Sheath and presheath in ion-ion plasmas via particle-in-cell simulation

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A full particle-in-cell simulation is developed to investigate electron-free plasmas constituted of positive and negative ions under the influence of a dc bias voltage. It is shown that high-voltage sheaths following the classical Child-law sheaths form within a few microseconds (which corresponds to the ion transit time) after the dc voltage is applied. It is also shown that there exists the equivalent of a Bohm criterion where a presheath accelerates the ions collected at one of the electrodes up to the sound speed before they enter the sheath. From an applied perspective, this leads to smaller sheaths than one would expect. © *2008 American Institute of Physics*.
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Ion-ion plasmas are plasmas that consist of positive and negative ions only (electron-free plasmas); in practice, a small amount of electrons can exist, provided that the main negative charge carriers remain the negative ions. These plasmas have been investigated both experimentally[1–4] and theoretically.[5–8] Ion-ion plasmas may be formed in the afterglow of pulsed discharges in electronegative plasmas,[9,10] in electron-beam-generated plasmas,[11,12] by magnetic filtering of electronegative plasmas,[2,4,13] etc. Ion-ion plasmas have many potential applications. In particular, Kanakasabapathy *et al.*[14] and Walton *et al.*[11,12] have shown that comparable fluxes of positive and negative ions can be extracted from an ion-ion plasma using a low-frequency sinusoidal bias, which could be useful in material processing to minimize charging in the fabrication of microelectronic devices. Ion-ion plasmas are also important in negative ion sources, dusty plasmas, and in the D layer of the atmosphere (see Ref. 15 and references therein). Finally, it was also recently proposed by Chabert[16] that ion-ion plasmas are a promising solution for electric space propulsion. Midha and Economou[6] and Midha *et al.*[7] have developed a time-dependent fluid model to investigate the dynamics of an ion-ion plasma under the influence of a rf and a dc voltage and found that the sheath structure differed profoundly from conventional electron-ion plasmas. However, the size of the sheath and existence of a presheath were not investigated in details. The sheath, the presheath, and their formation are fundamental features in the design of extracting grids for ion beam generation. In the present letter, a self-consistent particle-in-cell (PIC) simulation (no *a priori* assumption on the various energy distributions) is developed to investigate ion-ion plasmas. In particular, it is shown that under the influence of a dc bias, Child-law type sheaths form within a few microseconds (which corresponds to the ion transit time) and the charged species collected at one of the electrodes is preaccelerated up to the sound speed by a presheath. The consequence of this finding is twofold: the ion velocity at the entrance of the sheath of an ion-ion plasma is larger than the average velocity along one direction of a thermal distribution and, consequently, the sheath size is smaller, which, from an applied perspective, is crucial. Finally, the use of a full PIC simulation allows to investigate more complex situations (different masses for positive and negative ions, etc.): an example is given at the end of the letter.

The one-dimensional simulation that we have developed is based on the well-known particle-in-cell scheme.[17,18] The boundaries are absorbing; the left and the right electrodes are biased to the potential $V_0>0$ and $-V_0$, respectively (the total dc bias is $2V_0$). It is assumed that the ion-ion plasma is created *outside* the simulation and that it enters the simulation box from the top, which comes down to loading particles in the entire volume with a uniform probability profile (including in the sheaths). The initial velocity of each ion loaded into the simulation is chosen randomly from a 300 K Maxwellian distribution.[19] The conservative transport of the positive and negative ions is to be investigated; hence, no recombination between positive and negative ions is considered. Finally, the plasma is assumed collisionless.

The results presented in the following are for a 1-cm-long system represented by 1500–2500 cells. Simulations are between 10 and 100 ms long, with time steps between 10^{-10} and 10^{-9} s. Up to 2×10^6 macroparticles per species were used. Finally, the properties (mass, injection temperature, and charge) of positive and negative ions were taken equal ($m_+=m_-=40$ amu, $T_+=T_-=300$ K, and $q_+=-q_-=e$).

Figures 1(a) and 1(b) show the steady-state time-averaged electric potential and the charged species densities across a typical ion-ion plasma simulation, respectively. The dc bias was $2V_0=50$ V and the bulk density was $\sim10^{16}$ m^{-3}. The most striking feature observed in Fig. 1(a) is that the plasma potential in the bulk is not the most positive potential of the system (as opposed to electron-ion plasmas) and actually sits halfway between the cathode and the anode potentials. The second interesting feature is the existence of a negatively charged sheath at the anode (left side) and a positively charged sheath at the cathode (the negatively charged sheath edge is shown by the vertical dotted line and was defined as the position where the relative space charge exceeds 10%). Midha and Economou[6] and Midha *et al.*[7] found similar results using a fluid model but did not investigate the size of the sheath and the existence of a presheath.

The electric potential in the bulk of the ion-ion plasma looks almost perfectly flat [Fig. 1(a)], suggesting that ions enter the sheath with a thermal flux $\Gamma=n\bar{u}/4=n\overline{|u_x|}/2$

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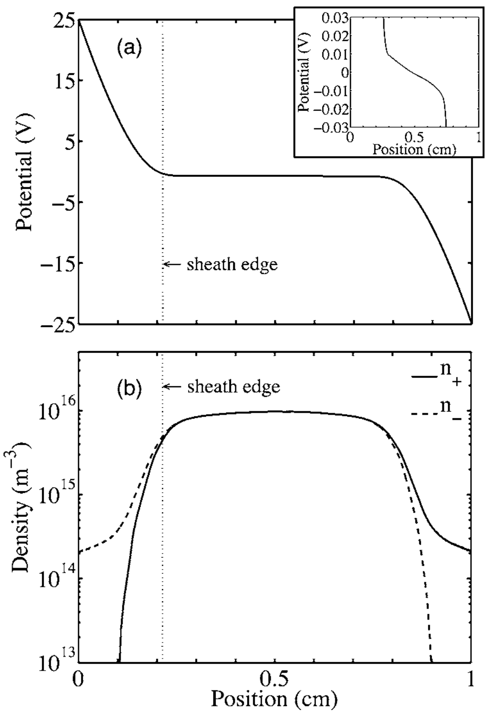

FIG. 1. (a) Electric potential across the plasma, averaged over 10 ms. The inset is a zoom on the same potential and shows the presheath. (b) Positive (solid line) and negative (dashed line) ion densities as a function of position, averaged over 10 ms. The vertical dotted lines in (a) and (b) show the anodic sheath-presheath boundary ($\Delta n/n > 10\%$).

$=n\sqrt{k_B T_{\pm}/2\pi m_{\pm}}$ (where $\bar{u}$ and $\overline{|u_x|}$ are the average velocity and the average along one direction of a Maxwellian distribution, respectively). However, a zoom [inset of Fig. 1(a)] reveals that there exists a small potential drop ($\sim$0.01 V) between the center of the discharge and the sheath edge. The potential drop is of the order of the ion temperature and more precisely around $k_B T_{\pm}/2e$. This suggests that, in the same fashion as in electron-ion plasmas, there exists a finite-field region, a presheath, preaccelerating the collected species to a critical velocity before it enters the sheath. Figure 2 shows the average positive (solid line) and negative (dashed line) ion velocities as a function of position. It appears that both positive and negative ions are accelerated to the directed velocity of around 250 m/s at the sheath edge (shown by the vertical dotted line). The velocity reached at the sheath edge

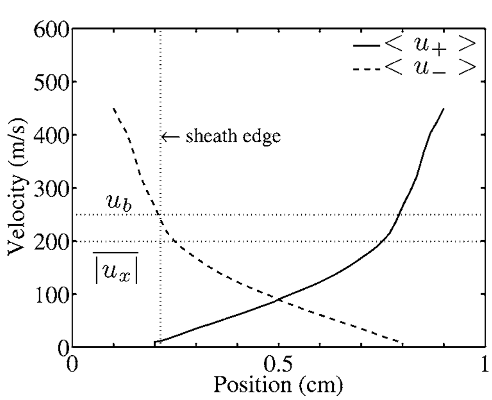

FIG. 2. Average velocity (absolute value) of the positive (solid line) and negative (dashed line) ions as a function of position corresponding to Fig. 1(a). The two horizontal dotted lines represent the Bohm velocity u_b and the average velocity $\overline{|u_x|}$ along one direction of a thermal distribution, while the vertical dotted line shows the anodic sheath edge ($\Delta n/n > 10\%$).

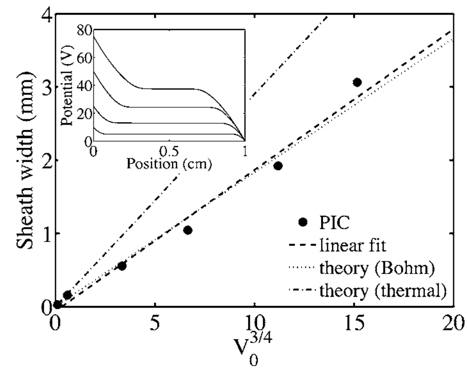

FIG. 3. Sheath width as a function of $V_0^{3/4}$. The black circles (●) are sheath widths from the simulation and the dashed line is the corresponding linear fit, while the dotted and the dotted-dashed lines are the sheath widths predicted by the theory assuming a Bohm velocity and a thermal velocity, respectively. The inset shows the electric potential across the plasma for various dc biases $2V_0$. Note that for clarity, the potential profiles in the inset were plotted with the right electrode shifted to the same potential reference.

corresponds almost perfectly to $u_b = \sqrt{k_B(T_+ + T_-)/(m_+ + m_-)}$, which is the Bohm velocity where the usual electron temperature was replaced by that of negative ions. This confirms that the collected species does not enter the sheath with a thermal velocity but is preaccelerated by a presheath and that the equivalent of a Bohm criterion exists for ion-ion plasmas.

The width s of the high-voltage sheath in classical electron ion is derived using the positive ion current continuity at the plasma/sheath interface, i.e., by equating the Child-law current to the Bohm current.[20] The sheath width is then given by

$$s = \frac{2}{3}\left(\frac{2}{ek_B}\right)^{1/4}\left(\frac{\epsilon_0}{n_s}\right)^{1/2}\frac{V_0^{3/4}}{T_e^{1/4}}. \tag{1}$$

where n_s is the sheath edge density, V_0 is the applied potential, and T_e the electron temperature. Since an equivalent of the Bohm criterion exists in ion-ion plasmas, it can be intuited that the size of the high-voltage sheath in such plasmas follows the same relation as depicted by Eq. (1), with T_e replaced by $T_{\pm}$. The inset in Fig. 3 shows the ion-ion plasma potential profile for various bias potential V_0: the sheath width increases with V_0. Figure 3 shows the sheath width s (where the sheath edge is defined as previously) as a function of $V_0^{3/4}$ (black dots). These widths can be well fitted by a straight line (dashed line) which the slope is very close (within 5%) to the theoretical one given by Eq. (1) and where the electron temperature T_e was replaced by the ion temperature T_+ (here, the negative ion sheath is considered). The dotted-dashed line shows the theoretical sheath width if ions were entering the sheath with a thermal velocity rather than with the sound speed (i.e., if there were no presheath). These results show that because of the existence of an equivalent of the Bohm criterion for ion-ion plasmas, the velocity of the ions entering the sheath is larger than just a thermal velocity and the sheath size is, therefore, smaller by a factor of almost 2.

As mentioned previously, the PIC simulations also allow us to investigate various complex ion-ion plasmas (as opposed to the previous ideal case with equal masses and temperatures); in particular, it is possible to investigate multi-ion plasmas, ion-ion plasmas where positive and negative ions do not have the same mass and temperature, the effect of

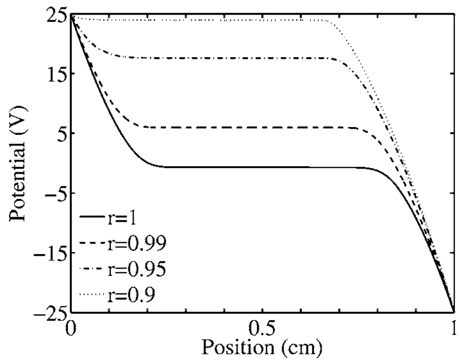

FIG. 4. Electric potential across the plasma, averaged over 10 ms for various negative to positive ion mass ratios; the solid, dashed, dotted-dashed, and dotted lines are for $r=m_-/m_+$ equal to 1, 0.99, 0.95, and 0.9, respectively.

collisions on the sheath size, the impact of the presence of a small amount of electrons, etc. As an example, Fig. 4 shows the plasma potential profiles for ion-ion plasmas for various positive to negative ion mass ratios. It is observed that even a slight difference in the masses (as small as 5%) yields a strong asymmetric potential, where the bulk potential sits much closer to one of the electrodes, hence, getting closer to a conventional electron-ion plasma.

In the present letter, we have shown that when a dc voltage is applied across an ion-ion plasma, a presheath appears in order to satisfy the sheath formation conditions: an equivalent of the Bohm criterion (where the usual electron temperature is replaced by that of negative ions) exists. The consequence of this finding is twofold: (i) in ion-ion plasmas, ions entering the sheath are faster than thermal ions; (ii) consequently, the sheath size is smaller by a factor of almost 2. From an applied perspective, these results are crucial as it has been suggested by many authors that ion-ion plasmas could be used in material processing and space propulsion, where the design of extracting grids to create an ion beam is strongly related to the size of the sheaths.

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[1]N. Sato, T. Mieno, T. Hirata, Y. Yagi, R. Hatakeyama, and S. Iizuka, Phys. Plasmas **1**, 3480 (1994).
[2]H. Amemiya, Jpn. J. Appl. Phys., Part 1 **30**, 2601 (1991).
[3]W. Oohara, R. Hatakeyama, and S. Ishiguro, Phys. Rev. E **68**, 066407 (2003).
[4]W. Oohara, D. Date, and R. Hatakeyama, Phys. Rev. Lett. **95**, 175003 (2005).
[5]V. I. Kolobov and D. J. Economou, Appl. Phys. Lett. **72**, 656 (1998).
[6]V. Midha and D. J. Economou, J. Appl. Phys. **90**, 1102 (2001).
[7]V. Midha, B. Ramamurthi, and D. J. Economou, J. Appl. Phys. **91**, 6282 (2002).
[8]M. Lampe, R. F. Fernsler, S. P. Slinker, S. G. Walton, and D. Leonhardt, *58th Gaseous Electronics Conference*, San Jose, CA (American Physical Society, Ridge, New York, 2005).
[9]I. D. Kaganovich, D. J. Economou, B. N. Ramamurthi, and V. Midha, Phys. Rev. Lett. **84**, 1918 (2000).
[10]V. Midha and D. J. Economou, Plasma Sources Sci. Technol. **9**, 256 (2000).
[11]S. G. Walton, D. Leonhardt, R. F. Fernsler, and R. A. Meger, Appl. Phys. Lett. **81**, 987 (2002).
[12]S. G. Walton, D. Leonhardt, R. F. Fernsler, and R. A. Meger, Appl. Phys. Lett. **83**, 626 (2003).
[13]W. Oohara and R. Hatakeyama, Phys. Rev. Lett. **91**, 205005 (2003).
[14]S. K. Kanakasabapathy, L. J. Overzet, V. Midha, and D. Economou, Appl. Phys. Lett. **78**, 22 (2001).
[15]D. J. Economou, Appl. Surf. Sci. **253**, 6672 (2007).
[16]P. Chabert, Patent Application No. WO 2007/065915 A1 (pending).
[17]R. W. Hockney and J. W. Eastwood, *Computer Simulation Using Particles* (IOP, Bristol, 1988).
[18]C. K. Birdsall and A. B. Langdon, *Plasma Physics via Computer Simulation* (IOP, Bristol, 1991).
[19]K. L. Cartwright, J. P. Verboncoeur, and C. K. Birdsall, J. Comput. Phys. **162**, 483 (2000).
[20]M. A. Lieberman and A. J. Lichtenberg, *Principles of Plasma Discharges and Materials Processing*, 2nd ed. (Wiley Interscience, New York, 2005), p. 177.