## Electrical Gas Discharges Research Group:

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**High frequency gas discharge operation in gas mixtures.** — Electric gas discharges, driven by periodic voltage waveforms in the radio frequency range, have proven to be useful fundamental tools for a wide variety of high technology applications. Even in the case of a single-component inert gas environment, the nonlinear and nonequilibrium electron and ion dynamics provide complex pathways for gas-phase and surface reactions such as etching, atomic layer deposition, implantation, activation, etc. The use of gas mixtures, typically with one reactive (molecular) and one inert (noble gas) component, allows the utilization of a variety of chemically active plasma particles for gas treatment and chemically assisted surface processing while maintaining stable plasma operation. In the case of the $Ar/O_2$ mixture at low pressures, we have applied phase-resolved optical emission spectroscopy (PROES) measurements to determine the spatio-temporal distribution of electron impact excitation processes with nanosecond time resolution. A particle-in-cell with Monte Carlo collisions (PIC/MCC) simulation model was constructed and validated against the experimental data. We have shown that, for otherwise identical discharge conditions, the operating characteristic strongly depends on the driving frequency, as shown in Figure 1 for the measured electron impact excitation rate. This results from the frequency-dependent contributions of the Ohmic and ambipolar terms to the electron power absorption[1]. At atmospheric pressure, a plasma jet configuration operated in a $He/O_2$ mixture was studied using a newly developed hybrid (fluid + Monte Carlo) simulation code, which preserves the non-locality of the electron dynamics while exploiting the computational efficiency of continuum models. The simulations have been validated against previous measurements and have shown that the observed saturation of the atomic oxygen concentration along the jet is due to the competition of electron impact mediated dissociation and chemical reactions favoring ozone formation[2].

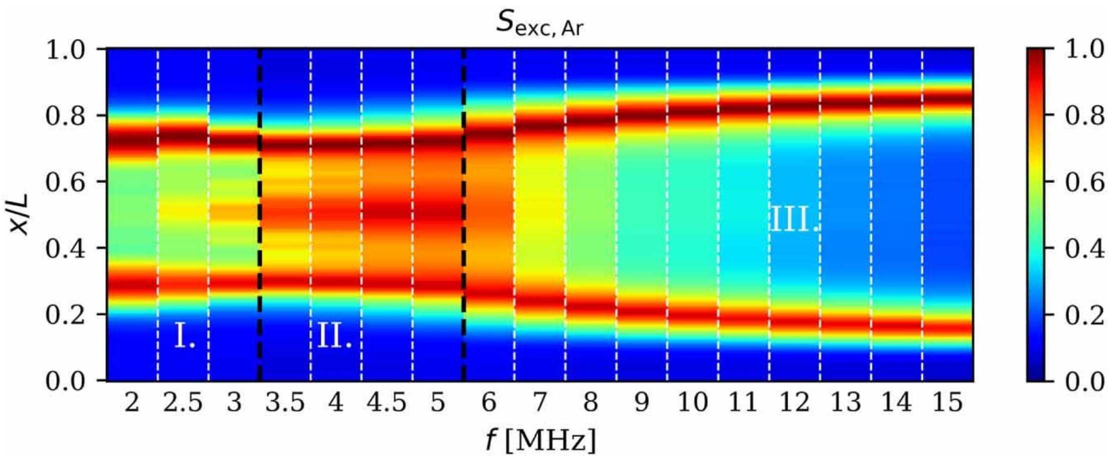


**Figure 1.** Time averaged results for the electron impact excitation rate from the ground state into the Ar $2p_1$ level measured by PROES [arb. units] for different driving frequencies *f*. Discharge conditions: 70% Ar/30% $O_2$ gas mixture, $L$ = 2.5 cm, $p$ = 120 Pa, $V_{pp}$ = 350 V.

**Self-consistent calculation of optical emission spectra.** — The spectral analysis of the emitted light is one of the most traditional methods of gas discharge diagnostics. It is undoubtedly useful for qualitatively determining the composition of the plasma. In principle, however, the intensity ratios of the detected spectral lines carry very detailed information about the plasma parameters, such as the density and energy distributions of all plasma species. Unfortunately, the relationships are very complex and indeterminate due to the multitude of reactions between the excited states, the plasma electrons, and the photons in the plasma. We have developed a computational framework for the calculation of the optical emission spectrum of a low-pressure argon capacitively coupled plasma (CCP) based on the coupling of a particle-in-cell/Monte Carlo collision simulation code with a diffusion-reaction-radiation code for 30 Ar I excited levels. The simulations were benchmarked against our experimental results on the intensities of 15 selected emission lines and tunable diode laser absorption (TDLAS) measurements on the density of Ar atoms in the metastable 1s5 state, with good overall agreement. The simulations provide insight into the contributions of various reaction channels to the excitation and de-excitation rates, including electron collisions, radiative processes, neutral quenching, and stepwise ionization[3]. The simulation results include the relative intensities of the selected spectral lines as well as detailed distributions of several plasma parameters, such as the electron density and the energy distribution function (EEDF). These results were used to train artificial neural network (ANN) and kernel regression for functional data (KRFD) machine learning (ML) models. The goal of these pre-trained models is to provide a diagnostic tool that can predict electron density and EEDF from measured emission spectra. The robustness of the ML models developed in this study was then tested. It was found that the ANN-based ML model was able to predict the normalized EEDF reasonably well at a pressure of 20 Pa or lower for the experimentally obtained relative line intensities and gas pressure. However, under the same conditions, the predictions of the KRFD-based ML model showed relatively large errors, while the performance seemed to be better at high pressure[4].

***References:***

[1] https://doi.org/10.1088/1361-6595/ad1fd5

[2] https://doi.org/10.1088/1361-6595/ad1f37

[3] https://doi.org/10.1088/1361-6463/ad4e42

[4] https://doi.org/10.1116/6.0003731