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3D PIC-DSMC Simulation of Strongly Coupled Cathode Spot Plasma Dynamics during Vacuum Arc Initiation:

A Cautionary Tale

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Introduction & Motivation

So I agreed to organize this workshop…

And then the vacuum arc funding I had was “deprioritized”!

But it hit me at GEC while Marco was presenting our work on Strongly Coupled Plasma (SCP) effects in atmospheric pressure discharges: Cathode spot plasmas in vacuum arcs are a SCP!

> When the cathode material takes the path of explosive transformation from solid to plasma, … , there is a certain, short-lived, high-density state that is best described as *non-ideal* plasma.
>
> -- André Anders, Cathodic Arcs (pg. 159)

Introduction & Motivation

- So what is a Strongly Coupled, or non-ideal, plasma?

- In an ideal plasma the kinetic energy of the plasma particles $\gg$ interaction energy (mainly from the shielded Coulomb potential). Equivalently, in an ideal plasma there are many charged particles in a Debye sphere.
  - For a non-ideal plasma we can no longer assume binary charged-charged collisions!

- A plasma is strongly coupled if the dimensionless coupling parameter is greater than 1:

$$\Gamma = \frac{q^2}{4\pi\varepsilon_0 k_B T}\left(\frac{4\pi n}{3}\right)^{1/3}$$

Motivation

- If the plasma during vacuum arc initiation is strongly coupled (e.g. non-ideal):
  - Implications on the physical dynamics, e.g. Disorder-Induced Heating (DIH) and pressure ionization*
  - And, as my talk title implies, implications on PIC's ability to properly simulate this phase of the vacuum arc!

- For atmospheric pressure spark discharge plasmas DIH results in significant heating on ω_p^{-1} timescales…

What about for cathode spot plasma?

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Letter

Disorder-induced heating as a mechanism for fast neutral gas heating in atmospheric pressure plasmas

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Abstract
Recent findings suggest that ions are strongly correlated in atmospheric pressure plasmas if the ionization fraction is sufficiently high ($\gtrsim 10^{-5}$). A consequence is that ionization causes disorder-induced heating (DIH), which triggers a significant rise in ion temperature on a picosecond timescale. This is followed by a rise in the neutral gas temperature on a longer timescale of up to nanoseconds due to ion–neutral temperature relaxation. The sequence of DIH and ion–neutral temperature relaxation suggests a new mechanism for ultrafast neutral gas heating. Previous work considered only the case of an instantaneous ionization pulse, whereas the ionization pulse extends over nanoseconds in many experiments. Here, molecular dynamics simulations are used to analyze the evolution of ion and neutral gas temperatures for a gradual ionization over several nanoseconds. The results are compared with published experimental results from a nanosecond pulsed discharge, showing good agreement with a measurement of fast neutral gas heating.

* Anders, et al., PSST **1**, 263-270 (1992)

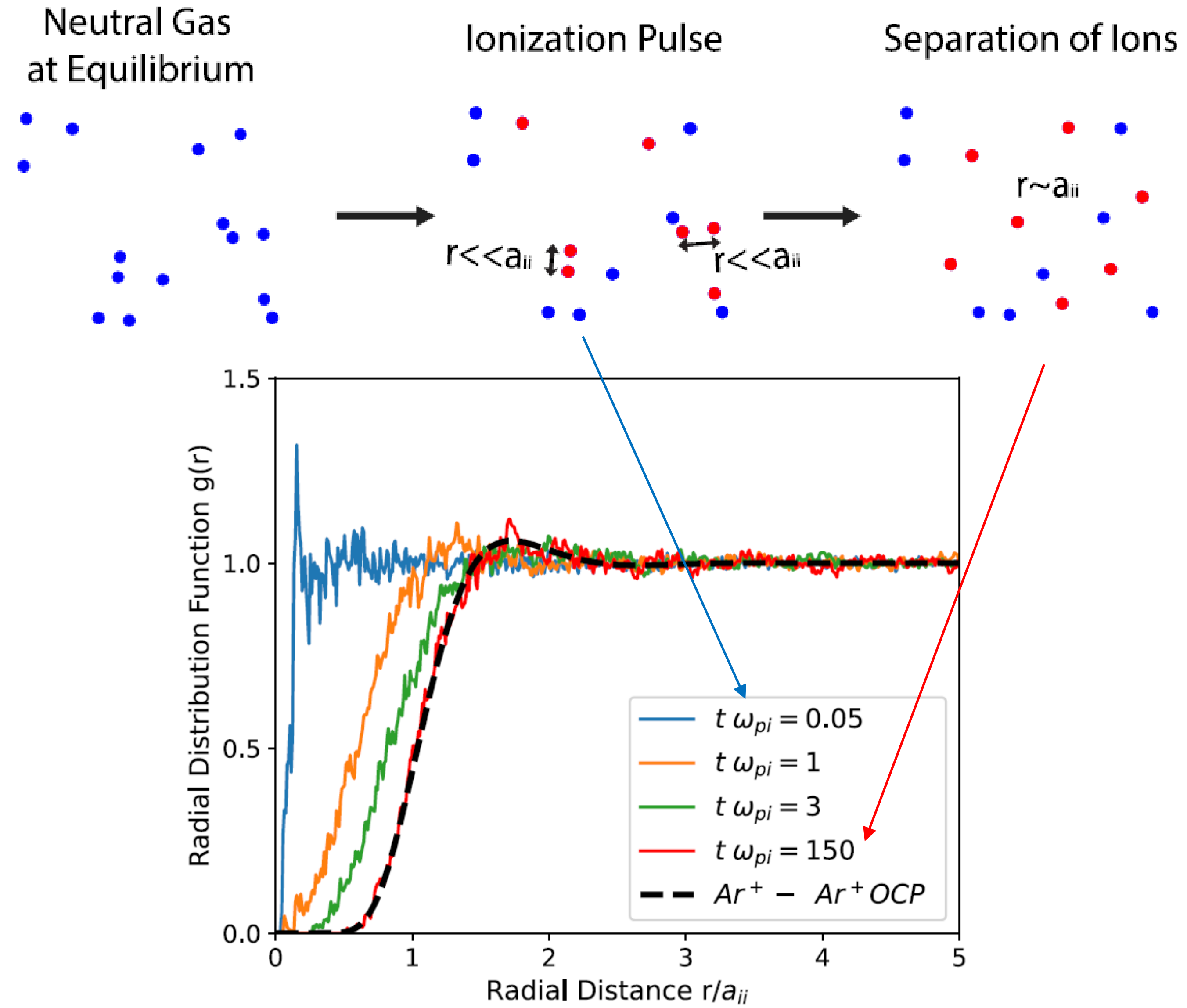
SCP Effects: Disorder Induced Heating

- Start with an uncorrelated state: The neutral atoms are randomly distributed and are, on average, $a_{NN} = \left(\frac{4\pi n_N}{3}\right)^{-1/3}$ apart

- Ionization occurs and now ions are too close together – their initial positions are based on the neutral state

- The ions fly apart due to Coulomb repulsion on the ion plasma period timescale:

→ The ions gain substantial thermal energy!



*These figures & results from MD simulations in M.D. Acciarri *et al*, PSST **31**, 125005 (2022)

SCP Effects: Disorder Induced Heating

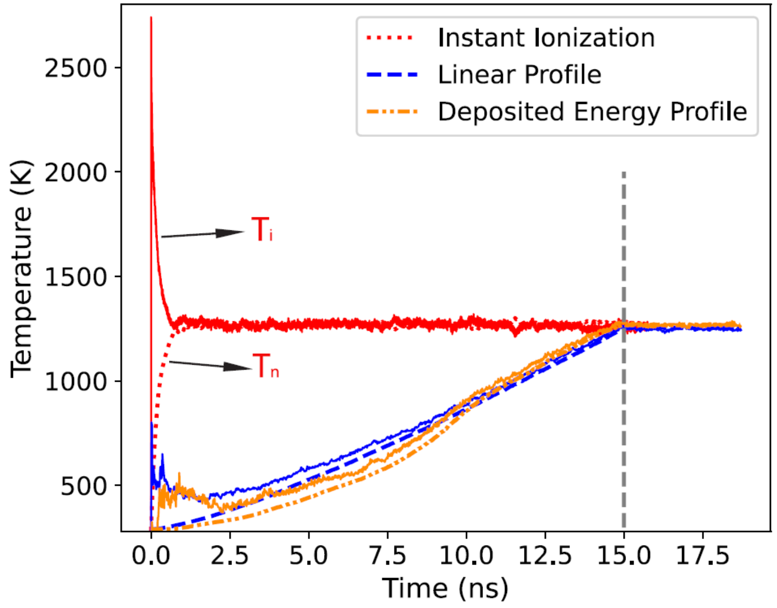
- The prior results were for a pulse of ionization all at once – will the heating still be significant if the ionization happens gradually?

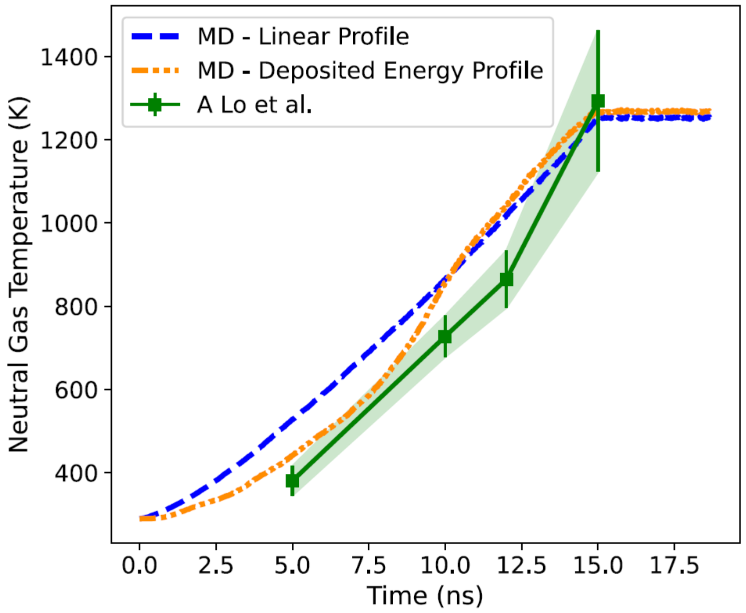
- Yes! The total energy released by DIH depends only on the end ionization fraction and coupling parameter and the equilibrium temperature will become:

$$x_i = \frac{n_i}{n_N + n_i} \qquad \frac{T_i^{max}}{T_0} = \frac{\Gamma_i}{1.91}$$

$$\frac{T_{eq}}{T_0} = x_i \frac{T_i^{max}}{T_0} + (1 - x_i)$$

- In fact, this mechanism is possibly the main ns-timescale heating mechanism for atmospheric pressure sparks





*These figures & results from M.D. Acciarri *et al*, PSST **33**, O2LT02 (2024)

Vacuum Arc conditions

- Let’s assume our cathode spot plasma has the following conditions:
- Copper thermally vaporizing off the surface at 2000K and $n_{Cu} = 10^{27}$ #/m^3
- Assume an applied E-field = 5 GV/m
- Pick j_e such that: $j_{GTF}(\beta=1) < j_e < j_{SCL}$ -- The exact value is not crucial to the talk takeaway since in the present model it just controls the ionization rate. We use 3×10^{10} A m^{-2} s^{-1}
- It is reasonable to assume based on prior observations and theory that $x_{Cu+} > 0.01$ and that the mean charge state, <*Z*>, is 2*

* Yushkov, et al., JAP **83**, 10, 5618-5622 (2000)

Vacuum Arc conditions

- So will we expect significant DIH?

- For these parameters, $\Gamma_i(x_i = 0.1) \cong 25 \;\rightarrow\; \frac{T_i^{max}}{T_0} \approx 13$

- If this system was a closed, triply periodic box, where the ions and neutrals can equilibrate we would expect: $T_{eq} \cong 4400\text{K}$

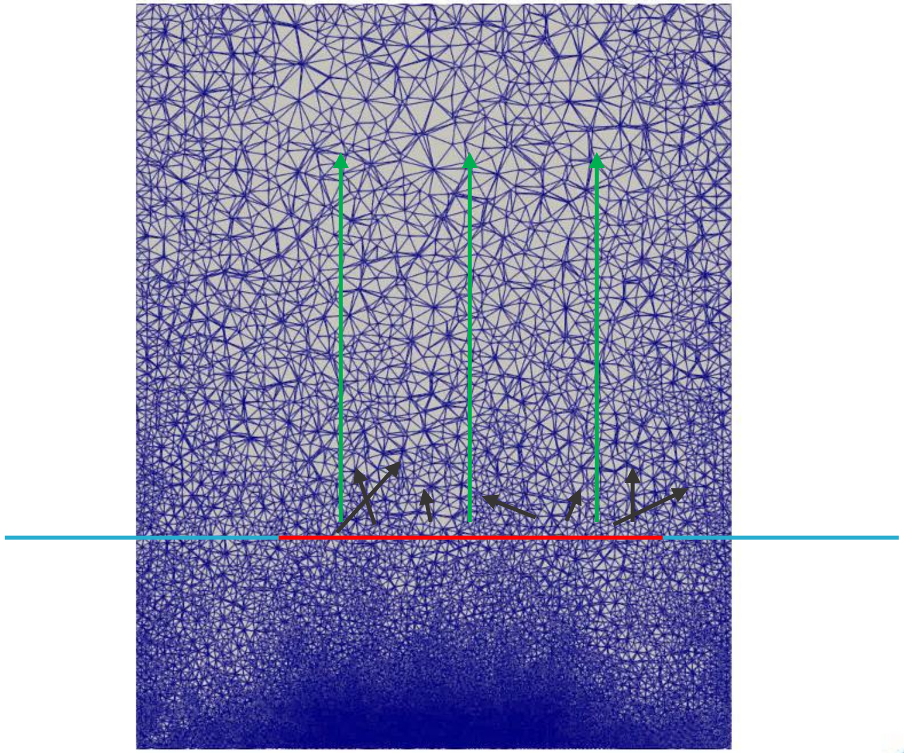
- But here we have the neutrals and plasma rapidly expanding into the vacuum and thus we might expect some level of “freezing” between the ions and neutrals

Model and 3D Simulation Domain

- Simulate a cathode spot with a 75nm radius and assume $n_e = 10^{24}$ m^{-3}; $n_i = 5\times10^{25}$ m^{-3} and $\langle Z \rangle = 1$
- Extend the domain out to a radius of 250nm and a height of 500nm
- To avoid numerical instabilities for a warm plasma, $\Delta t \leq 1.62\omega_p^{-1} \cong 2.9 \times 10^{-14}$s $\rightarrow \Delta t = 0.5$fs
- Size the mesh "near" the cathode spot to resolve the Debye length ($\sum_j \frac{Z_j^2 n_j}{T_j} \gg \frac{n_e}{T_e}$) at the *initial temperature* (2000K) and then allow Δx to grow away from that region:

$$\Delta x = f\lambda_D \cong f\sqrt{\frac{\varepsilon_0 k_B T_i}{(Ze)^2 n_i}} \approx 0.436f \text{ nm}; \; f{\leq}1 ???$$

- Mesh ultimately has O(10^7) elements for f=2



The PIC-DSMC Modeling Challenge

- Mean spacing between physical particles is: $a_{jj} = \left(\frac{4\pi}{3} n_j\right)^{-1/3}$ → a_{nn} ~ 0.63nm
- Thus, if we resolve the Debye length (0.4nm), there are fewer than one physical neutral particle per element volume and many fewer than one physical ion or electron per element!
- Even with computational particle weights equal to 1 we will not have good statistics resulting in numerical heating over 100's ω_p^{-1}
- Additionally, the minimum density that can be represented by a single, weight=1 particle is O(0.4^{-3}) ~ 6×10^{29} m^{-3}
- Since the ionization rate is non-linear* with E/n, the integrated ionization along the e$^-$ path will be wrong

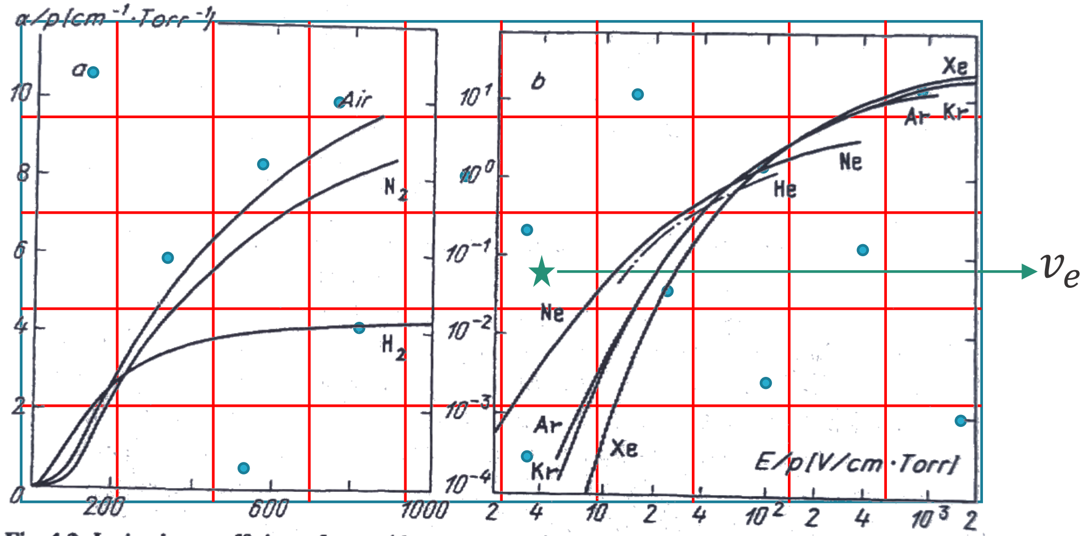


Fig. 4.3. Ionization coefficients for a wide range of E/p values (a) in molecular gases, (b) in inert gases. From [4.3]

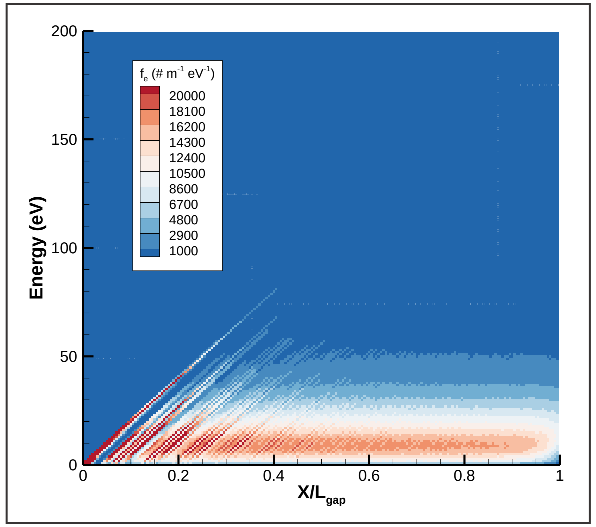
*Raizer, *Gas Discharge Physics*, 1991

The PIC-DSMC Modeling Challenge

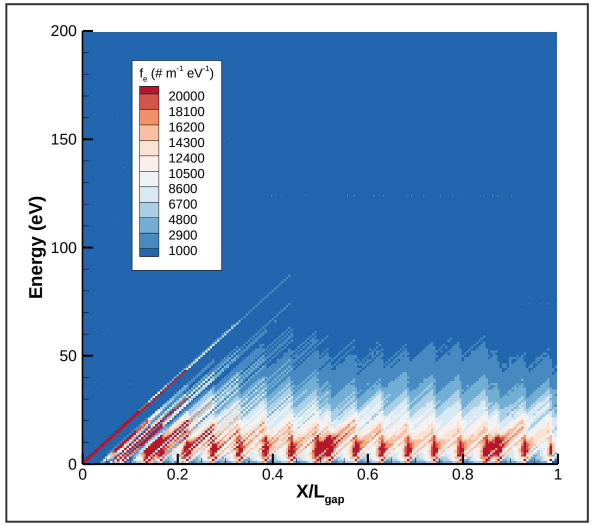
- We could solve the collision rate issue several ways:
  - Use a separate collision mesh and field solve mesh
  - Just use larger elements, forget about resolving the Debye length

- We have looked at separate collision and field-solve meshes in the past and it does improve the accuracy for avalanche calculations:

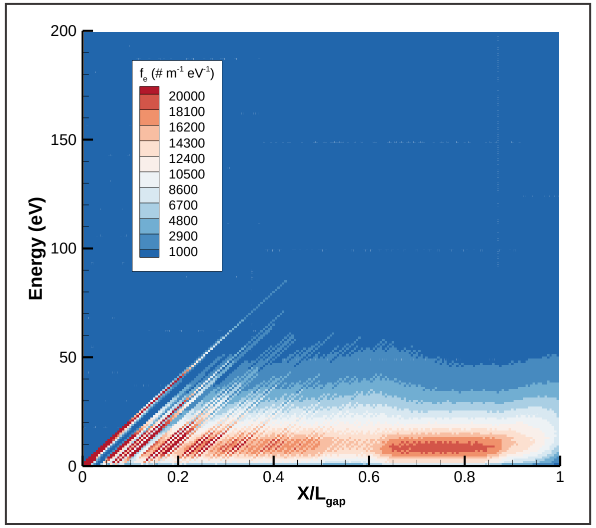
10 particles/cell



0.1 particles/cell



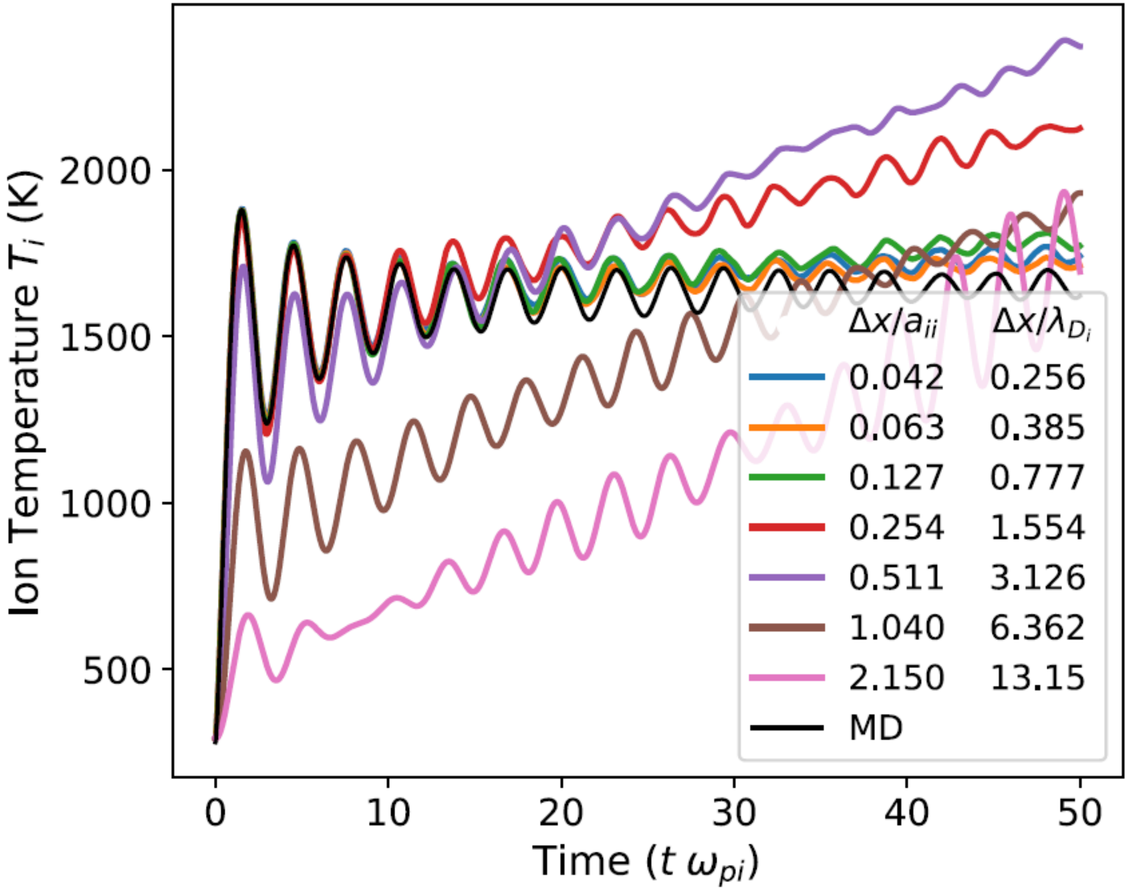
~10 particles/collision cell



* S. Moore, P. Crozier, C. Moore, M. Bettencourt, and M. Hopkins, “Automatic Coarsening of the Particle Interaction Mesh in a Hybrid PIC-DSMC Simulation”, DSMC workshop, 2013

The PIC-DSMC Modeling Challenge

- Can we use a mesh size greater than the Debye length and just accept some numerical mesh heating on the timescale of 10's ω_p^{-1}?
- Unfortunately we must still resolve the mean ion spacing if we hope to capture the physical Disorder Induced Heating and the many-body charged-charged "collisions" via the fields on the mesh
- So we still are left with unphysically large e- densities unless the e- density is larger than the ion density
- And, since we are forced to have less than one ion per cell, we cannot avoid numerical heating on the timescale of 100's ω_p^{-1}



*These figures & results from M.D. Acciarri *et al*, "When should PIC simulations be applied to atmospheric pressure plasmas? Impact of correlation heating", PSST *under peer review* -- arXiv:2403.00656

The PIC-DSMC Modeling Challenge

- Can we just use computational particle weights, W<1 in order to have more than one ion per cell and avoid numerical heating on the timescale of 100's ω_p^{-1}?

- Unfortunately not as this changes the radial distribution function, g(r), and thus the amount of DIH. Furthermore, it's possible when using W>1 to introduce Artificial Correlation Heating (ACH)!

- A possible path forward is to use a Particle-Particle-Particle-Mesh scheme** that does MD inside the element and accounts for far-field charges via the fields on the mesh. This allows for $\Delta x > \lambda_D$ while still capturing DIH. However, one must still use W=1.

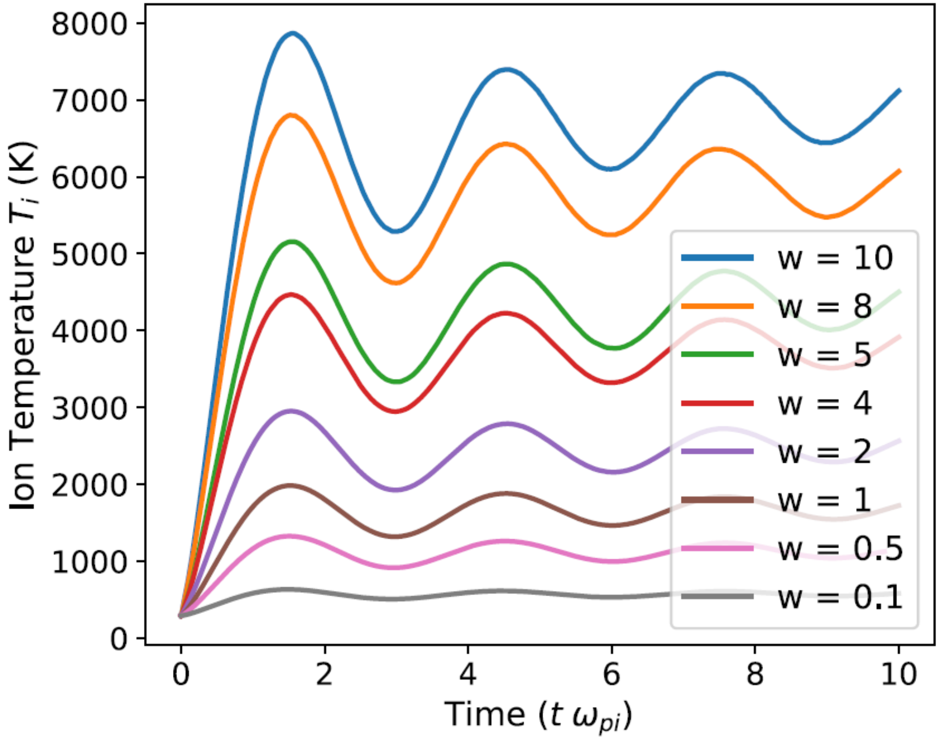


FIG. 4. Evolution of the ion temperature using a grid spacing of $\Delta x/a_{ii} \approx 0.042$ for different macroparticle weights w.

*These figures & results from M.D. Acciarri *et al*, "When should PIC simulations be applied to atmospheric pressure plasmas? Impact of correlation heating", PSST *under peer review* -- arXiv:2403.00656
Bettencourt, IEEE Transactions on Plasma Science, **42, 5, 1189-1194 (2014).

EMPIRE Simulation Model

- We choose to use W=1 particles and resolve (or very nearly resolve) the Debye length such that numerical mesh heating is small and accept late time particle count heating with the goal of gaining insight about DIH on shorter timescales.

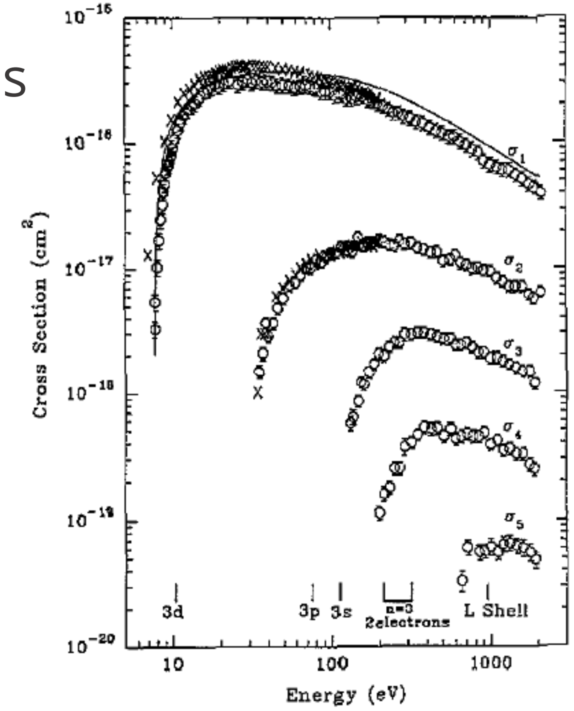
- Using standard DSMC collisions would give wrong ionization rates thus as an approximation we use a constant ionization rate where the neutral has a probability of ionizing ($Cu \rightarrow Cu^{+} + e^{-}$):

$$P_{iz} = 1 - exp^{-\Delta t n_e \langle \sigma v_e \rangle}$$

- Where we let $\langle \sigma v_e \rangle \sim \sigma_{max} v_e \approx 3 \times 10^{-20} (4 \times 10^{6}) = 1.2 \times 10^{-14}$ [m³/s]

- We include double ionization at 5% of the single ionization rate

- Note, we have neglected field and pressure ionization and are not accounting for ionization rate changes as the neutrals get further from the cathode. We also do not include e+Cu elastic or excitation collisions.



Bolorizadeh et al, J. Phys. B: At. Mol. Opt. Phys. **27**, 175

EMPIRE Simulation Model

- Inject neutrals on a regular lattice inside cathode spot to approximate starting from a solid Cu lattice

- Charge-Charge collisions are directly computed via the fields on the mesh since $N_{elem} \ll 1$

- Ion collisions:
  - Elastic collisions → Use approximate VHS parameters for Cu+Cu collisions*

    $d_{ref} = 0.57$ nm and $\omega = 0.92$

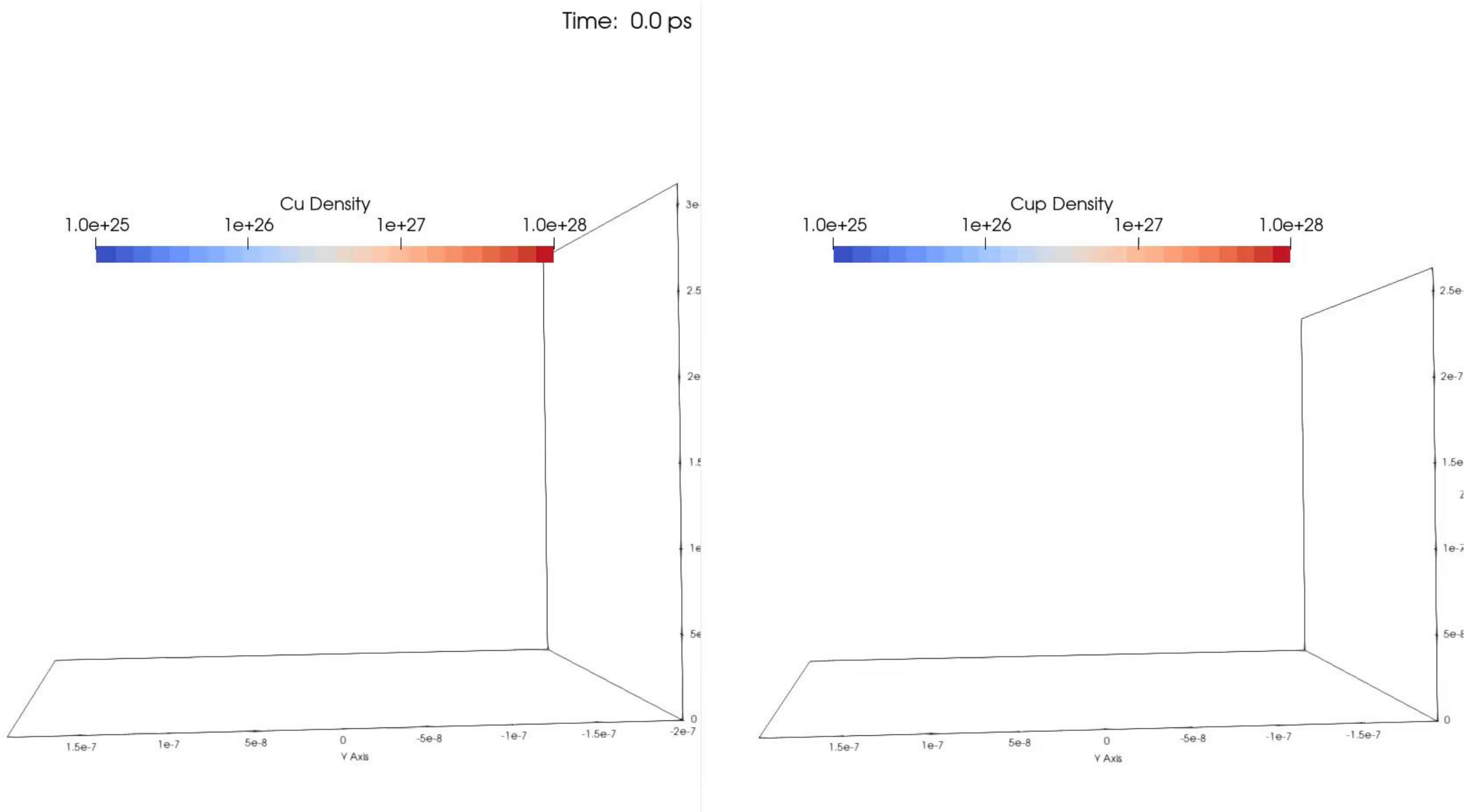
  - Charge exchange* → $\sigma_{CEX} \sim \frac{1}{I_B}\left(C_1 - C_2 ln(v)\right)^2, C_1 = 6.5 \times 10^{-7}, C_2 = 3 \times 10^{-8}$

  - However, note that charge exchange is a tunneling process and thus extremely short ranged (~Å) but DSMC allows collisions to occur across the element (which is ~8Å). This results in unphysically large ion “transport” across the element.

  - We neglect $Cu^+ + e^- \rightarrow Cu^{++} + 2e^-$ and all ion-cathode feedback BCs (sputtering, SEE, heating, etc.)

*Venkattraman, “Direct Simulation Monte Carlo modeling of e-beam metal deposition”, 2010. http://dx.doi.org/10.1116/1.3386592
*Fridman and Kennedy, “Plasma Physics and Engineering”, 2004.

Results: Without Charge Exchange



- Neutrals expand out from the cathode spot and are gradually ionized
- Note that, until the mesh coarsens after ~18nm, the mesh is so small that we don't accurately capture the ion or neutral densities in a given element

  → The rest of our results will show quantities computed using all the particles in the domain (or a subset of it) in order to reduce noise since we typically have <1 particle/cell

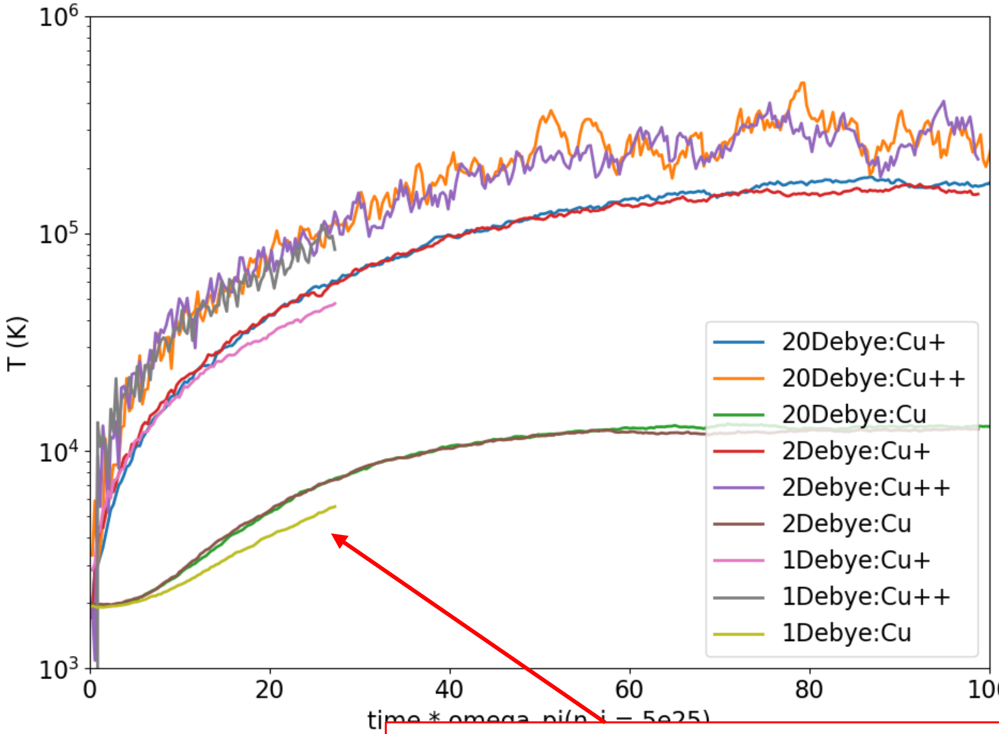
Results: Without Charge Exchange

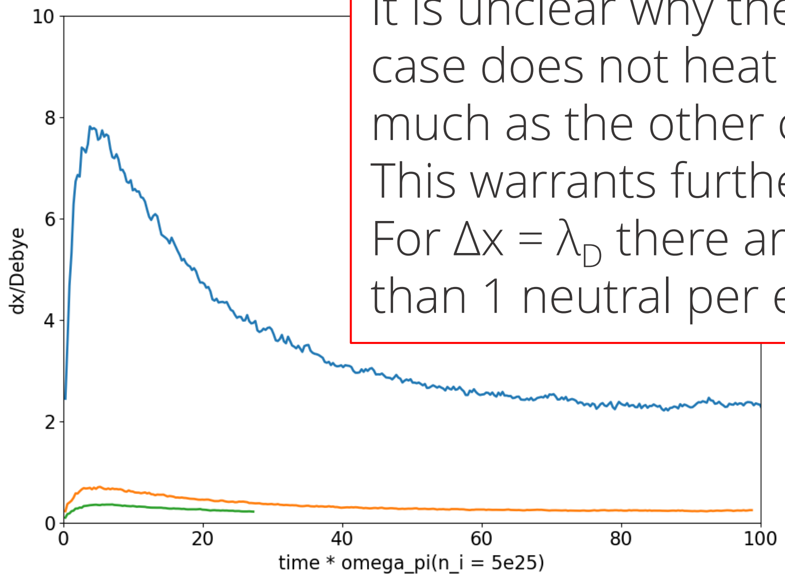
- Significant Disorder Induced Heating is seen to occur on the timescale of $\sim 50\omega_{pi}^{-1}$ as it takes time for the neutrals to expand and ω_{pi} is **not** constant!

- However! Given the large applied fields, the ion velocity distribution is NOT an equilibrium Maxwellian so "temperature" is not particularly meaningful in the usual sense.

- The $\Delta x = 20\lambda_D(n_i = 5\times10^{25}\ \mathrm{m}^{-3}, T_i = 2000\mathrm{K})$ case does not actually ever reach a mesh that is 20× Debye as the ions are rapidly heating (similarly for all mesh sizes)

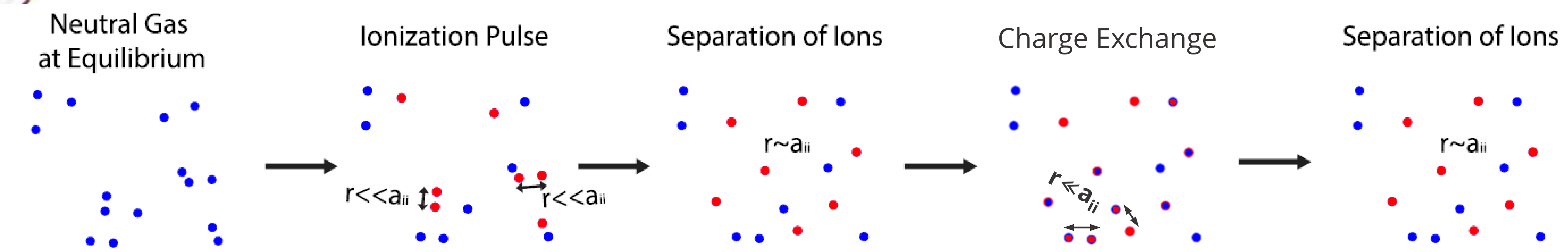
- Ion and neutral temperatures do not reach equilibrium as they expand into the vacuum and the collision rates are not fast enough to fully equilibrate



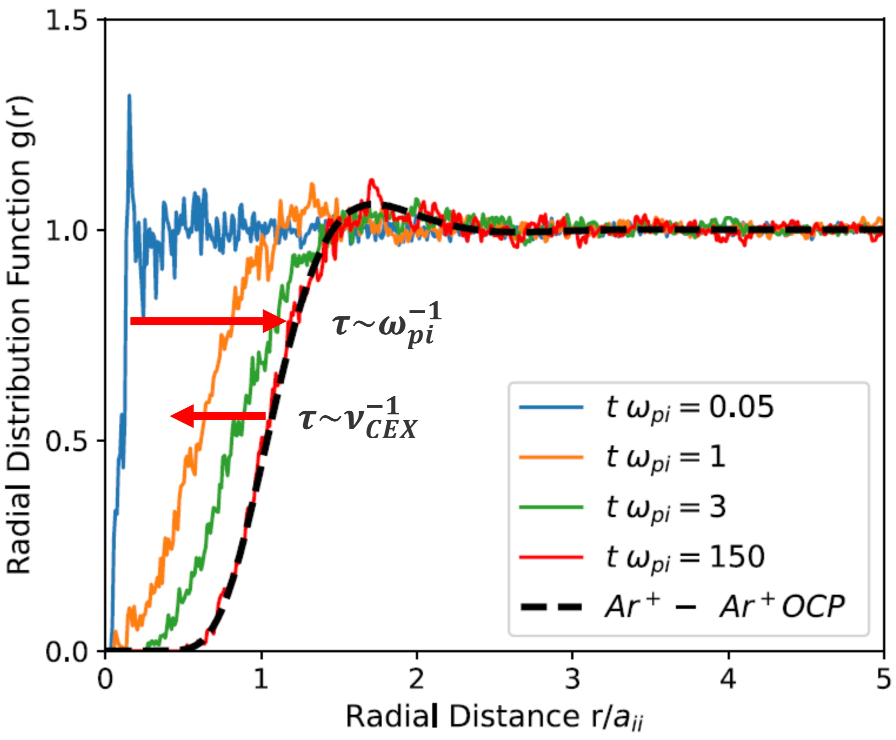


It is unclear why the $\Delta x = \lambda_D$ case does not heat quite as much as the other cases. This warrants further study. For $\Delta x = \lambda_D$ there are fewer than 1 neutral per element.

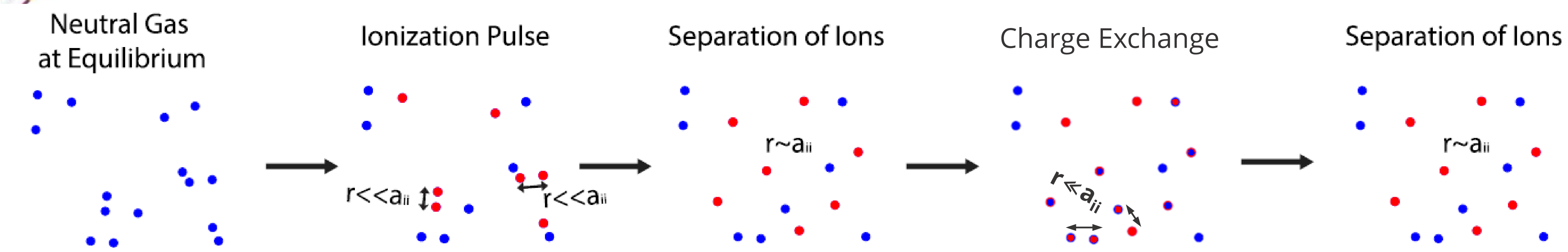
Disorder Induced Heating with Charge Exchange



- As ionization occurs the ions are too close together – some fraction of their positions are based on the former-neutral locations
- The ions fly apart due to Coulomb repulsion on the ion plasma period timescale and the ions gain thermal energy
- At the same time, charge exchange (tunneling of charge to the neutral) occurs as ions and neutrals pass closely by each other
- This results in more uncorrelated ions again and additional heating!



Disorder Induced Heating with Charge Exchange

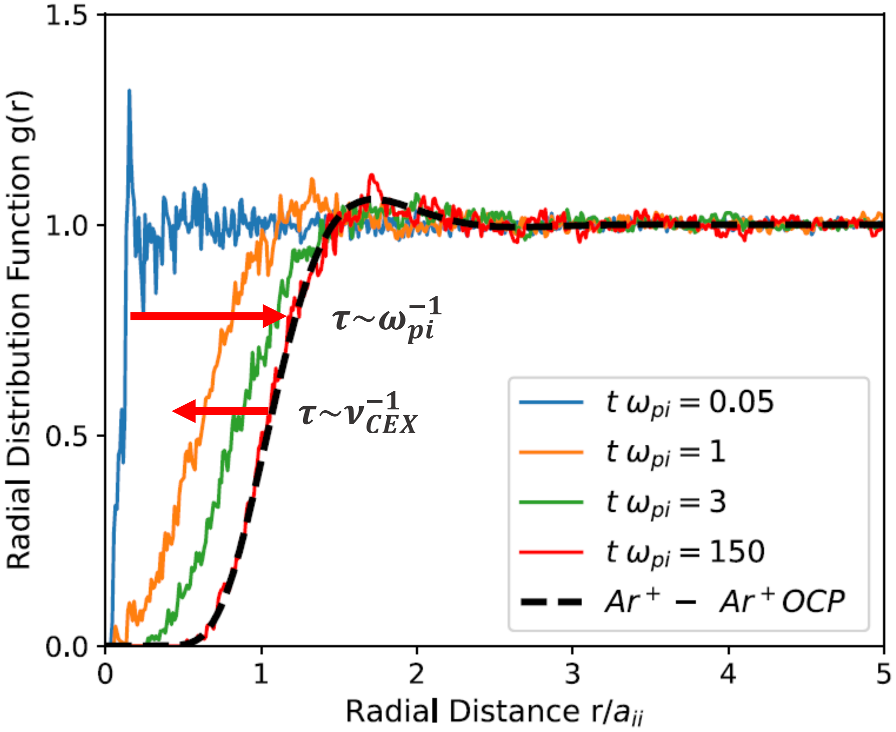


- Will this just continue forever and T → ∞ ?
- No, for at least two reasons:

$$\sigma_{CEX} \sim \frac{1}{I_B}\left(C_1 - C_2 ln(v)\right)^2, C_1 = 6.5 \times 10^{-7}, C_2 = 3 \times 10^{-8}$$

- So as the temperature increases, ν_{CEX} will decrease

- Second, the densities rapidly decrease as the gas/plasma expands into the vacuum further decreasing $\nu_{CEX}(n_i)$ (faster than $\omega_{pi}(\sqrt{n_i})$)

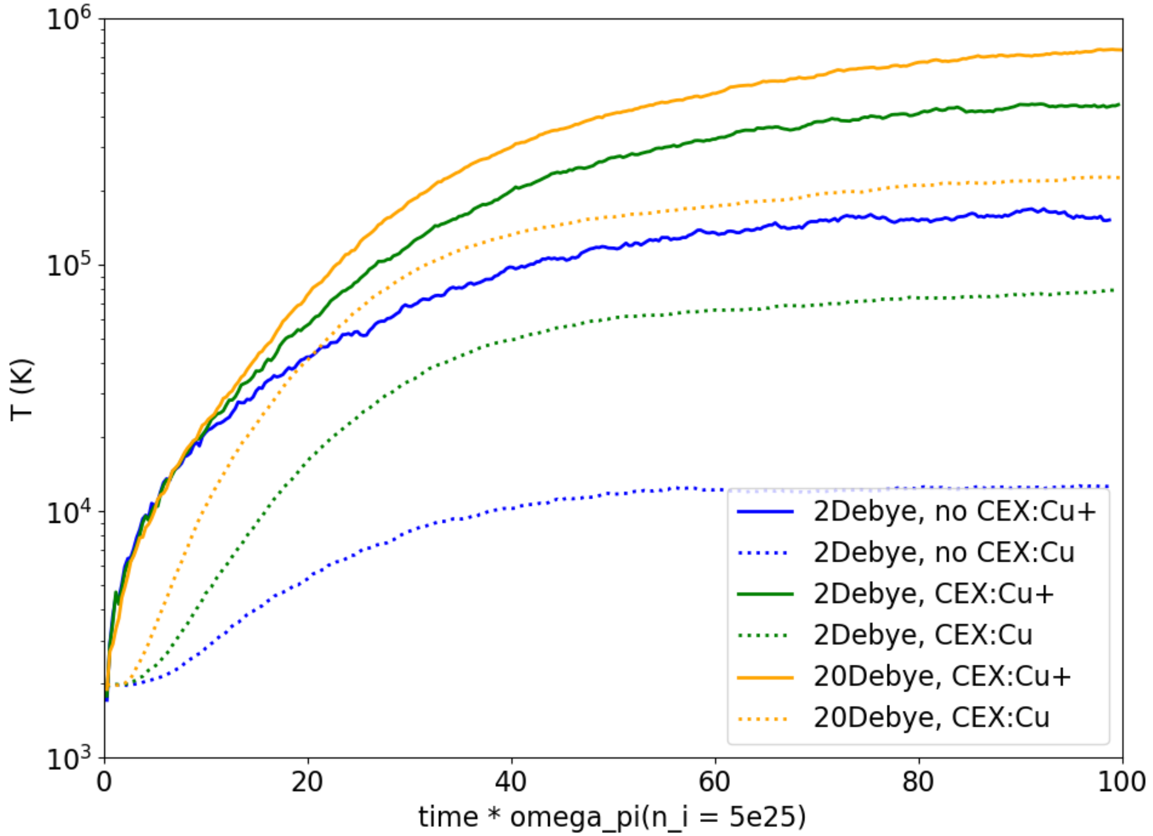


Results: With Charge Exchange

- As expected allowing charge exchange does result in additional DIH

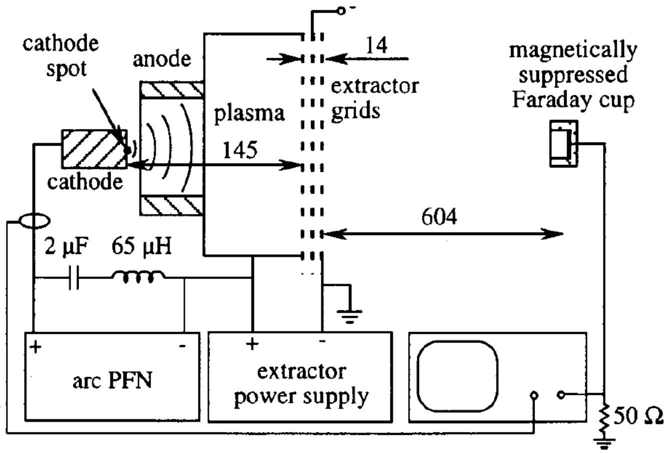
- Furthermore, as we decrease the size of the mesh, the additional DIH decreases (versus the no charge exchange case)
  - Due to charge exchange distances that scale with Δx

- Note, we did not include Cu^{++} charge exchange in the model; however there is increased Cu^{++} DIH due field interactions with the Cu^{+}



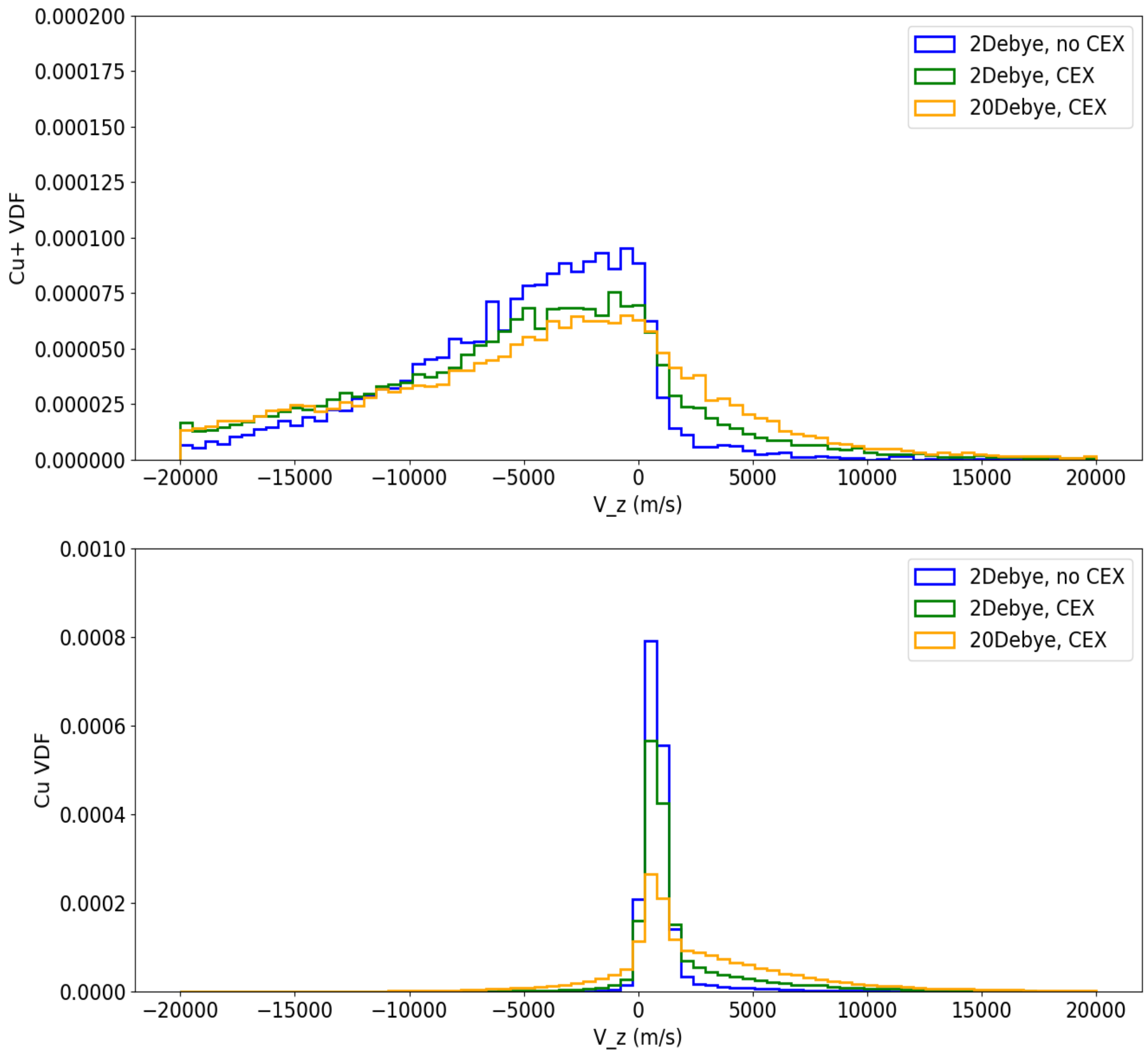
Results: With Charge Exchange

- With charge exchange we now get a non-negligible population of ions with large velocities (5-10km/s) away from the cathode
- Ions are rapidly accelerated via DIH and then charge exchange results in a fast neutral which is later ionized after traveling some distance from the cathode spot
- Similar in magnitude to the mean 12.8km/s Cu^+ velocity (for the ions that escape the cathode spot) reported in Yushkov et al. (2000)

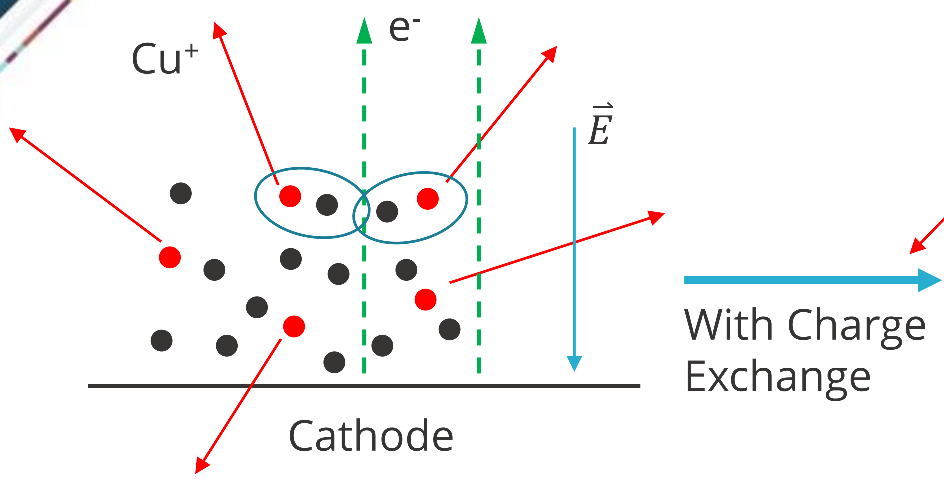


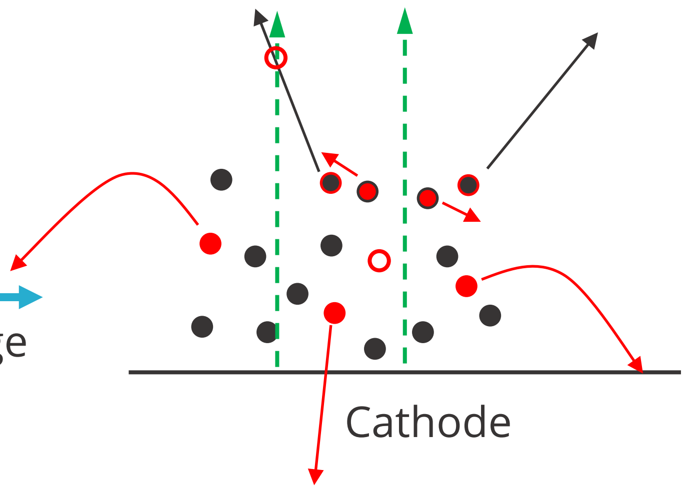
Yushkov, et al., JAP **83**, 10, 5618-5622 (2000)

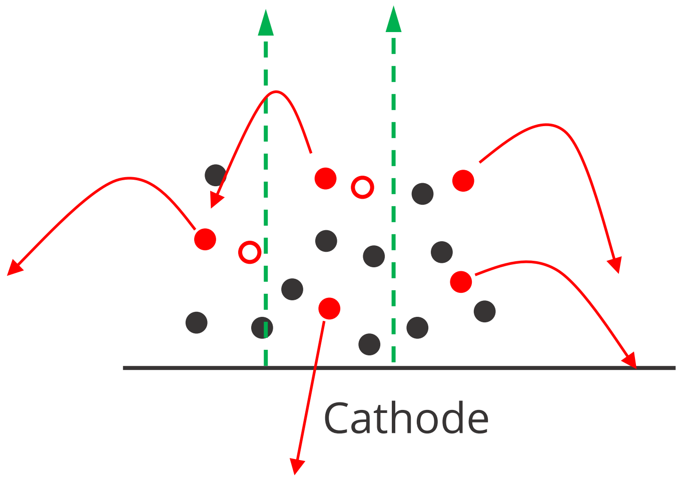
t=83.5ps -- $\omega_{pi}t$ ~ 98



Results: With Charge Exchange





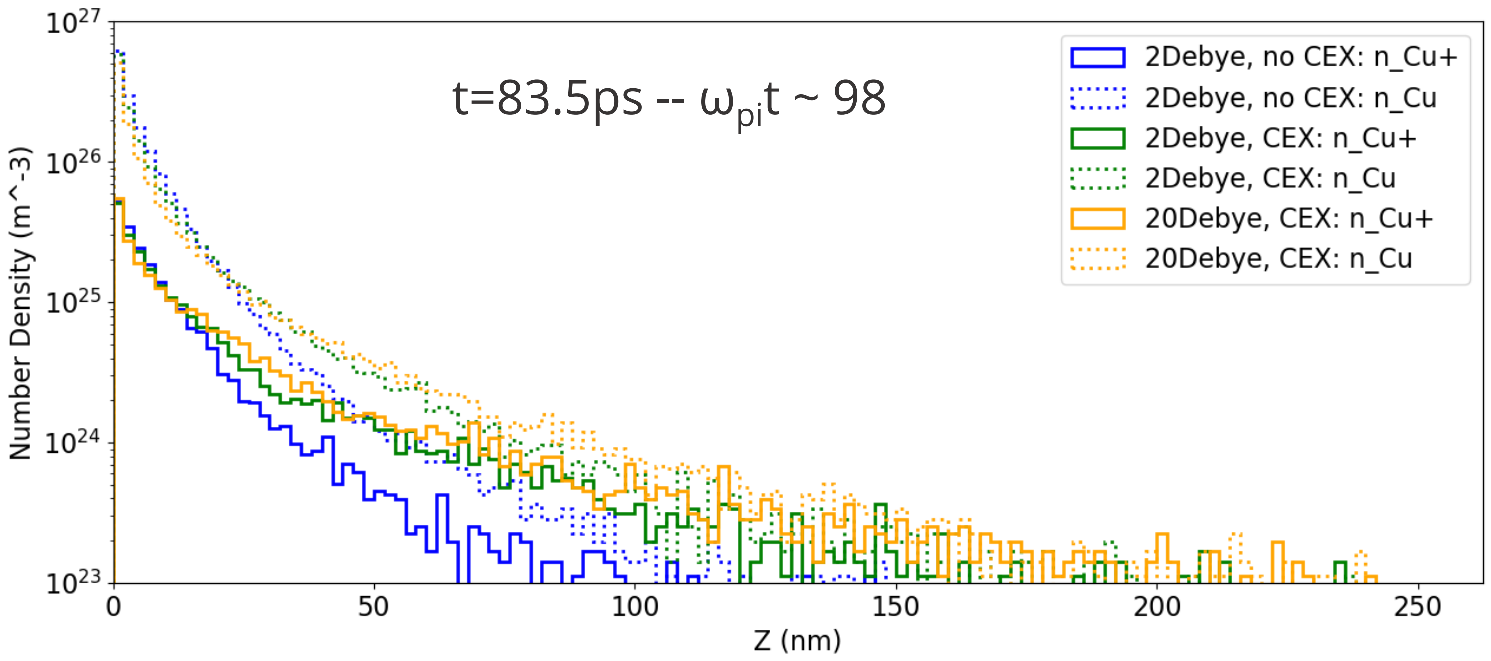


Ions are rapidly accelerated via DIH

Charge exchange results in a fast neutrals and additional DIH

The neutrals are then ionized after traveling some distance from the cathode spot

→Faster expansion of the plasma away from the cathode



Conclusions

- The cathode spot plasma in a vacuum arc is very likely a SCP (this is not really "news") and thus we have several physical mechanisms we need to account for that are not present for ideal plasmas. At the very least be aware of:
  - Pressure Ionization (covered by Anders, et al., PSST **1**, 263-270 (1992))
  - Disorder Induced Heating

- DIH can result in much higher ion (and neutral) temperatures than present in the vaporizing cathode material surface temperature

- DIH (especially with charge exchange) can provide some explanation for the observed ion expansion velocity *away* from the cathode

- Modeling Strongly Coupled Plasmas with traditional PIC-DSMC is challenging at best, and should really only be attempted for short timescales.
  - → See M.D. Acciarri *et al*, "When should PIC simulations be applied to atmospheric pressure plasmas? Impact of correlation heating", PSST *under peer review* -- arXiv:2403.00656

- To model component-scales we will need a meso-scale model for the cathode material supply that accounts for SCP effects in the very-near (<1μm) cathode region!