Simulations of Argon Plasma Decay in a Thermionic Converter

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The dynamics of an argon plasma in the gap of a thermionic diode is investigated using particle-in-cell (PIC) simulations. The time-averaged diode current, as a function of the relative electrical potential between the electrodes, is studied while the plasma density depletes due to recombination on the electrode surfaces. Simulations were performed in both 1D and 2D and significant differences were observed in the plasma decay between the two cases. Specifically, in 2D it was found that well defined plasma sheaths formed in front of both electrodes, while in 1D, the sheath heights varied continuously. This creates significant differences in the time-averaged diode current. In 2D simulations, it was found that the maximum time-averaged current is collected when the diode voltage is set to the flat-band condition, where the cathode and anode vacuum biases are equal. This suggests a novel technique of measuring the difference in work functions between the cathode and anode in a thermionic converter.

Introduction

Thermionic energy converters (TECs) are devices that directly convert heat into electrical energy [1, 2]. The lack of moving parts and scalability (core conversion efficiency is independent of system size) of the technology makes this type of converter appealing in a wide range of applications [3]. Furthermore, thermionics are agnostic to the source of heat used, further widening its potential for impact. Examples of heat sources include solar [4], thermonuclear [5] and natural gas [6]. In its simplest form, a thermionic diode consists of two electrodes physically separated by some gap distance (referred to as the inter-electrode gap). One electrode (the cathode) is heated to a temperature at which thermionic emission of electrons occur at a desired current density. The emitted current density is given by the Richardson equation, which relates the thermionically emitted current density to the electrode temperature and work function [7]. The other electrode (the anode) absorbs some of the thermionically emitted electrons. If the two electrodes are externally connected across a load, this process drives an electrical current through the circuit. Depending on the work functions of the two electrodes and the applied bias from the external circuit, the system can be either power producing or power consuming. Figure 1 shows a typical electron motive diagram of a thermionic diode. The electron motive diagram plots the negative of the electrical potential ($\psi = -eV$). The device produces power whenever the anode Fermi level is at a lower electrical potential than the cathode’s i.e. $V_{\text{out}} > 0$. The diagram also shows that as long as $V_{\text{out}} + \phi_a < \phi_c$, electrons are accelerated towards the anode, called the accelerating regime. Conversely, when $V_{\text{out}} + \phi_a > \phi_c$, electrons are decelerated as they move towards the anode, termed the retarding regime. The middle point, when $V_{\text{out}} + \phi_a = \phi_c$, is called the flat-band condition. This corresponds to the case where $V_{\text{out}}$ equals the contact potential difference, $\phi_c - \phi_a$.

In reality, for a vacuum thermionic diode in which the interelectrode gap is more than a few microns wide, only a small fraction of the emitted electrons make it through the gap to the anode. A space charge barrier forms in front of the cathode that reflects most of the emitted electrons back to the cathode. In such a case the diode current obeys the Child-Langmuir law [8, 9]. Various strategies have been reported to increase the fraction of emitted current that makes it to the anode. Belbachir et al. (2014) [10] used spacers to maintain a sufficiently small interelectrode gap (10 $\mu$m) to avoid the space charge problem. Meir et al. (2013) [11] and Wanke et al. (2016) [12] used additional electrodes biased positively to reduce the space charge barrier height. Unfortunately, these methods have so far been unable to produce stable, long term operation of a thermionic converter. Another approach, used more successfully in previous TEC development programs, is to use positive ions in the gap to neutralize the space charge barrier [13, 14]. Cesium plasmas have been heavily employed for this purpose, since the ionization energy of cesium is low [15, 16]. While these plasmas are effective at mitigating space charge, the energy required to maintain an arc-discharge, defined as the arc-drop, heavily reduces the efficiency of the converter [2]. This is due to the large neutral scattering cross section of cesium atoms for low

![Figure 1. Electron motive diagram to show relation of different physical parameters of interest in a thermionic diode.](image-url)
energy electrons. As a solution to this problem, using inert gas plasmas have been suggested where the Ramsauer minimum makes these gases mostly transparent to low energy electrons. Using an inert gas plasma requires the plasma ignition be engineered to be very energy efficient. This can be achieved by including highly biased auxiliary electrodes that are optimally placed to produce an inert gas plasma in the gap [17, 18]. Another way is to apply short high voltage pulses across a diode [19, 20]. As electrons accelerate towards the anode they collide with neutral atoms in the gap, causing ionization and eventually striking a plasma in the gap. A schematic of this is shown in Fig. 2. When the plasma producing pulse is turned off, the plasma starts to slowly decay to the electrodes (the dynamics of this decay are discussed in detail later). During this time, a large portion of the space charge cloud from thermionically emitted electrons is neutralized and the diode current remains high. Once the plasma density has decayed to such a level where it can no longer support high diode current, the plasma ignition pulse is repeated to start the process over again. By keeping a very low duty cycle of on-to-off phases of the ignition pulse, high time-averaged diode current can be sustained with relatively little energy spent to repeatedly strike the plasma [21].

While pulsed argon plasma thermionics have been studied concerning the energy required to repeatedly strike the plasma, little is known about the impact of output voltage on the decay dynamics of the plasma, or phrased differently, how the relative bias between cathode and anode affects the average diode current. Understanding the IV-curve of a pulsed plasma converter is important since often this is the only diagnostic available which researchers have to deduce several system parameters such as cathode and anode work functions, plasma density, gap, etc. In the following, this question is explored using particle-in-cell (PIC) simulations. The decay of an argon plasma in the gap of a thermionic converter as a function of time was studied with different biases applied to the anode relative to the cathode. Specifics of the simulation setup are discussed in the Methods section. It was found that the plasma lifetime is strongly dependent on the anode bias, and is slowest at flat-band. Thereby a characteristic of the IV-curve was identified that allows extraction of the difference in electrode work functions. Furthermore, simulations were performed in both 1D and 2D, and it was found that the decay characteristics of the plasma are strongly dependent on the dimensionality of the system. The Results section describes the differences in the plasma decay under different anode biases as well as the differences that arise from dimensionality. In the Discussion section the plasma sheaths are studied to understand why the plasma decay is slowest at flat-band. The origin of the dimensional dependence is also explored.

Theoretical considerations

A well documented characteristic of pulsed inert-gas plasma thermionic converters is that once the plasma producing pulse is turned off, the plasma sheath in front of the cathode rapidly inverts from an ion-accelerating to an ion-retaining (electron-rich) sheath [21]. This is a desirable situation, since if instead the plasma producing pulse created a dense enough plasma to completely mitigate the thermionic space charge barrier for an extended amount of time, it means for some number of produced ions their decay doesn’t affect the diode current. Therefore, the energy used to create those ions was wasted. It consequently would be more energy efficient to pulse for a shorter amount of time and instead re-pulse more frequently so that each produced ion has a maximal impact on the power producing diode current. For this reason, we can assume that during the power producing phase, the cathode sheath will always be ion-retaining. According to McVey (1990) [20] the electron and ion currents can be described by the following equations:

$$J_e = \frac{2}{3} \left( J_R \exp \left( \frac{eV_c}{kT_c} \right) - J_{re} \right)$$  \hspace{1cm} (1a)$$
$$J_i = (J_i/2 - J_{ri}) \exp \left( \frac{eV_c}{kT_c} \right)$$  \hspace{1cm} (1b)$$

where $J_R$ is the Richardson current emitted from the cathode, $V_c$ is the height of the sheath in front of the cathode, $T_c$ is the cathode temperature, and $J_{r(i,e)}$ are the random ion/electron currents given by,

$$J_{r(i,e)} = \frac{en}{4} \sqrt{\frac{8k_B T_{r(i,e)}}{\pi M_{r(i,e)}}}$$  \hspace{1cm} (2)$$

where $e$ is the electron charge, $n$ the plasma density, $T$ the species temperature in the bulk plasma, $k_B$ Boltzmann’s constant, and $M$ the particle mass. Notice that
the same barrier, $V_c$, that hinders thermionically emitted electrons from entering the plasma also retains ions in the bulk plasma. This clearly indicates that achieving higher diode currents also leads to faster ion decay.

The direction of the anode sheath depends on the applied bias. Warner and Hansen (1967) [22] noted that if the anode vacuum potential is sufficiently low (compared to the cathode’s), the anode sheath will be electron-retaining (ion-accelerating). In this configuration the ion current at the anode is simply given by $J_i = 2J_{ri}$. Seeing as the lack of an anode barrier doesn’t increase the diode current, this configuration only serves to deplete the ion density, leading to shorter plasma lifetimes and consequently lower time-averaged currents. Clearly, a more favorable configuration is to also have an ion-retaining sheath on the anode side, which similarly as before gives,

$$J_e = 2J_{re}$$

$$J_i = (J_i/2 + J_{ri}) \exp \left( \frac{eV_a}{kT_a} \right).$$

If we assume a perfectly neutral and uniform plasma without sheaths, an electric field will exist in the gap with $E = (V_c - V_a)/d$, where $d$ is the interelectrode gap distance. This field vanishes when $V_c = V_a$ or equivalently (see Fig. 9 of Ref. [13]) when $V_{int} = \phi_e - \phi_a$. Although this argument serves to form intuition, in a real system plasma sheaths will be present and their heights will be affected by the energy distribution of the plasma particles. Seeing as the sheaths determine the plasma decay rate, correctly calculating their properties are vital to obtaining an accurate picture of the plasma decay. For this reason PIC simulations were used since the first principle nature of these calculations provide the required accuracy in describing the plasma sheaths. The PIC simulations discussed in the following sections show that the critical point that leads to the longest plasma lifetime and highest time-averaged current corresponds to the flat-band condition.

The approximate plasma decay constant at flat-band was derived by Rasor (1991) [13], as

$$\tau = 2\tau_i \left[ \frac{2J_s/J_0}{1 + \frac{3}{8} \frac{d}{\lambda}} \right]^{T_e/T_i},$$

where $\tau_i$ is the ion crossing time, $d$ is the gap distance, $\lambda$ the electron mean free path, $J_k$ the Richardson saturation current density emitted from the cathode, $J_0$ the initial diode current density, $T_i$ the average ion temperature in the gap and $T_c$ the cathode temperature. The ion crossing time, $\tau_i = d/\bar{v}$ can be estimated by noting that the ion current is given by $J_i = ne\bar{v}$, where $n$ is the plasma density and $\bar{v}$ is the drift velocity of the ions (Eq. 2), giving

$$\tau_i = \frac{d}{\bar{v}} = 4d\sqrt{\frac{\pi M_i}{8kBT_i}}.$$  

Using typical values of the diode parameters $d = 0.5$ mm, $T_c = 1100$ °C, $T_i = 700$ °C, $d/\lambda \approx 2$ and $J_s/J_0 \approx 2$ the pulse repetition period is found to be $4\tau \approx 50$ µs. For this reason the diode current density was averaged over a 50 µs time interval of the plasma decay in the simulations discussed in this article.

Methods

The simulations discussed in this paper were performed with an adapted version of the PIC code Warp [23]. The simulations were performed by introducing a quasi-neutral plasma of a specified density between two parallel plates, as in the schematic in Fig. 2. The parallel plates are modelled as perfect conductors, thereby creating Neumann boundary conditions for the ends of the $\hat{x}$ domain and charges are absorbed when entering the conductor domains. During 2D simulations, periodic boundary conditions are used for the $\hat{x}$ domain. The conductor plate on the left of the computational domain will be referred to as the ‘cathode’, and is modelled as a thermionic emitter i.e. electrons are emitted from the face of the conductor. The emitted electrons have velocities sampled from the thermionic emission distribution derived in the Supplemental Material. The conductor plate on the right of the computational domain will be referred to as the ‘anode’.

In all simulations the cathode vacuum potential is used as the zero potential reference while the anode’s vacuum potential is varied in order to study the impact of changing the output voltage of the thermionic diode. The simulations are seeded with a neutral argon plasma of specified average density. The seeded plasma density follows a sine-distribution that peaks in the middle of the gap. Simulations of plasma ignition indicate that this is close to the expected plasma density profile (see Supplemental Material for further details), confirming the same result from Ref. [20]. The seed ions are assumed to be at the neutral gas temperature (for simplicity taken as the average of the cathode and anode temperatures) while the seed electrons are injected with a temperature equal to the cathode temperature, an assumption commonly made in modelling the beam electrons in inert-gas plasma thermionic converters, see Ref. [13] for example.

The PIC simulations are evolved up to 50 µs during which the current through the diode is continuously tracked, along with several other quantities such as the spatially resolved plasma density and electrostatic potential. Simulations were performed varying several aspects of the system including the spacing between the electrodes, the density of the initial plasma, the current density emitted from the cathode, and the density of the background neutral gas. To verify accuracy and resolution convergence of the simulations, benchmark calculations are presented in the Supplemental Material along with further details of the computational parameters.
Simulated IV-curves

Figure 3. Simulation results for a system with a 500 µm inter-electrode gap, 10 Torr background argon, initial plasma density of $10.2 \times 10^{12}$ cm$^{-3}$ and 2.2 A/cm$^2$ thermionic current emitted from the cathode ($T_C = 1100$ °C and $\phi_C = 2.1$ eV). The diode current as a function of time is shown in the top panel for different anode potentials. The average plasma density in the gap is shown in the bottom panel.

Results

2D Simulations. The first set of results, shown in Fig. 3, is for a system where the inter-electrode gap was set to 500 µm, the initial plasma density was set to $10.2 \times 10^{12}$ cm$^{-3}$, and the cathode emission current density was set to 2.2 A/cm$^2$. The simulation results show that as the diode output voltage is increased, moving into the retarding regime, the diode current is suppressed. As the diode output voltage is decreased, moving into the accelerating regime, the diode current at the start of the simulation is increased, but the plasma lifetime is significantly decreased. This leads to a rapid decrease in the diode current as the plasma density diminishes. The slowest plasma decay is seen when the diode is in the flat-band configuration, and in this configuration the time-averaged diode current is also the highest, as shown in Fig. 4. The same simulations were done with different initial plasma densities for which the time-averaged diode current is also shown in Fig. 4. It was found in all simulated cases that the slowest plasma decay (and therefore highest time-averaged current) occurred at flat-band. This same result was also seen with simulations of different gap values ($250 \mu m, 1 \ mm$), different background pressures (15 Torr, 25 Torr) and other emission current densities (8.5 A/cm$^2$, 3.9 A/cm$^2$).

1D Simulations. The computational benefit of being able to do 1D simulations that accurately describe systems with translational invariance is clear. Unfortunately, it was found that the specific simulations discussed in this paper do not have the same results when performed in 1D as in 2D.

As shown in Fig. 4, it was found that the plasma decay simulated in 2D did not match results from performing the same simulation in 1D. Specifically, 1D simulations consistently showed a slower decay of the plasma density at both the positive and negative bias extremes. This leads to higher average current densities through the diode except around flat-band where the 1D simulations predict lower current density than the 2D cases, despite the higher plasma density. This causes the 1D simulations to predict flatter IV-curves with peaks in the retarding regime rather than at flat-band.

The difference in plasma decay characteristics between the 1D and 2D simulations are manifested in the elec-

Figure 4. Time-averaged diode current for the output voltage cases shown in Fig. 3 as well as cases with different initial plasma densities. In all three cases the time-averaged current peaks at the flat-band condition.

Figure 5. Average plasma density as a function of time for different output voltages showing results from 1D (dashed) and 2D (solid) simulations. Note the stark differences in the final plasma density between the two cases, which is the cause for the differences in time-averaged collected current. The simulation parameters were as follows: 500 µm gap, 10 Torr background argon, initial plasma density of $2.2 \times 10^{12}$ cm$^{-3}$, $T_C = 925$ °C and $\phi_C = 2.1$ eV.
Figure 6. Time evolution of the electron motive for both 1D and 2D simulations. The simulations are started with the same plasma density ($10.2 \times 10^{12}$ cm$^{-3}$), electron temperature, and ion temperature. The case shown is where the anode vacuum level is biased 0.1 V relative to the cathode’s.

electron motive evolution, as shown in Fig. 6. In 2D, the plasma screening is well captured leading to relatively smooth electrostatic potential profiles throughout the plasma decay. The time-averaged RMS deviation between the motive at $x = 0$ and the motive averaged over the x-domain is only 3.1 meV, showing that small charge inhomogeneities are well screened by the surrounding plasma. In 1D, however, the reduced dimensionality of the simulations is unable to capture the plasma screening sufficiently leading to abrupt changes in the electrostatic potential as small regions of charge separation form. Around flat-band, these potential variations lead to a higher average barrier for beam electrons (see Fig. 6) resulting in an under-prediction of the diode current compared to the 2D case. A cut of the electron phase space ($z$ vs $v_z$) is shown in Fig. 7 at different times. The phase space plots show a beam instability in both 1D and 2D. However, in 2D the wavelength of the beam instability increases as time progresses, indicating a damping of its growth (not seen in 1D). This damping is due to transverse scattering of the electrons off electrostatic waves, something that cannot happen in 1D since there $\vec{E} = 0$. Evidence of this is that at $t = 12 \mu$s, the transverse temperature, $T_L = \frac{m}{2k_B} \sigma v_L$, is $\sim 2964$ K in 2D but only $\sim 1939$ K in 1D. This artificially contains the plasma in the gap, leading to slower decay as shown in Fig. 5.

Discussion

The impact of diode output voltage was studied for argon plasma-based thermionic diodes. It was found that the maximum time-averaged current is collected when the diode is in the flat-band configuration. This result can be understood by studying the electron motive for differently biased cases, as shown in Fig. 8. These results confirm the intuition discussed earlier. At highly negative biases the anode sheath becomes ion-accelerating which understandably leads to fast plasma decay. At highly positive biases the plasma potential forms a minimum that is lower than either electrode’s vacuum potential. In this condition ions from the bulk plasma easily have enough energy to overcome the ion-retaining sheaths in front of either electrode, again causing a fast plasma decay. Towards the flat-band condition, the sheaths in front of both electrodes become ion-retaining and single valued, which is the desired condition for slow plasma decay. As discussed earlier, precisely at flat-band the anode sheath height reaches its maximum (which leads to the slowest ion decay to it). Interestingly, for the time interval considered, the averaged cathode sheath height is also larger at flat-band than for the positively biased cases considered. This also contributes to slower plasma decay. The result of considering the full 50 $\mu$s decay time shows that the benefit of the slower decay here outweighs the penalty of a slightly larger barrier index, since the flat-band condition was found to collect the highest time-averaged diode current. Seeing as at flat-band the plasma density decay is the slowest it is easy to see that this condition will provide the optimal output power from a pulsed plasma thermionic converter. In this condition the remaining plasma density is highest when the next pulse is started, therefore the required pulse to restore the plasma density to a desired level will be the shortest. This leads to lower energy cost to maintain high diode current, which gives the maximal net output power.

Furthermore, this result provides a novel technique to measure the difference in work functions between the
cathode and anode in a thermionic converter. In practice, it is very difficult to determine electrode work functions in operating thermionic diodes. Typically, the work functions will be sensitive to temperature, as is the case with dispenser cathodes [27] and refractory metal electrodes that rely on cesium-oxide coverage to achieve useful work functions [28]. Furthermore, evaporation and deposition of electrode material on the opposite electrode greatly alters the electrode work functions. For these reasons, measurements have to be done in operating conditions to be reliable. The results discussed here indicate that an \textit{in situ} measurement of work function differences can be done by sweeping the output voltage of an operating pulsed argon plasma diode while recording the time-averaged current. A peak in the time-averaged IV-curve indicates the difference in electrode work functions. This in turn allows one to study more carefully the impact of changing operating conditions by tracking changes to work functions rather than solely the output power of the converter, which is a convoluted measurement of many factors. Experimental work is currently ongoing to test this proposed method.

It was also observed that simulating the plasma decay, using a PIC approach, resulted in different behavior in 1D than in 2D. Specifically, enhanced plasma lifetimes were seen in 1D as compared to the 2D simulations. Therefore, in its current implementation, this type of simulation cannot be done with high fidelity in 1D. It is believed that the dominant electron thermalization mechanism simulated is scattering off electrostatic waves, which excludes transverse scattering in the 1D case. Adding an anomalous scattering cross section in this case to enable transverse thermalization could recover fidelity in such simulations. This is left to future work.

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AUTHOR CONTRIBUTIONS

All authors contributed to the code development needed for the discussed simulations. RG ran the simulations and wrote the manuscript with input from the other authors.

SUPPLEMENTAL MATERIAL TO: SIMULATIONS OF ARGON PLASMA DECAY IN A THERMIONIC CONVERTER

VELOCITY DISTRIBUTION OF THERMIIONICALLY EMITTED ELECTRONS

We start by assuming the velocities of electrons that could participate in thermionic emission (electrons close to the top of the conduction band) can be well described by a Maxwellian distribution function,

\[
f_{\vec{v}}(v_x, v_y, v_z) = \left(\frac{1}{\sqrt{2\pi\sigma}}\right)^3 \exp\left[-\frac{v_x^2 + v_y^2 + v_z^2}{2\sigma^2}\right], \quad (6)
\]

where \(\sigma = \sqrt{\frac{k_B T}{m}}\) is the thermal velocity of an electron. Let the cathode work function be \(\phi\) and assume an idealized step function in the potential between the interior of the cathode and the vacuum. By assumption there is no barrier to escape in the \(\hat{x}\) or \(\hat{y}\) directions so these velocity components are not perturbed. In the \(\hat{z}\) direction, however, only particles with \(v_z > 0\) and \(\frac{1}{2}mv_z^2 > \phi\) can escape from the cathode. Hence, the electrons that can be thermionically emitted are characterized by

\[
v_z^* > \sqrt{\frac{2\phi}{m}}. \quad (7)
\]

The cumulative distribution function for the longitudinal velocity of electrons that will be thermionically emitted just prior to emission, is thus given by:

\[
P\left(v_z \leq v_z^* \Big| v_z > \sqrt{\frac{2\phi}{m}}\right) = \begin{cases} 0, & v_z^* < \sqrt{\frac{2\phi}{m}} \\ \frac{4}{\pi}, & v_z^* \geq \sqrt{\frac{2\phi}{m}} \end{cases} \quad (8)
\]
where

\[
A = \int_{\frac{v_z^*}{\sqrt{2m}}}^{v_z^*} f(v_z) dv_z = \frac{1}{2} \left[ \text{erf} \left( \frac{v_z^*}{\sqrt{2}\sigma} \right) - \text{erf} \left( \frac{\sqrt{2\phi/m}}{\sqrt{2}\sigma} \right) \right]
\]

\[
B = \int_{\frac{v_z^*}{\sqrt{2m}}}^{\infty} f(v_z) dv_z = \frac{1}{2} \left[ 1 - \text{erf} \left( \frac{\sqrt{2\phi/m}}{\sqrt{2}\sigma} \right) \right].
\]

(9a)

(9b)

We can now get the distribution function by differentiating the CDF above, giving

\[
f_{\text{inside}}(v_z') = \begin{cases} 
0, & v_z' < \sqrt{\frac{2\phi}{m}} \\
\frac{1}{\sqrt{2\pi}\sigma} \exp \left( -\frac{v_z'^2}{2\sigma^2} \right), & v_z' \geq \sqrt{\frac{2\phi}{m}}
\end{cases}
\]

(10)

Finally, we compute the velocity distribution function immediately outside the cathode. Conservation of energy requires that the electron kinetic energy be reduced by \(\phi\) upon escaping the cathode, so

\[
v_z' = \sqrt{v_z^2 - \frac{2\phi}{m}}.
\]

(11)

We now use the change-of-variables rule for probability distributions to calculate the distribution of \(v_z'\) from Eq. (10) giving,

\[
f_{\text{outside}}(v_z') = \begin{cases} 
0, & v_z' < 0 \\
\frac{1}{\sqrt{v_z'^2 + \frac{2\phi}{m}}} \exp \left( \frac{v_z'^2 + \frac{2\phi}{m}}{2\sigma^2} \right), & v_z' \geq 0
\end{cases}
\]

(12)

Seeing as there is no barrier in the \(\hat{x}\) or \(\hat{y}\) directions we have

\[
\begin{align*}
&f_{\text{outside}}(v_x') = f_{\text{inside}}(v_x) \\
&f_{\text{outside}}(v_y') = f_{\text{inside}}(v_y).
\end{align*}
\]

(13a)

(13b)

In the typical case of thermionic converters, cathode work functions are on the order of a few eV while temperatures are on the order of 0.1 eV, thus \(k_B T \ll \phi\). In this regime we can take

\[
v_z'^2 = \frac{2\phi}{m}
\]

and Eq. (12) simplifies to

\[
f_{\text{outside}}(v_z') = \begin{cases} 
0, & v_z' < 0 \\
\frac{1}{\sqrt{-v_z'^2}} \exp \left( -\frac{v_z'^2}{2\sigma^2} \right), & v_z' \geq 0
\end{cases}
\]

(14)

This distribution is used to sample the \(\hat{z}\) direction velocities of electrons injected in the PIC simulations discussed in the main paper.

PLASMA DENSITY PROFILE AFTER IGNITION PULSE

The simulations discussed in this article started with seeded plasma densities distributed according to a sine function. This distribution was chosen after simulations of plasma ignition indicated that it is a good approximation for the plasma density formed, as shown in Fig. [9]. The seed density specified in the labels of figures refers to the plasma density at the maximum point (in the middle of the gap).

Figure 9. Plasma density after ignition as simulated in Warp, by applying a 25 V bias across a diode of 500 \(\mu\)m gap for 100 ns. Also shown is a sine function scaled to have a wavelength of \(d/2\).

CODE MODIFICATIONS

As mentioned in the main manuscript, the PIC simulations discussed in this article were performed using an adapted version of the code Warp [23, 25]. The main modifications made to the code included:

- a reimplementation of the MCC scheme using the collision cross-sections as parameterized in the oopd1 [29] code
- direct solvers were written to solve Poisson’s equation in the field solve step of the PIC procedure as this was found to be much faster than the multi-grid solver implemented in Warp (specifically for 2D problems where the \(z\)-domain is much larger than the \(x\)-domain). The 1D solver uses Gaussian elimination to efficiently solve the 1D Poisson equation while the 2D solver uses superLU to decompose the finite difference matrix and quickly solve the linear system.
**CODE BENCHMARK**

The MCC implementation, we added to Warp, was benchmarked against the PIC code *opd1*, through the python wrapper *pypd1* [29]. The plot in Fig. 10 shows the ion density evolution during plasma ignition in a 1 mm diode over 200 ns.

As a second test, the plasma ignition in a 500 µm gap diode with 1 Torr of argon and the anode biased to 25 V was simulated. The current collected on the anode as a function of time as calculated with *pypd1* was compared to the same calculation done in 1D and 2D in *Warp*. Results for this test are shown in Fig. 11. The test shows that the MCC implementation in the modified *Warp* code behaves the same in 1D as in 2D and that the implementation is correct (compared to the independent code *pypd1*). This indicates that the differences seen in 1D and 2D as highlighted in the article are due to the dimensional dependence of the problem, not the PIC implementation.

**COMPUTATIONAL PARAMETERS AND CONVERGENCE STUDY**

The simulations discussed in this article were all done with spatial resolution of 0.7 µm. This value was chosen as it is at least 30% less than the Debye length of the densest plasma simulated, which was 1.03 µm. The PIC timestep was chosen as the maximum value such that the CFL condition is still satisfied, assuming a maximum electron energy of 5 eV (much higher than the average energy simulated). This resulted in a timestep of $6.15 \times 10^{-13}$ s. The 1D simulations injected 5 macroparticles per timestep and assumed an emission area of 1 m². The macro-particle weighting was then determined by the Richardson saturation current for the temperature conditions simulated. The 2D simulations used 24 cells in the x-direction from which 1 macroparticle was emitted every timestep. The y-length was taken as 1 m for the calculation of the emission area and consequently macro-particle weight. In both 1D and 2D the initial plasma density was simulated with 100 macro-particles per cell, with the weights scaled according to a sine-distribution in order to have the plasma density follow a sine-distribution as discussed earlier. A study to check whether the number of particles injected per timestep was sufficient to achieve converged results was performed by running a case with a 500 µm gap, cathode temperature of 1100 °C, cathode work function of 2.1 eV, initial plasma density of $6.1 \times 10^{12}$ cm⁻³ and background argon pressure of 10 Torr. The simulation was run up to 20 µs of simulation time and the average current compared
for different macro-particle injection settings. The results are shown in Fig. 12. The middle case (NPPC = 5) is what was used for the results discussed in the article. As can be seen in Fig. 12, the simulation results do not change significantly when increasing the macro-particle injection rate.

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