Mathematical Formulation and Numerical Modelling of the Extraction of H⁻ ions

Reinard Becker
Institut für Angewandte Physik der Johann Wolfgang Goethe – Universität, Fach 180
D-60054 Frankfurt/M, Germany

Abstract. In the past, ion extraction of volume produced H⁻ ions has either been simulated with programs for the extraction of positive ions [1] or by programs, which wrongly claimed to have a “real” and “genuine” option for H⁻ ions [2]. Although “reasonable” results have been obtained in both ways, the mathematical formulation of the physics at the plasma sheath is wrong, and the modelling of electrodes near the sheath [3] must fail. In this paper a self consistent formulation of the extraction problem for H⁻ ions is presented, which takes into account any number of positive ions, like fast or thermal protons, thermal cesium and molecular ions like H₂⁺ and H₃⁺, which all are essential for the generation of H⁻ ions in the plasma volume. Equally important is the porting of this formulation to a simulation program and the verification of experimental results. This has lead to the development of the program nlGUN⁷.

INTRODUCTION

The present theory is the result of several steps of development: In 1997 the virtual cathode behaviour of protons, entering the plasma sheath and being reflected by the field for H⁻ extraction has been pointed out [4], however, without considering the role of thermal positive ions, like molecules and cesium ions in the case of cesium seeding. This feature has been added in 2002 [5] for one kind of thermal ions. In 2003 the attempt has been made, to include the whole sheath from the plasma potential to the extraction in one theory [6]. This, however, is too comprehensive, because the important effect of changing the electron to H⁻ fraction by a bias of the plasma electrode [7] cannot be treated in a linear sheath model. The present formulation therefore is an extension of the 2002 theory, allowing for any number and kind of positive ions in front of the plasma electrode, like protons coming from the plasma potential and protons, molecules, and cesium ions with thermal energy, being created in the neutralized vicinity of the plasma electrode. Since H⁻ are assumed to be thermal there, it will not matter, if these will be produced by surface or by volume processes. Other work on the extraction of H⁻ ions is reviewed in ref. [6]. PBGUNS [2] uses wrong expressions for the electron space charge and ignores fast positive ions as well as additional thermal ones, like cesium and molecules.
THE INVERTED SHEATH

In contrast to positive ion extraction, where the potential fall in the sheath is continued by the acceleration field of the extraction potential [8], ion sources for H\textsuperscript{-} production are more complex: The natural potential fall of the plasma sheath needs to be reversed for the extraction of negative ions (and electrons). In general this is provided by a transverse magnetic field (filter) in front of the plasma electrode, which forces fast electrons to follow the flux lines, while slow ones may have enough collisions to move across them by ambipolar diffusion. This localized changes of the electron velocity distribution and of the electron density will cause a fall of potential towards the plasma electrode, favouring the migration of H\textsuperscript{-} ions into this region [9]. According to the axial potential model shown in Fig. 1, we can formulate the space charge term for each kind of particle in the extraction region, which is the region of interest for this paper:

\[ U(Z) \]

\[ U_p \]

\[ U = 0 \]

\[ \text{birth of protons and other fast positive ions} \]

\[ \text{plasma potential} \]

\[ \text{region of interest} \]

\[ \text{birth and trap for thermal positive ions} \]

\[ \text{birth of H}^- \]

**FIGURE 1.** Axial potential model for the definition of space charges in the extraction region

The density of electrons with energy \( U_e \) will be reduced by acceleration in the same way as the H\textsuperscript{-} density:

\[ n_e(U) = \frac{n_e(0)}{\sqrt{1 + \frac{U}{U_e}}} \]

\[ n_-(U) = \frac{n_-(0)}{\sqrt{1 + \frac{U}{U_-}}} \]  

(1)

the density of fast protons (and other fast ions) is dieing out by the virtual cathode process [4]:

\[ n_p(U) = n_p(0) \left( 1 - \frac{U}{U_p} \right) \]

(2)

other positive ions are considered to be thermal and trapped between the extraction field and the plasma, hence will obey a Boltzmann distribution:
This problem now has 2 unknowns for each charged particle, the density and the energy (either directed or thermal). While the energies must be known to obtain solutions, the densities can be expressed by the definition of the electron to H- current ($\Gamma$)

$$\frac{n_e}{n_-} = \Gamma \frac{m_e U_-}{M U_e}$$  \hspace{1cm} (4)

$$\frac{n_p}{n_-} = 1 + \frac{n_e}{n_-} - \frac{n_1}{n_-} \sum \frac{n_i}{n_i}$$

and by the condition of quasineutrality at $U=0$

We then calculate from the balance of charged particle currents at the plasma electrode with wall potential $U_w$ the relation of the density of the first kind of positive thermal ions to the density of H- ions:

$$n_i = \frac{1 + \Gamma - \left(1 + \Gamma \sqrt{\frac{m_e U_-}{M U_e}} \right) \left(1 - \frac{U_w}{U_p} \right)^3 \sqrt{\frac{\pi M U_p}{M U_-}}}{\sum \frac{n_i}{n_i} \left(\sqrt{\frac{M U_i}{M U_-}} \exp \left[-\frac{U_w}{U_i}\right] - \left(1 - \frac{U_w}{U_p}\right)^{\frac{3}{2}} \sqrt{\frac{\pi M U_p}{M U_-}}\right)}$$  \hspace{1cm} (5)

PARAMETER RELATIONS OF SOLUTIONS

By solving eq. 6 for assumed values of the directed or thermal ion energies and for choosing $M_1=1$ or $=133$, relations will be obtained for the parameters of solutions either without or with cesium seeding. The assumption of a negative wall potential, as used in a former presentation [5] has been dropped, because the potential model (Fig. 1) and the associated space charge terms (eq. 1-3) then will break down. In Fig. 2, the relation of parameters is shown with cesium seeding for a directed proton energy of 10 times the H-, cesium, and electron temperature. A positive wall potential always will reduce the electron to H- ratio, as observed in experiments, and the cesium ion density always must be lower than the H- density. Lower values of $\Gamma$ exist with cesium, as observed in experiments, too.
FIGURE 2. Relation of parameters for solutions of the inverted sheath with cesium seeding

FIGURE 3. Relation of parameters for solutions of the inverted sheath without cesium seeding
IMPLEMENTATION INTO nIGUN©

The 2D simulation program for positive ion extraction, IGUN© [8] has been modified to simulate negative ion extraction on the basis of the theory presented in this paper and given the name nIGUN©. The evaluation of eq. 6 is part of the input procedure. For the "real" solution, however, the densities of the different particles must be known absolutely. This is achieved by the integration of Poisson's equation with the space charge terms eq. 1-3, resulting in eq. 7:

$$\frac{E_z U^2}{2e} = n_e \left( 2 \frac{n_e}{n_-} \left[ \frac{1}{\sqrt{1 + \frac{U}{U_n}}} - 1 \right] + 2 U \left[ \frac{1}{\sqrt{1 + \frac{U}{U_n}}} - 1 \right] - \frac{n_p}{n_-} \left( U - \frac{U_p^2}{2U_p} \right) + \frac{n_i}{n_-} \sum \frac{n_i}{n_i} \left( \exp \left[ -\frac{U}{U_i} \right] - 1 \right) \right)$$

(7)

For any combination of the potential and the field strength in the extraction region the absolute H⁻ density can be determined from eq. 7. The other densities are following then from eq. 4-6. It has been found that this determination of densities is done reasonably at $U=U_p$, where the space charge of fast positive ions has disappeared. As a result, the densities of a cesium seeded plasma are shown in fig. 4 from the quasineutral plasma (on the left) towards the extraction region (right side) together with the increase of the potential function for a planar diode of 20 mesh thickness.

**FIGURE 4.** Self-consistent densities of electrons, H⁻ ions, fast protons and thermal cesium ions in an inverted plasma sheath according to the presented theory and its implementation into nIGUN©
THE 3/2 POWER LAW

Poisson’s equation for charged particles, being accelerated in a diode from zero velocity, reads:

\[
\Delta U = -\frac{\rho}{\varepsilon_o} = \frac{j}{2e \varepsilon_o \sqrt{\frac{U}{M}}} \tag{8}
\]

For H⁻ extraction, the expression for the space charge term looks quite different:

\[
\Delta U = \frac{e}{\varepsilon_o} \left\{ \frac{n_e}{\sqrt{1 + \frac{U}{U_e}}} + \frac{n_i}{\sqrt{1 + \frac{U}{U_i}}} - n_p \left( 1 - \frac{U}{U_p} \right) - n_i \sum n_i \exp \left[ -\frac{U}{U_i} \right] \right\} \tag{9}
\]

If the energy is sufficiently high, however, the contributions from positive ions disappears and the electron and H⁻ term may be approximated by:

\[
\Delta U \approx \frac{j_{H^-}}{2e \varepsilon_o \sqrt{\frac{U}{M}}} \left( 1 + \frac{\Gamma}{42} \right) \tag{10}
\]

**FIGURE 5.** Simulations with nIGUN© for a plane diode compared with the voltage\(^ {3/2} \)-law.
This shows, that for high voltages there will be approximately a 3/2 power law, but the current will be an effective one, just as described by Leitner et al. [1], when using a computer program for positive ion extraction in order to simulate the extraction of negative ions. It should be emphasized, that this asymptotic appearance of the 3/2 power law may be useful only for the prediction of the current in a planar diode, but other questions, like the shape of the plasma electrode in the vicinity of the beam boundary need a correct consideration of the potential function there. It has been found [6], that an angle of 45° between the beam boundary and the plasma boundary will provide an aberration free beam boundary, in similar way as the famous Pierce angle of 62.5° for solid emitters.

CONCLUSIONS

The presented theory for H⁻ extraction is self-consistent and can take into account any number of fast and of thermal positive ions. The axial potential function starts with vanishing field strength at the potential of the wall electrode (if there is no bias on the PE). This model accepts birth of H⁻ ions in the volume around the extraction aperture as well as on the wall electrode. In agreement with measurements, the proton energy is much lower with added cesium than without and lower values for the electron to H⁻ current are found for cesiated plasmas than for cesium free ones. The mathematical formulations have been implemented into a new program, called nIGUN© [10], for the simulation of the extraction of H⁻ ions.

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