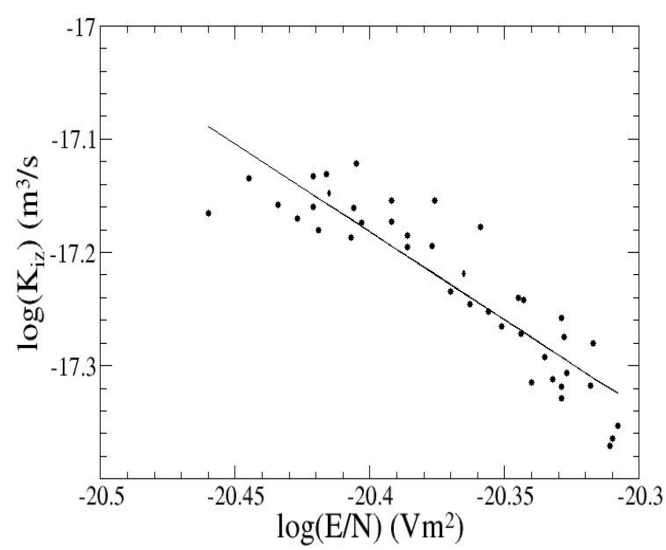


Fig. 1 – Log plot of ionization rate coefficient K_{iz} vs. E/N in the bulk region of an unstable discharge with C_{rec}=1. Solid line is least squares linear regression fit.

References

[1] E. Kawamura, M.A. Lieberman, A.J. Lichtenberg, P. Chabert and C. Lazzaroni, Plasma Sources Sci. Technol., **23**, 035014 (2014).

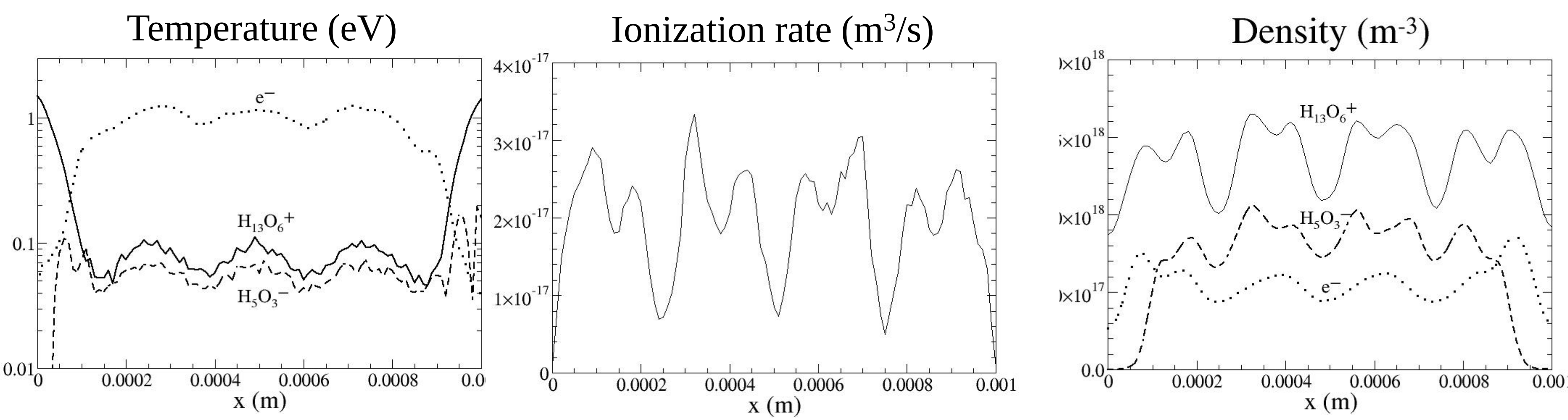
DOE Center for Control of Plasma Kinetics

Highlight

Center for Predictive Control of Plasma Kinetics: Multi-Phase and Bounded Systems
Department of Energy Plasma Science Center

STRIATIONS IN PIC SIMULATIONS OF ATMOSPHERIC PRESSURE DISCHARGES: A NEW INSTABILITY REGIME

- **Narrow gap, atmospheric pressure plasmas are critical components of energy and biomedical applications, and reproducibility requires stability.**
- **Particle-in-Cell simulations reveal that the stability of narrow gap He/H_2O = 98/2, discharges (27.12 MHz) is determined by a fine balance between bulk ionization and recombination processes due to kinetic effects.**
- **The ionization rate is out of phase with the electron temperature and electric field, due to non-local transport of electrons, important even at 1 atm.**



- **Results of PIC simulations showing striation instabilities.**

Ion velocity distributions in argon and helium discharges: Comparison between numerical simulation and experimental data

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Optimizing low temperature plasmas (LTPs) for materials processing and energy applications requires fine control over ion velocity distributions. (IVDs). This is particularly true for those processes which are activated by ion bombardment, such as etching and plasma catalysis. Although the majority of the energy imparted to ions comes from the sheath, the angular distribution of ions striking the surface is limited by the shape of the IVD entering the sheath from the bulk plasma. Recently, IVDs in argon plasmas were measured making use of a planar one-sided probe.[1] These experimental data allow for careful benchmarking of simulations of IVDs and, indirectly, of elastic and charge-exchange differential cross sections, which determine the angular IVD. Since the fundamental data for both charge exchange and elastic scattering collisions required to perform the calculations is sparse, we have developed an approximate numerical model of differential cross sections for these collisions.[2]. Good agreement between measured [1] and simulated IVDs [3], as shown in Fig. 1, validates both the fundamental data and the numerical methods. These techniques can now be extended to investigate plasma surface interactions.

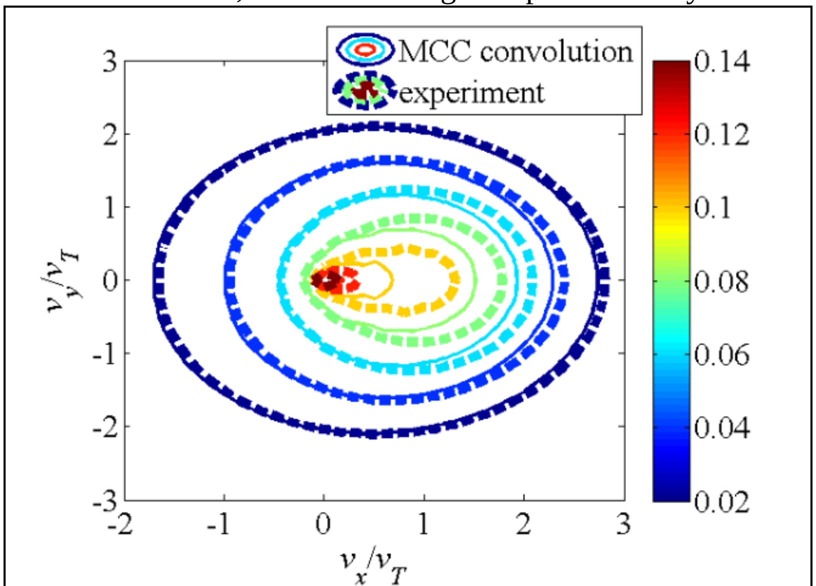


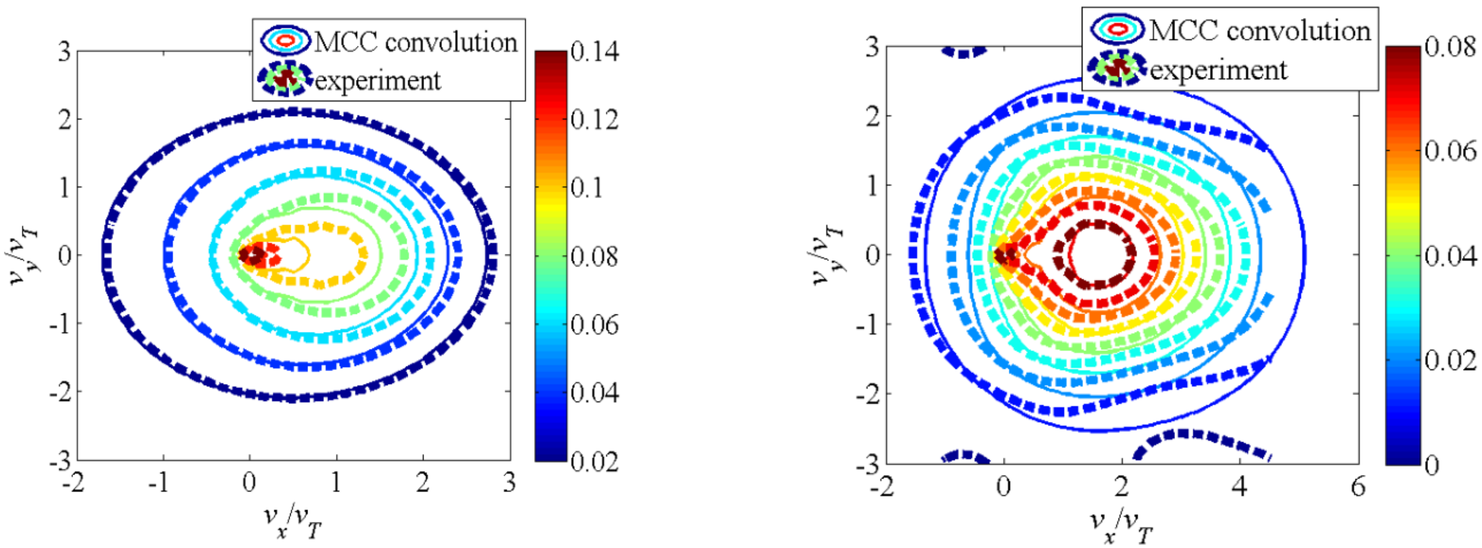
Figure 1 – Comparison of calculations with experimental data for IVD in argon. E/P =9 V/cm-Torr p=0.2Torr

References

[1] A S Mustafaev, V S Sukhomlinov and M A Ainov, Technical Physics **60**, 1778 (2015).
[2] H. Wang, V S Sukhomlinov, I D Kaganovich, A S Mustafaev "Monte Carlo simulations of ion-atom collisions for ion velocity distributions" submitted to Plasma Sources Science and Technol. (2016).
[3] H. Wang, V S Sukhomlinov, I D Kaganovich, A S Mustafaev, "Ion velocity distribution functions in argon and helium discharges: detailed comparison of numerical simulation and experimental data" submitted to Plasma Sources Science and Technol. (2016).

ION VELOCITY DISTRIBUTION FUNCTIONS IN ARGON AND HELIUM DISCHARGES

- Control of ion velocity distributions (IVDs) is critical to optimizing low temperature plasmas for energy and material processing applications.
- Using a flat probe IVDs were measured with excellent angular resolution. These IVDs were simulated with a particle-in-cell simulation.
- To match experimental data a more accurate model for ion-atom scattering cross sections was implemented.
- The validated simulations can be applied to optimizing LTP energy systems.



- Angular IVDs simulated by PIC and measured by flat probe. (left) Argon, (right) Helium.

September 2016 **HIGHLIGHT**

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