PIC Simulation of a Double Layer Formation in a Hydrogen Plasma with Negative Ions

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1. Introduction

Plasmas containing negative ions have been and still are investigated very intensively because of their importance in various technological processes for treatment of materials [1]. Negative ion hydrogen and deuterium plasma sources are used in installations for netral beam heating of fusion plasmas. In this contribution we present results from computer simulation experiments on potential double layer formation in negative ion hydrogen plasma. They are compared with analytically obtained results from a fully kinetic treatment.

2. Model

The kinetic plasma-sheath model considers a planar source of half-Maxwellian positive and negative ions and electrons. Such planar source aproach to the presheath/sheath theory is based on work by Emmert et al. [2] in which they showed that the potential drop through the distributed plasma source region is independent of the source width, and can be therefore modelled as a planar source with a subsequent source sheath potential drop [3]. The collisionless source sheath and presheath region is bounded on the other side by the presheath/sheath interface. In the system the potential is assumed to decrease from the source towards the collector and, according to the solutions of the steady-state Vlasov equation, negative ions and electrons are described by a truncated full Maxwellian velocity distribution and positive ions by an accelerated half-Maxwellian distribution function. The collector potential and the plasma source sheath potential drop are evaluated as functions of negative ion fraction and negative ion to electron temperature ratio using Poisson equation.

3. Simulation

The plasma system is only 2 cm (~ 100 \( \lambda_D \)) long in order to complete simulations in a reasonable time span. The simulations are run in a similar way as in our study of the plasma...
with two electron populations [4]. Initially the simulation region is empty. Positive ions, electrons and negative ions are then injected with equal fluxes, \( j^\pm = j_0 = j_{\text{e}0} \). The particles that return to the source are refluxed in the system with a velocity characteristic of their source temperature. There is no charge accumulation at the source, the electric field is zero. Since all negative ions are always reflected to the source, except at very high density ratios, the system would never reach the steady state. For this reason we run the simulation in the following way: at the moment when the total number of negative ions reaches the predetermined value on which the final value of \( \alpha \) depends, the process is stopped and the situation saved as dump file. The simulation is then restarted with the same input file but with zero negative ion injection current, \( j^\pm = j_{\text{e}0} \). The system is then allowed to reach the steady state. The results are analysed by the use of several built-in diagnostic tools.

**Fig.1.** a) Potential profiles in a hydrogen plasma for different values of \( \alpha \) density ratio \( \alpha_\text{e} \). A double layer-like potential step formation is clearly observed in plasmas with certain values of \( \alpha_\text{e} \). b) Density profiles of \( H^+ (\text{pi}), H^- (\text{ni}) \) and electrons (e) in the same plasma. Double layer stratification of the plasma is observed.

### 4. Results and conclusions

Since the main objective of the investigation is the formation of a double layer structure and the corresponding stratification of the plasma system, we choose for the simulation the appropriate parameter regime as already indicated in theoretical analysis [5]: \( \tau_\text{e}^{-1} = T_e/T_\text{e} = \gamma = 10 \) and \( 40, \tau_\text{e} = T_e/T_\text{e} = 0.1, T_e = 2 \text{ eV} \). We investigate a hydrogen plasma, therefore we put \( \mu = M_\text{e}/M_\text{e} = 1 \). The value of \( \gamma = 10 \) lies just below the critical value \( \gamma_c = 12.20 \) above which multiple solutions for presheath potential boundary value \( \psi_P \) were found. Under certain conditions, determined by the values of the negative ion fraction \( \alpha_\text{e} = n_-/n_+ \) and depending on \( \gamma \), a double layer potential structure is formed in the presheath region. At this
Fig. 2. a) Relative density difference (= net space charge) in a plasma with $\alpha_+ = 0.63$ and $\gamma = 40$. On the expanded plot b) a clear formation of space charge double layer is observed.

Fig. 3. a) Electron velocity distribution functions obtained from simulation, plotted in a logarithmic scale to show the truncation at negative (reflected electrons) high velocity tail more clearly. The acceleration of electrons through the double layer can be seen (cs – ss). b) Comparison of electron velocity distribution functions at two locations in the system (ss – source side, cs – collector side of the double layer) with those from simulation. Theoretical curves represent full Maxwellian distribution functions.

special potential drop the negatively charged species are separated and a structured plasma system is formed as can be observed from Fig.1.and Fig.2. Potential profiles, density profiles and particle velocity distributions along the axis of the system are studied for different values of $\alpha_+$. and the results compared with the results obtained from a fully kinetic theoretical model [5]. Good accordance is found as can be seen on Figs 2., 3, 4 and 5. It should be pointed out that the region of $\alpha_+$ in which the double layer is formed is different than found by other investigators [6]. In our case the double layer is formed after the floating potential solutions transfer to the lower branch as can be seen on Fig. 5. As presented by [6], at these values of $\alpha_+$, the double layer already disapeared in the collector sheath and a uniform plasma was formed. The discrepancy will be further investigated.
Fig. 4. a) Positive ion velocity distribution functions from simulation shown at two locations in the plasma system (ss – source side, cs – collector side of the double layer) and compared with theoretical accelerated half-Maxwellian distribution functions. b) Negative ion velocity distribution function from simulation compares very good with calculated full-Maxwellian distribution function.

Fig. 5. The normalized potential $\psi_P$ at the presheath-sheath boundary (left) and the normalized collector potential $\psi_C$ (right) as a function of negative ion density fraction $\alpha$ for two values of negative ion temperature ratio $\gamma$. Solid data points indicate values from simulation.

5. References