Particle-in-Cell Simulations of Multi-Peak Ion Impact Energy Distributions in RF Capacitively-Coupled Discharges using the hPIC2 Code

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Background

- Capacitively-Coupled Plasma (CCP) discharges exhibit complex behavior in their ion impact energy distribution function (IED), exhibiting multiple peaks at different discharge regimes, observed both experimentally and computationally.
- In this work we analyze the occurrence of this multi-peak structure of the IED through Particle-in-Cell simulations using the hPIC2 code by Meredith [1] of an argon CCP operating between 20 and 200 mTorrs of background neutral pressure.
- We also use the original Koidl [2] model exploring this phenomena, as well as a modification using a Monte Carlo random walk, and compare the results of all three models.

Methodology

Koidl [2] uses a parametric model for the sheath electric field ***E(x,t)*** with normalized time τ and normalized position ***s***. We extend this by adding a 1D Monte Carlo ion trajectory model.

$$E(x,t) = E_0' x^{\nu}(1 - cos(\omega_{rf} t)) \qquad \tau = \omega_{rf} t \qquad s = \frac{x}{d}$$

We solve the differential equation (right) for the ion motion given starting phase ρ_0 using scipy.integrate.solve_ivp (RK45).

$$\frac{d^2 s}{d\tau^2} = (\nu + 1)\eta s^{\nu}(1 - cos(\tau + \rho_0))$$

$$E_{impact} = \frac{1}{eU_b}\frac{(dx/dt)^2}{2m_i} = \frac{(ds/d\tau)^2}{2\eta}$$

$$P_{impact}(S_0) = exp(-\alpha(1 - S_0))$$

The resulting ion impact energies E_{impact} are binned in a histogram using impact probability P_{impact} as a weight, to calculate the IED. This approximates ion-neutral collisions by assuming an expotential profile in the ion start positions.

The following parameters are used in both the Koidl and Monte Carlo models:

1. Sheath size ***d***, obtained from hPIC2 electric potential profile.
2. Sheath electric field parameter ν.
3. Normalized sheath size α, the sheath size in units of the number of ion mean free paths λ_{mfp}.

$$\alpha = \frac{d}{\lambda_{mfp}}$$

4. Effective potential U_b, the time-averaged integrated electric field.

$$U_b = \frac{1}{T_{rf}}\int_0^{T_{rf}}\int_0^d E(x,t)\,dx\,dt = \frac{d^{\nu+1}E_0'}{\nu + 1}$$

5. Discharge scaling parameter η. Physically, this is the ratio between the effective potential U_b and the potential energy of an ion oscillating across the sheath at the RF potential.

$$\eta = \frac{eU_b}{m_i \omega_{rf}^2 d^2}$$

$$d_{coll} = \frac{-ln(1 - \xi)}{\alpha} \qquad \lambda_{mfp} = \frac{1}{n\sigma}$$

The Monte Carlo model predetermines a collision distance d_{coll}, and attempts to integrate the equation of motion until either d_{coll} has been traversed or the ion has impacted a wall. ξ is a uniform random variable over (0,1).

The ion mean free path depends on the gas density and interaction cross section. The ion-neutral interactions considered in this study follow the methodology of Phelps [3], where interactions are either backscattering or isotropic scattering.

At sufficient energy, most of the backscattering interactions are due to charge exchange. In our Monte Carlo model, these charge exchange collisions reset the ion motion to stationary and restart the motion integration, while preserving the RF phase.

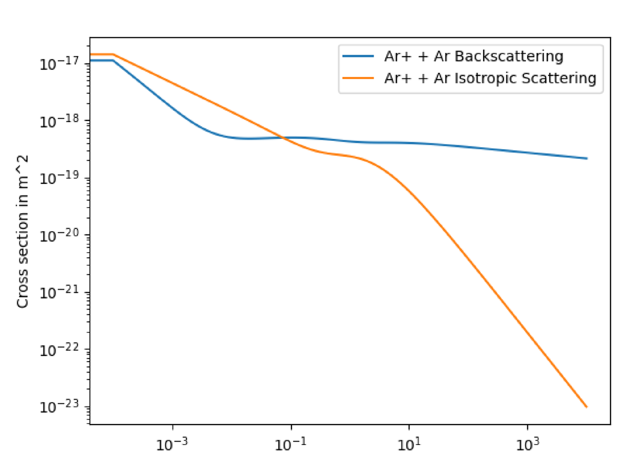

Figure 1: Argon ion – neutral scattering cross sections from Phelps database, www.lxcat.net, retrieved May 2, 2024. The backscattering cross section is nearly constant with a value of ~3.5*10^{19} m^2 and at least an order-of-magnitude dominant over the isotropic scattering cross section across the energy range of a few eV to 10^3 eV.

Finally, the Particle-in-Cell code hPIC2 uses the aforementioned Phelps database for ion-neutral interactions, as well as the Biagi-v7.1 database, www.lxcat.net, retrieved on May 2, 2024. The simulations scan over a range of 10 pressures from 20 to 200 mTorr in increments of 20 mTorr, as well as a range of 5 voltages from 200 V to 600 V in increments of 100 V. The discharge gap was 25 mm with one RF (13.56 MHz) electrode. The simulation parameters (ex: number of sample particles for the Koidl and Monte Carlo models, or timestep, RF cycles, particles-per-cell, etc. for hPIC2) are not shown on this poster but will be made available on the github page (bottom right of poster) or at request to the author.

Model Comparison

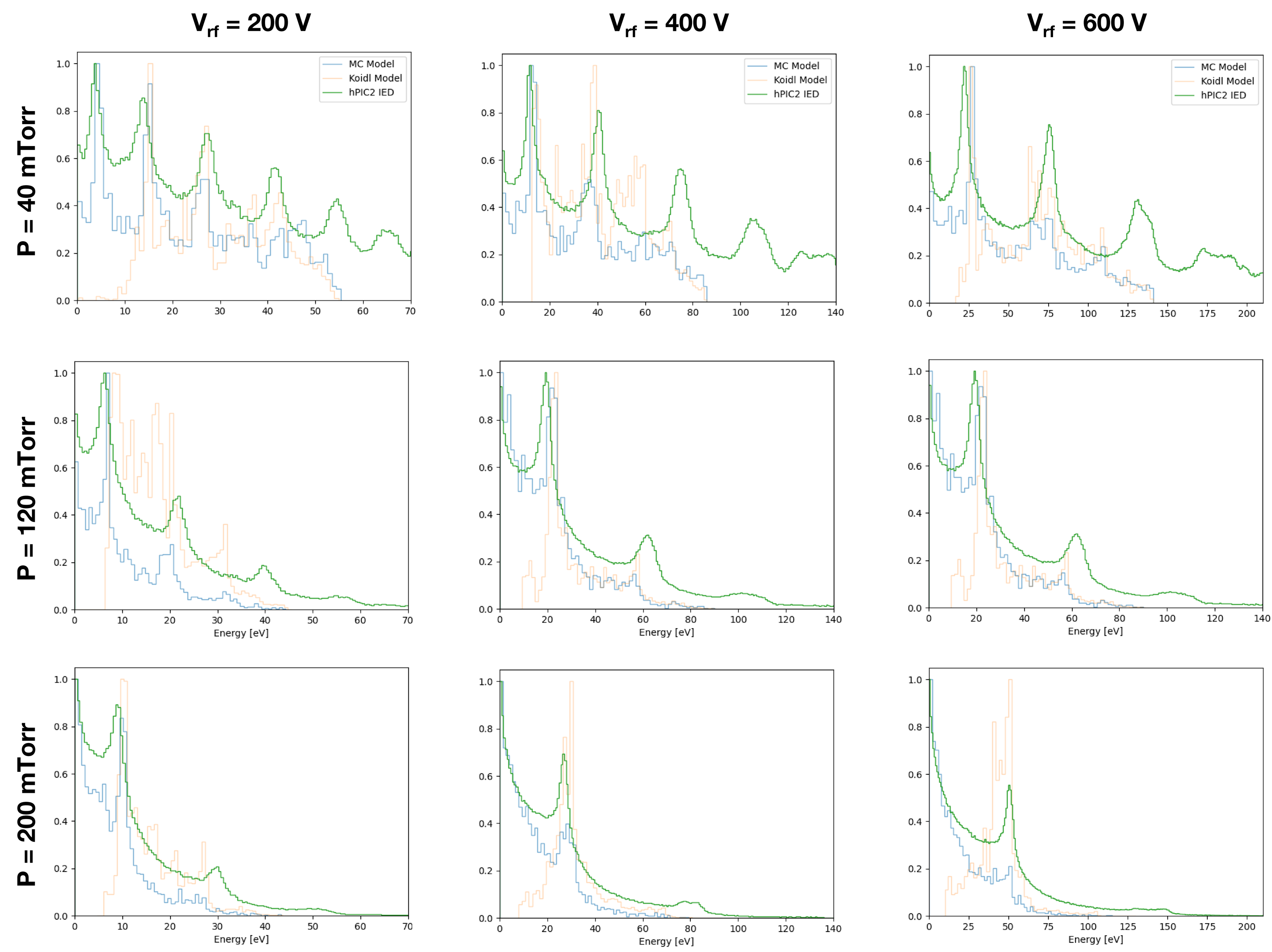

Figure 5: Peak-normalized ion energy distributions (IED) from hPIC2, Koidl model, and Monte Carlo model for pressures of 40, 120, and 200 mTorr, and RF voltages of 200, 400, and 600 V.

Both hPIC2 and the Monte Carlo model feature a zero-energy peak because both models actually track the ions; the Koidl model just assumes a distribution of ions across the sheath to be decreasing exponentially as the distance to the wall decreases. These ions are assumed to be removed due to charge exchange collisions, instead of accounting for the creation of a low energy ion.

On the other hand, the zero-energy peaks with the hPIC2 and Monte Carlo models may not be entirely physically realistic, since at low enough ion energy, there may be three-body recombination processes that take place to remove those ions from the population. The possible effect of considering recombination was beyond the scope of this study.

The Monte Carlo and Koidl models required fitting to the hPIC2 peaks' energies. In the Koidl [2] paper, peak fitting was used to find ν and η, as well as Gaussian smoothing.

The number of peaks increases with both decreasing pressure and with decreasing voltage, which is detailed in Figures 6 and 7.

Discharge Parameter Scaling

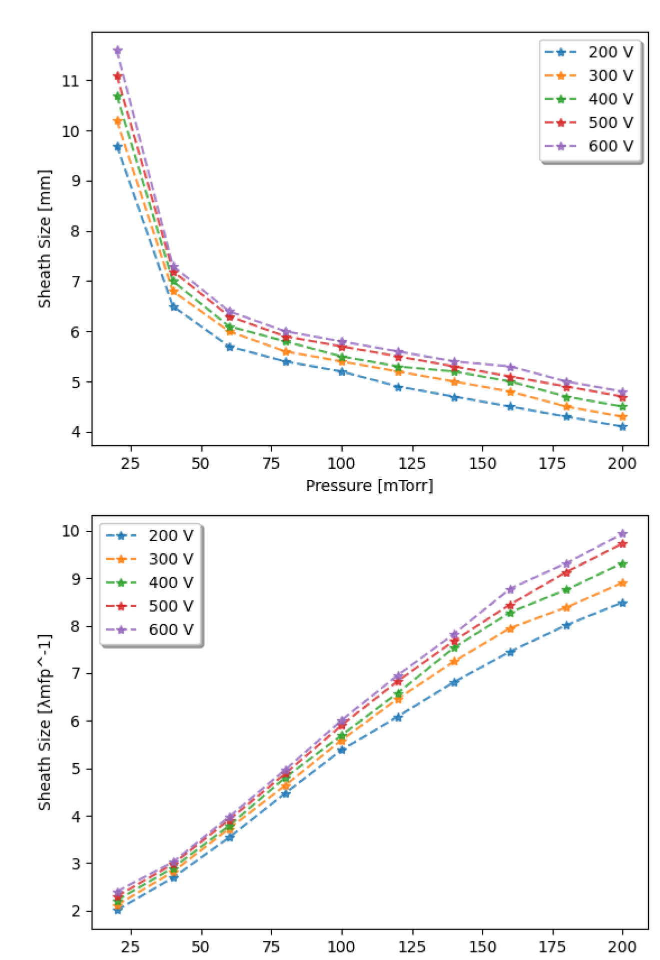

Figure 2: Raw (top) and α, *the* λ_{mfp} - normalized sheath size (bottom), as a function of pressure. Although the raw sheath size decreases as a function of pressure, the effect of increasing pressure on ion mean free path is dominant. The 20 mTorr data points can be considered outliers due to an observed order-of-magnitude drop in the steady-state hPIC2 simulated ion density, possibly due to a numerical or "real" instability.

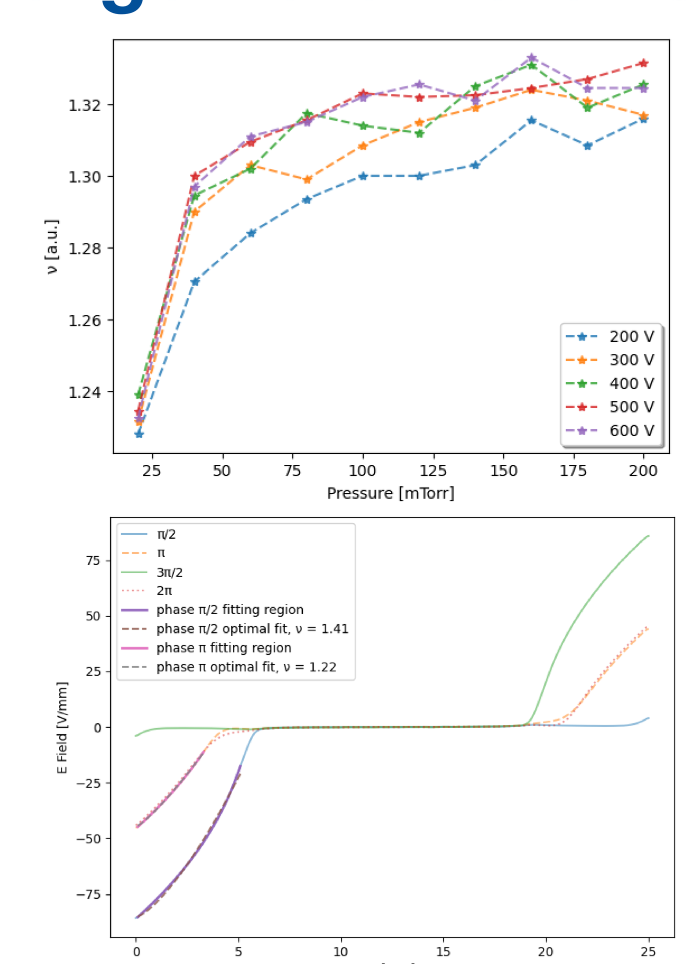

Figure 3: Sheath field parameter ν as a function of pressure (top) and example fitting of ν using hPIC2 Electric field profile for 120 mTorr, 300 V discharge (bottom). The original Koidl [2] paper reported ν values < 1, resulting in a concave down sheath profile. The hPIC2 sheath profiles are concave up due to low-energy ions that are not removed, possibly due to a lack of 3-body recombination reactions, and instead contribute to the electric potential. In Koidl [2], the sheath ion population is assumed to be an exponential drop with characteristic length of λ_{mfp}.

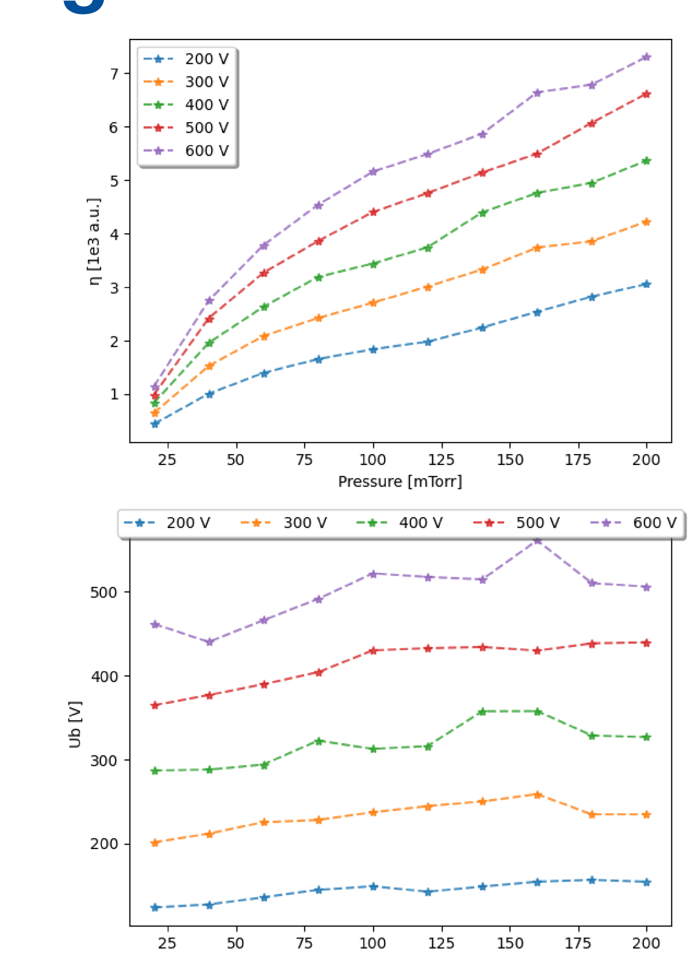

Figure 4: Discharge parameter η (top) and effective potential U_b (bottom) as a function of pressure. The discharge parameter increases with both pressure and peak RF voltage, which is in good agreement with Koidl [2]. The effective voltage U_b scales strongly with peak RF voltage but weakly with pressure. The latter is explained by the only effect of increasing pressure being a slight decrease in sheath size.

IED Structure Scaling with hPIC2

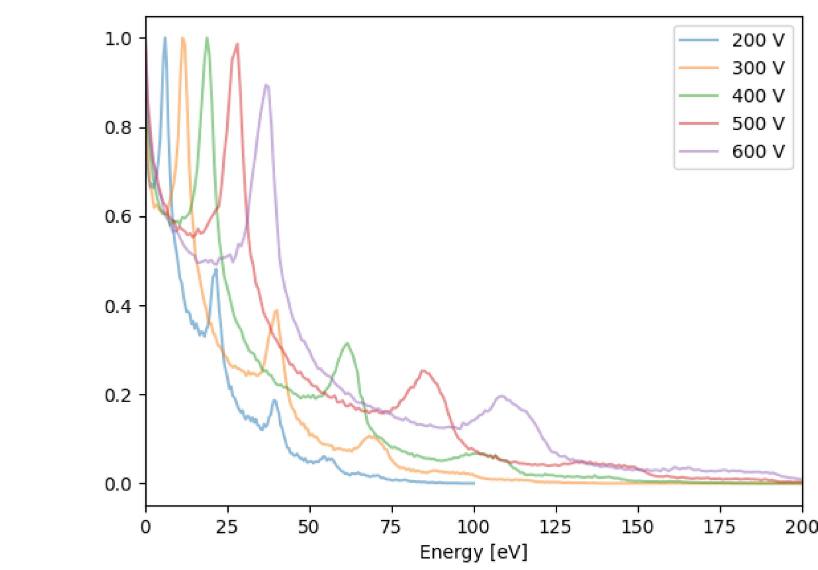

Figure 6: Peak-normalized IEDs at various peak RF voltages for discharges at 120 mTorr. The distributions broaden out with increasing voltage; while the collision frequency remains the same, the energy gained during the time between collisions is larger. In accordance with Figure 4, the number of peaks increases with decreasing voltage, since decreasing voltage increases the relative contribution of RF modulation. The RF modulation "bunches" up the ions in energy, creating more peaks in the IED.

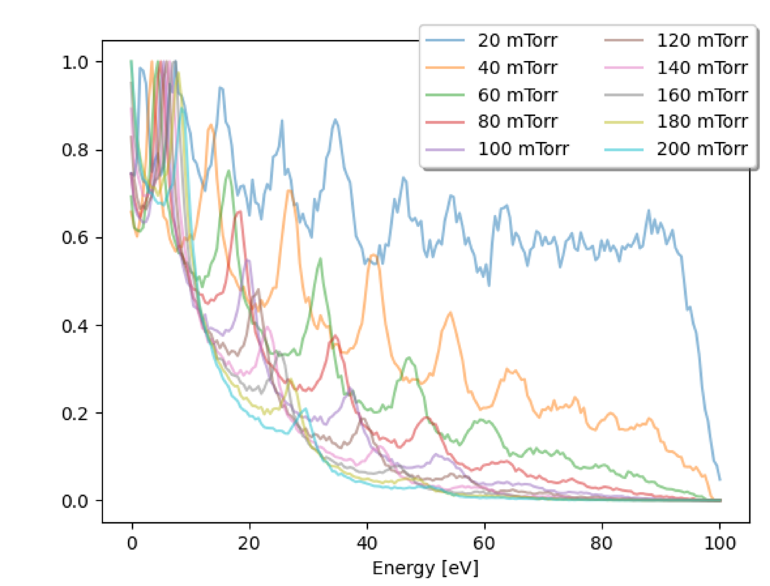

Figure 7: Peak-normalized IEDs at various pressures for discharges at a peak RF voltage of 200 V. The distribution thins out with increasing pressure; the ions are thermalizing with the background gas as they traverse the sheath, in accordance with Figure 2. This thermalization diminishes the height of the higher energy peaks, so the total number of peaks decreases with increasing pressure.

Conclusions

- The energy peaks are a result of radio-frequency sheath modulation and ion-neutral interactions, dominated by symmetric charge exchange collisions.
- Ion-neutral collisions create low energy ions within the sheath, which cannot respond to the full sheath potential.
- It is observed that the number of low-energy peaks increases with decreasing voltage (increasing the effect of RF sheath modulation) as well as decreasing pressure (less thermalization of the ion energy distribution).

Future Work

- Figure out why the Monte Carlo model shows good qualitative agreement with the hPIC2 IEDs, but still requires further scaling of U_b.
- Add recombination reactions into hPIC2 to remove the low energy ion group, making the electric field structure more realistic.
- Vary the RF frequency (which will affect U_b) and observe how the IED scales with respect to the ratio between ion collision frequency vs RF frequency.

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https://github.com/lcpp-org/aps-dpp-2024-liu