

Comment on “Ar⁺ and Xe⁺ Velocities near the Presheath-Sheath Boundary in an Ar/Xe Discharge”

A recent Letter by Gudmundsson and Lieberman [1] (GL) presents results of a 1D particle-in-cell Monte Carlo simulation of an Ar/Xe plasma. The authors conclude that Ar⁺ and Xe⁺ ions each reach their own sound speed, $V_i = c_{s,i} = \sqrt{T_e/M_i}$, at the presheath-sheath interface. This result contradicts experimental measurements in the configuration that the authors sought to model [2], which found the ion speeds to be closer to a common system sound speed $c_s = \sqrt{(n_1 c_{s1}^2 + n_2 c_{s2}^2)/n_e}$. Scientific validity entails giving precedence to an established and rich set of experimental results over subsequent theoretical contributions that disagree with those results. We argue this disagreement is due to too wide of grid spacing in the simulations to resolve beam instabilities and neglect of instability-enhanced collisional effects.

The GL simulations were initialized with the same 0.5 and 0.2 mTorr partial pressures for argon and xenon, respectively, that were used in [2]. The resultant plasma parameters at the sheath edge ($n_{\text{Ar}^+}/n_{\text{Xe}^+} = 0.75$ and $T_e = 0.34$ eV), differed from the experiment ($n_{\text{Ar}^+}/n_{\text{Xe}^+} = 1$ and $T_e = 0.7$ eV) for reasons likely related to elements (hot filament source of electrons, 3D multidipole confinement chamber, secondary electron emission, etc.) that were not simulated. Nevertheless, the feature that the simulated ion speeds are close to individual sound speeds qualitatively differs from the experimental measurements.

Previous theories have also argued that ions obtain their own sound speed at the sheath edge [3]. The primary question driving research in this area has been to explain why experiments contradict this prediction. Several experiments [2,4–6] have shown that when the densities of Ar⁺ and Xe⁺ are similar, the speed of Ar⁺ is significantly slower than its sound speed, and the speed of Xe⁺ is significantly faster than its sound speed. The most recent experiments [5,6] have shown that the density ratio of ion species is also important. When the density ratio is large or small, individual sound speeds are measured, but when the ratio is near unity, the speeds merge toward the system sound speed.

This merging suggests that ion-ion friction is important. Although the friction predicted from standard Coulomb collision theory is weak, a recent theory [7,8] shows that it is rapidly enhanced by ion-ion beam instabilities. Ion beams are formed when the presheath electric field accelerates species of different mass, or charge, to different speeds. Instabilities become excited when the difference in beam speeds surpasses a threshold determined by the ion species density ratio and thermal speeds. The theory uses this threshold and the generalized Bohm criterion to determine the speed of each species at the sheath edge [8]. The theoretical predictions have been tested

experimentally in both Ar/Xe [5] and He/Xe [6] plasmas. In both cases, good agreement is found over a broad range of ion density ratios. Experiments have also directly measured the two-stream instabilities predicted by the theory [6,9]. There is substantial evidence that Coulomb collisions and ion-ion beam instabilities are important in these plasmas, but neither effect is included in [1].

In order to capture the instability-enhanced collision process, a particle-in-cell simulation needs to include an algorithm for the instability-enhanced collision operator [10]. In addition, sufficiently fine grid spacing is required to resolve unstable waves. The lack of any Coulomb collision algorithm is an obvious flaw of the simulations, but GL also claim to see no instabilities. For the simulation parameters, theory predicts a spectrum of unstable waves centered about $k\lambda_{\text{De}} \approx 2$ (see Fig. 2 of Ref. [8]). Several grid points per Debye length are required to resolve this spectrum of instabilities. For the simulation parameters, the electron Debye length is $\lambda_{\text{De}} = 5.7 \times 10^{-3}$ cm. The grid spacing of 2000 cells in the 10 cm domain is $l_{\text{cell}} = 5 \times 10^{-3}$ cm, approximately one Debye length, which is insufficient to resolve the waves.

The authors acknowledge an anonymous referee for pointing out that the electron impact excitation cross section for argon that was used in [1] did not account for resonances that are important at low electron temperatures [11]. This may be an additional source for discrepancies between the simulations and experiments.

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