Ar\(^+\) and Xe\(^+\) Velocities near the Presheath-Sheath Boundary in an Ar–Xe Discharge

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Introduction

In a weakly collisional plasma with a single ion species a presheath develops in the plasma and ions are accelerated to the Bohm speed (ion sound speed) at the presheath-sheath edge

\[ u_B = \left( \frac{eT_e}{M} \right)^{1/2} \]

where \( T_e \) is the electron temperature and \( M \) is the ion mass


Introduction

For multiple-ion species there is a generalized Bohm criterion

$$\sum_j \left( \frac{n_j}{n_e} \right) \frac{u_{Bj}^2}{u_j^2} \leq 1$$

where the sum is over the number of ion species, $u_j$ is the ion drift velocity at the presheath-sheath edge, $n_j$ is the ion density, $n_e$ is the electron density, and the equality is usually assumed.

However, this criterion leads to an infinite number of possible solutions.

Two simple solutions are apparent.

- All ions reach the sheath edge with the same velocity, the ion sound speed of the system.
- Each ion species has its own Bohm speed at the sheath edge.

Outline

- The oopd1 – 1D3V particle-in-cell/Monte Carlo code
  - The reaction set for the Ar/Xe discharge
- Measurements of Ar\(^+\) and Xe\(^+\) velocities at the sheath-presheath boundary
- Simulations to determine the Ar\(^+\) and Xe\(^+\) velocities
- The search for ion-ion two stream instability
- Summary
The oopd1 particle-in-cell/Monte Carlo code
To model the discharge we use the object oriented plasma device 1D3V (oopd1) particle-in-cell/Monte Carlo code.

This code is currently being developed at the University of California at Berkeley to replace the XPDx1 codes.

The oopd1 was developed to combine XPDP1, XPDC1, and XPDS1 family of codes into an object oriented code written in C++.

The oopd1 will be more user friendly than the earlier codes and its easier to add new chemistry and external circuit elements than in the earlier codes.
The reaction set for the Ar/Xe discharge

- The cross section set for argon was significantly revised from what is used in the XPDP1, XPDC1, and XPDS1 family of codes.
The reaction set for the Ar/Xe discharge

- A reaction set was constructed for xenon as well as the Ar–Xe cross terms
## The reaction set for the Ar/Xe discharge

**Ar reactions**
- \( e + Ar \rightarrow Ar + e \) \(
  \text{elastic scattering} \quad \text{(Ferch et al., 1985; de Heer et al., 1979)}
\)
- \( e + Ar \rightarrow Ar^+ + 2e \) \(
  \text{electron impact ionization (15.76 eV)} \quad \text{(Krishnakumar and Srivastava, 1988; Vikor et al., 1989)}
\)
- \( e + Ar \rightarrow Ar^r + e \) \(
  \text{electron impact excitation (11.62 eV)} \quad \text{(Hayashi, Hayashi)}
\)
- \( e + Ar \rightarrow Ar^{in} + e \) \(
  \text{electron impact excitation (11.55 eV)} \quad \text{(Hayashi, Hayashi)}
\)
- \( e + Ar \rightarrow Ar(4p) + e \) \(
  \text{electron impact excitation (13.2 eV)} \quad \text{(Eggarter, 1975)}
\)
- \( e + Ar \rightarrow Ar(II) + e \) \(
  \text{electron impact excitation (14.09 eV)} \quad \text{(Eggarter, 1975)}
\)
- \( e + Ar \rightarrow Ar(III) + e \) \(
  \text{electron impact excitation (14.71 eV)} \quad \text{(Eggarter, 1975)}
\)
- \( e + Ar \rightarrow Ar(\text{higher}) + e \) \(
  \text{electron impact excitation (15.20 eV)} \quad \text{(Hayashi, Hayashi)}
\)
- \( Ar + Ar^+ \rightarrow Ar + Ar^+ \) \(
  \text{elastic scattering} \quad \text{(Cramer, 1959)}
\)
- \( Ar + Ar \rightarrow Ar + Ar \) \(
  \text{elastic scattering} \quad \text{(Phelps et al., 2000)}
\)
- \( Ar + Ar^+ \rightarrow Ar + Ar^+ \) \(
  \text{elastic scattering} \quad \text{(Hegerberg et al., 1982; Cramer, 1959)}
\)

**Xe reactions**
- \( e + Xe \rightarrow Xe + e \) \(
  \text{elastic scattering} \quad \text{(Mozumder, 1980)}
\)
- \( e + Xe \rightarrow Xe^+ + 2e \) \(
  \text{electron impact ionization (12.13 eV)} \quad \text{(Rapp and Englander-Golden, 1965)}
\)
- \( e + Xe \rightarrow Xe^m + e \) \(
  \text{electron impact excitation (8.315 eV)} \quad \text{(Sakai et al., 1991)}
\)
- \( e + Xe \rightarrow Xe^r + e \) \(
  \text{electron impact excitation (8.437 eV)} \quad \text{(Sakai et al., 1991)}
\)
- \( e + Xe \rightarrow Xe^h + e \) \(
  \text{electron impact excitation (9.570 eV)} \quad \text{(Sakai et al., 1991)}
\)
- \( Xe + Xe^+ \rightarrow Xe + Xe^+ \) \(
  \text{elastic scattering} \quad \text{(Piscitelli et al., 2003)}
\)
- \( Xe + Xe \rightarrow Xe + Xe \) \(
  \text{elastic scattering} \quad \text{(Phelps, 2009)}
\)
- \( Xe + Xe^+ \rightarrow Xe^+ + Xe \) \(
  \text{charge exchange} \quad \text{(Miller et al., 2002)}
\)

**Xe/Ar reactions**
- \( Xe^+ + Ar \rightarrow Xe^+ + Ar \) \(
  \text{elastic scattering}
\)
- \( Ar^+ + Xe \rightarrow Ar^+ + Xe \) \(
  \text{elastic scattering}
\)
- \( Ar + Xe \rightarrow Ar + Xe \) \(
  \text{elastic scattering}
\)
Measurements of $\text{Ar}^+$ and $\text{Xe}^+$ velocities at the sheath-presheath boundary
Measurements of $\text{Ar}^+$ and $\text{Xe}^+$ velocities indicate that the velocities approach the ion sound speed of the system near the sheath-presheath boundary.

Measurements of $\text{Ar}^+$ and $\text{Xe}^+$ velocities

The measured drift velocities of $\text{Ar}^+$ and $\text{Xe}^+$-ions at the sheath edge, with respect to the ion concentration ratio at 0.7 mTorr.

The velocities differ only slightly for approximately equal ion concentrations.

When either ion concentration greatly differs from the other, each species leaves the plasma at its own Bohm velocity.

Measurements of Ar$^+$ and Xe$^+$ velocities

Recent theoretical work claims that for roughly equal densities of cold ions a collisional friction associated with ion-ion two stream instability will bring the two ion species drift velocities closer together, and each ion species leaves the plasma at the common sound speed.


Simulations to determine the Ar$^+$ and Xe$^+$ velocities at the sheath-presheath boundary
Simulations to determine the $\text{Ar}^+$ and $\text{Xe}^+$ velocities

- The simulation attempts to model the multidipole experimental configuration described by Lee et al.

- The simulation discharge is maintained between two equal-area electrodes ($1.77 \times 10^{-2}$ m$^2$) separated by a gap of 10 cm.

- The left hand electrode is biased at $-30$ V to generate an ion sheath.


Simulations to determine the Ar$^+$ and Xe$^+$ velocities

To model the ionization created by the energetic electrons in the multidipole chamber, we use a volume source with a uniform ionization rate of $4.3 \times 10^{-19}$ m$^{-3}$s$^{-1}$ to maintain the steady state.

Electrons are created with electron temperature of 0.88 eV, and ions with temperature of 32 meV.

Three cases were simulated:
- a pure argon discharge at 0.7 mTorr
- a pure xenon discharge at 0.7 mTorr
- an argon-xenon discharge with argon and xenon partial pressures 0.5 and 0.2 mTorr, respectively

Simulations to determine the $\text{Ar}^+$ and $\text{Xe}^+$ velocities

- The density profiles of the charged particles for
  - (a) a pure argon discharge
  - (b) an argon-xenon discharge with argon and xenon partial pressures 0.5 and 0.2 mTorr, respectively
  - (c) a pure xenon discharge
Simulations to determine the Ar\(^+\) and Xe\(^+\) velocities

- The effective electron temperature in the presheath region.
- For comparison, the measured electron temperature is 880 meV.
- The xenon ion temperature is roughly the same for a pure xenon discharge and Ar/Xe mixture.
- The argon ion temperature is higher for argon ions in an Ar/Xe mixture than for a pure argon discharge.
Simulations to determine the $\text{Ar}^+$ and $\text{Xe}^+$ velocities

- The velocity of argon and xenon ions versus distance from the biased plate shifted by the location presheath-sheath boundary.
- The solid horizontal lines show the Bohm speed for a pure argon and pure xenon discharge.
- The dashed horizontal lines show the Bohm speed in an Ar/Xe mixture for argon and xenon ions.
Simulations to determine the Ar$^+$ and Xe$^+$ velocities

- For the Ar/Xe mixture the two ions have very distinct velocity profiles within the presheath.
- For a pure argon discharge the argon ion has almost the same velocity profile as it does in the mixture of argon and xenon.
- Similarly for a xenon discharge the xenon ion has almost the same velocity profile as it does in the mixture of argon and xenon.
Simulations to determine the $\text{Ar}^+$ and $\text{Xe}^+$ velocities

<table>
<thead>
<tr>
<th>Disch.</th>
<th>$T_{\text{eff}}$ [meV]</th>
<th>$x_0$ [cm]</th>
<th>$u_{\text{eff}}^{\text{B, Ar}^+}$ [m/s]</th>
<th>$u_{\text{B,x}^+}$ [m/s]</th>
<th>$u_{\text{B, Ar}^+}^{x_0}$ [m/s]</th>
<th>$u_{\text{B,x}^+}^{x_0}$ [m/s]</th>
<th>$n_e/10^{15}$ [m$^{-3}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ar</td>
<td>336</td>
<td>0.300</td>
<td>898</td>
<td>-</td>
<td>985</td>
<td>-</td>
<td>4.7</td>
</tr>
<tr>
<td>Ar/Xe</td>
<td>344</td>
<td>0.295</td>
<td>907</td>
<td>501</td>
<td>926</td>
<td>544</td>
<td>5.6</td>
</tr>
<tr>
<td>Xe</td>
<td>398</td>
<td>0.285</td>
<td>-</td>
<td>540</td>
<td>-</td>
<td>584</td>
<td>6.6</td>
</tr>
</tbody>
</table>

- The ion speed at the presheath-sheath boundary is roughly the same for an ion in a pure argon or xenon discharge and for the same ion in a mixture of argon and xenon.
- Therefore we draw the conclusion from our simulation that each ion reaches its own Bohm speed at the presheath-sheath interface.
- These findings contradict the experimental findings of Lee et al. where the ion velocities near the presheath-sheath boundary approach the common ion sound speed for both argon and xenon ions in the Ar/Xe discharge.

The search for ion-ion two stream instability
For the Ar-He system ion-ion two stream instabilities have been measured in the presheath, and they are strongest when the relative concentration of each ion species is similar.


Furthermore, it is argued that ion-ion two stream instability leads to a collisional friction that slows down one ion species and accelerates the other, while this collisional friction can be ignored in a stable plasma.

Baalrud et al., *Phys. Plasmas* **18** 023505 (2011)
The search for ion-ion two stream instability

Thus to understand the simulation results, we have calculated the instability condition from kinetic theory.

The Vlasov dispersion assuming drifting Maxwellian velocity distribution for each of the species involved

\[ \epsilon(k, \omega) = 1 - \sum_j \left( \frac{\lambda_j^2}{2k^2} \right) Z'(\zeta_j) \]

where the plasma dispersion function is

\[ Z(\zeta) = i\pi^{1/2} e^{-\zeta^2} \text{erfc}(-i\zeta) \]

\[ \zeta_j = (\omega/k + i\nu_j/k - u_j)/(2^{1/2}\nu_j) \]

For plasma that consists of electrons and two positive ions we can write the dispersion relation

\[ 2k^2 \lambda_e^2 = Z'(\zeta_e) + \sum_j (V_j/v_j)^2 Z'(\zeta_j), \]

where

- \( k \) is the wavenumber
- \( \lambda_e \) is the electron Debye length
- \( V_j = u_{B,j}(n_j/n_e)^{1/2} \) (\( j = 1, 2 \) corresponds to argon and xenon ions, respectively) are the density-weighted ion Bohm speeds
- \( v_j = (eT_j/M_j)^{1/2} \) are the ion thermal velocities

The search for ion-ion two stream instability

Also

\[ \zeta_j = \left( \frac{\omega}{k} + i\nu_j/k - u_j \right) / \left(2^{1/2}v_j\right) \]

- \(\omega\) is the radian frequency
- \(u_j\) and \(\nu_j\) are the drift and thermal velocities of the species, respectively
- \(\nu_j\) is the collision frequency with the background gas

The least stable solutions are a slow (ion thermal) wave with phase velocity \(v_{ph} \sim \nu_j\), and a fast (ion acoustic) wave with \(v_{ph} \sim u_B\)

Both fast and slow waves can be driven unstable if the relative ion drift velocity is large compared to the ion thermal velocities
The search for ion-ion two stream instability

- The real (solid line) and imaginary (dashed line) parts of the phase velocity $v_{ph} = v_{phr} + jv_{phi}$ and the frequency $\omega = \omega_r + j\omega_i$ for the simulation parameters
  - Assuming $T_{eff} = 0.34$ eV (Top)
  - Assuming $T_{eff} = 0.85$ eV (Bottom)
- The slow wave is unstable for $\omega_i > 0$
The search for ion-ion two stream instability

- We find no evidence of unstable waves in our simulation, which is the proposed mechanism for a common system speed.
- Reducing the ion temperatures 60% below the self-consistent simulation values, we obtain the onset of instability for the ion acoustic wave at $k\lambda_e \approx 0.44$. This corresponds to unrealistic (below room temperature) values of 19 meV for argon and 16 meV for xenon.
- Alternatively, increasing $T_{\text{eff}}$ by a factor of 2.5 above the simulation value can lead to the onset of instability.
Summary
Summary

- The velocities of Ar\(^+\) and Xe\(^+\) ions near the presheath-sheath boundary in an Ar/Xe discharge are studied by particle-in-cell/Monte Carlo simulation.
- For a pure argon discharge the argon ion has almost the same velocity profile as it does in the mixture of argon and xenon.
- Similarly, for a xenon discharge the xenon ion has almost the same velocity profile as it does in the mixture of argon and xenon.
- The ion speed at the sheath-presheath boundary is the same for an ion in a pure argon or xenon discharge and for the same ion in a mixture of argon and xenon.
- We conclude that in our simulation, each ion reaches its own Bohm speed at the presheath-sheath interface.


Hayashi, M. A set of electron-Ar cross sections with 25 excited states. ftp://jila.colorado.edu/collision_data/electronneutral/hayashi.txt.


