Analysis and particle-in-cell simulation on the similarity relation during an ion extraction process

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Abstract. Ion extraction time is one of the key parameters for an ion extraction process. Particle-in-cell (PIC) simulation can provide a detailed description on the charged-particle behaviours during the ion extraction process in a decaying plasma. However, the PIC modelling is a very time-consuming task with very small space step (~ Debye length) and time step (~ inverse of plasma frequency), as well as a massive number of macro-particles, especially for the cases in multi-dimensions and large geometrical sizes. In this paper, based on the sheath expansion and ion-acoustic rarefaction wave propagation model, a similarity relation of ion extraction time with different geometrical sizes of the ion extraction regions is established. The theoretical analysis shows that, by changing the magnitude of the externally applied voltage to keep the ion extraction flux equal, the ion extraction time is proportional to the geometrical size ratio. Then, the PIC simulations on the ion extraction process are conducted, which show that there exists a good consistency with the theoretical analysis and previous experimental data. This research is helpful for promoting numerical simulations facing actual ion extraction processes with large geometrical sizes and provides theoretical guidance for improving the ion extraction efficiencies in applications.

1. Introduction

In recent years, the laser-induced isotope separation method has attracted more and more attention of researchers due to its low energy consumption and high separation coefficient. During the laser-induced isotope separation process, the target isotope is firstly heated to form an atomic vapor, and subsequently selectively ionized by a laser beam at a specific wavelength. Then, under an externally applied electrostatic field, the target ions are extracted to the collectors (ion extraction process). Effective extraction and collection of target ions are the key points of the ion extraction process. Currently, analytical method, fluid method, and particle-in-cell (PIC) method are the major theoretical research methods for studying the ion extraction process. And numerous studies have been conducted, such as analytical expressions for the ion extraction time, one- and two-dimensional simulations of the whole ion extraction process under different collector configurations (c.f., Ref. [1] and papers cited therein).

A high vacuum environment is necessary during the ion extraction process to obtain a longer existence time of charged particles. Thus, species collisions are negligible due to the relatively larger ion mean free path length compared to the characteristic length of the collector. In addition, low collision frequency brings high kinetic effects in the laser-induced plasmas indicating that the PIC method shows more appropriateness than the fluid method. However, meeting the needs of resolving electron behaviors requires enormous computing resources. For a typical laser-induced plasma with the plasma density of...
\( n_{i,0} = 10^{16} \text{ m}^{-3} \) and electron temperature of \( T_{\text{e},0} = 0.5 \text{ eV} \), the Debye length is \( \lambda_{\text{De}} = 5.3 \times 10^{-5} \text{ m} \) and the electron plasma frequency is \( \omega_k = 5.6 \times 10^9 \text{ s}^{-1} \). Therefore, the restrictions for the space and time steps with being smaller than \( \lambda_{\text{De}} \) and \( 2\pi/\omega_k \) \( (1.1 \times 10^9 \text{ s}^{-1}) \) have to be imposed in the PIC simulations to ensure correctly resolving the electron dynamics. While for a practical ion extraction device, its characteristic length is usually on the order of 10 cm. Therefore, at least 2000 grids are required in each dimension for simulating the ion extraction process, and at least \( 2.7 \times 10^4 \) time steps are needed for a 30 \( \mu \text{s} \) physical time simulation. In consequence, the preceding restrictions on the space and time intervals bring great computing challenges for the full-scale PIC simulations, especially under the multi-dimensional conditions.

In order to take the advantages of the PIC method to provide useful guidance for practical applications, a similarity law for predicting the ion extraction time in the actual devices is proposed based on the analysis of the ion extraction process in this study. The analysis and PIC simulations of the extraction process are provided in Section 2, and the theoretical derivation and simulation verification are given in Section 3. Finally, a brief conclusion is presented in Section 4.

2. PIC simulations and analysis of the ion extraction process

A parallel plate conductor configuration is employed in this section [2, 3]. A barium plasma is generated and uniformly distributed between two parallel plates at \( t = 0 \). During the ion extraction process, the left negative plate \( (x = 0) \) is fixed at potential \( -V_0 \), while the right positive plate \( (x = L) \) is grounded, as shown in figure 1(a). The species collisions are neglected due to the low environment pressure which is on the order of \( 10^{-5} \text{ Torr} \). The detailed description on the simulation method can be referred to our previous paper, and the simulation parameters are listed in Table 1 [3].

The PIC simulation results show that the stage of the sheath expansion and ion rarefaction wave (IRW) propagation play an important role in the ion extraction process. The IRW is excited due to the disturbance of the ion density and propagates with the velocity of the local ion sound velocity, \( c_s \) [4]. The sheath expansion and the IRW propagation contribute greatly to the evolution of the ion density distributions. As shown in figure 1(b), the direction of the IRW propagation is from the collector surface to the central part of the plasma, which is the same as that of the sheath expansion. When the sheath expansion velocity, \( v_{sh} \), exceeds \( c_s \), the sheath is in the phase of the supersonic expansion; in consequence, the disturbance of the ion density caused by the sheath expansion exceeds the ion sound velocity, therefore, the IRW cannot be excited. Under such a situation as illustrated by line A in figure 1(b), the ion density discontinuity appears at the interface between the sheath and the central plasma, which makes the ion density of the central plasma remain unchanged. With the continuous sheath expansion, the ions are gradually accelerated by the sheath electric field and extracted from the plasma core region. The corresponding ion extraction flux caused by the sheath expansion can be denoted by \( \Gamma_s \). On the other hand, if the value of \( v_{sh} \) is lower than that of \( c_s \), the sheath is in the phase of subsonic expansion, in which the IRW front will exceed the sheath front with the formation of the density gradient as shown by Line B in figure 1(b). For this case, the ions in the area between the IRW front and the sheath front will also be accelerated to form an extra ion extraction flux, which is expressed as \( \Gamma_{\text{IRW}} \). According to the Child-Langmuir’s Law,

\[
\Gamma_i = \Gamma_{\text{IRW}} + \Gamma_s = \Gamma_{\text{CL}} = \frac{4e_0}{9} \left( \frac{2}{em_i} \right)^{1/2} \frac{U^{3/2}}{s^2},
\]

where \( U \) is the externally applied voltage, \( e_0 \) is the vacuum permittivity, \( \Gamma_{\text{CL}} \) is the Child-Langmuir flux, \( s \) refers to the sheath thickness. When the sheath is in the phase of supersonic expansion, \( \Gamma_{\text{IRW}} \) is reduced to zero, thus,

\[
\Gamma_s = n_{i,0}v_{sh} = n_{i,0} \frac{dx}{dt} = \frac{4e_0}{9} \left( \frac{2}{em_i} \right)^{1/2} \frac{U^{3/2}}{s^2}.
\]

Since the ion sound speed can be expressed as
Figure 1. Schematics of the calculation domain for the ion extraction process (a), spatial profiles of the ion number density under different IRW propagation speeds (b), and calculated evolutions of the ion number density distributions between two parallel plates under the supersonic sheath expansion (c) and subsonic sheath expansion (d) conditions [3].

Table 1. Typical simulation parameters [3]

| Case No. | 1 | 2 |
|----------|---|---|
| Plasma width, $L$ (cm) | 2.0 |   |
| Ion mass, $m_i$ (amu) | 137 |   |
| Externally applied voltage, $U$ (V) | 400 |   |
| Initial ion temperature, $T_{i,0}$ (eV) | 27.9 |   |
| Initial electron number density, $n_{i,0}$ ($\times 10^{16}$ m$^{-3}$) | 1.0 |   |
| Initial electron temperature, $T_{i,0}$ (eV) | 0.1 | 5.0 |

The sheath thickness ($s_D$) can be obtained when the sheath front separates from the front of IRW by introducing Equation (3) into Equation (2) as follows

\[ v_{sh} = c_s \Rightarrow s_D^2 = \frac{4\varepsilon_0}{9n_{i,0}} \left( \frac{2}{eT_e + 3eT_i} \right)^{1/2} \cdot U^{3/2}. \]

The PIC modelling results revealed the spatiotemporal evolutions of the ion number density ($n_i$) under the conditions of supersonic and subsonic sheath expansions, as shown in figures 1(c) and (d), respectively [3]. It is seen clearly that, besides the sheath expansion, the IRW propagation may influence
the non-equilibrium transport characteristics of the ion extraction process. Under the subsonic sheath expansion condition, the IRW can accelerate the ions in the bulk plasma to the sheath and brings considerable ion flux to both the positive and negative electrodes, as shown in figure 1(d). In addition, our modelling results show that the higher the electron temperature is, the more ions will be accelerated in the bulk plasmas [3].

3. Similarity law for the ion extraction time

In this section, the theoretical derivation of the similarity law and the PIC simulation validations are conducted for the Π-type electrode configuration. Although the ion extraction process under the Π-type electrode configuration is no longer a one-dimensional case, the fundamental physical process is still similar to that discussed in Section 2 [5]. It is assumed that the geometrical dimensions in the PIC simulations, as shown in figure 2, are proportional to those of the full-scale experimental setup, i.e.,

\[
X = \frac{L_F}{L_S} = \frac{H_F}{H_S} = \frac{D_{x,F}}{D_{x,S}} = \frac{D_{y,F}}{D_{y,S}} = \frac{s_{o,F}}{s_{o,S}} = \frac{M_F}{M_S} = \frac{Q_F}{Q_S},
\]

where the subscripts “F” and “S” represent “full scale” and “simulated scale”, respectively.

Figure 2. Schematic of the ion extraction with a Π-type electrode configuration.

For the ion extraction with a Π-type electrode configuration, the ions are mainly collected by the two negative electrodes [5]. According to Equation (1), the total ion flux at each negative electrode can be expressed as the Child-Langmuir flux. Thus, we can adjust the magnitude of the externally applied extraction voltage to make the value of \( \Gamma_{CL} \) in the simulation equal that in the full-scale experiment, i.e.,

\[
\left[ \frac{4e_0}{9} \frac{2}{em} \frac{U^{3/2}}{s^2} \right]_F = \left[ \frac{4e_0}{9} \frac{2}{em} \frac{U^{3/2}}{s^2} \right]_S \Rightarrow \frac{U_F}{U_S} = X^{4/3}.
\]

When the sheath is in the phase of supersonic expansion, \( \Gamma_{IRW} \) can be neglected, and we can get

\[
\frac{d}{dt} n_{i,0} = \frac{4e_0}{9} \frac{2}{em} \frac{U^{3/2}}{s^2}.
\]

Do the integration on both sides of Equation (7) from \( s_0 \) to \( s_D \), we can obtain
where \( \tau_1 \) is the time of the sheath expansion. Equation (8) can be simplified if the plasma parameters are the same in the simulation and the experiment, i.e.,

\[
\frac{\left(s_d^3 - s_0^3\right)_E}{\left(s_d^3 - s_0^3\right)_S} = \left(\frac{U^{3/2} \tau_1}{\epsilon_{em}}\right)_E = \left(\frac{U^{3/2} \tau_1}{\epsilon_{em}}\right)_S.
\]

Thus, according to Equations (4), (6) and (9), we can have

\[
\frac{\tau_{1,E}}{\tau_{1,S}} = X.
\]

Equation (10) means that the ratio of the ion extraction time in the full-scale experimental setup to that of the small-size simulation case equals the scaling ratio, \( X \), under the supersonic sheath expansion condition.

For the subsonic sheath expansion process, the ion extraction time depends on the time required by the propagation of IRW from \( s = s_0 \) to the sheath front near another negative electrode, which can be given as follows

\[
\frac{\tau_{1,E}}{\tau_{1,S}} \approx \left(\frac{L - 2s_0}{c_s}\right)_E = X.
\]

Therefore, according to Equations (10) and (11), regardless of the phase of the sheath expansion and ignoring the process after the disappearance of the IRW, the similarity law for the ion extraction time, \( \tau \), can be expressed as

\[
\frac{\tau_{E}}{\tau_{S}} \approx \frac{\tau_{1,E}}{\tau_{1,S}} + \frac{\tau_{2,E}}{\tau_{2,S}} = X.
\]

With the reduction of the geometrical sizes, the computing consumption can be reduced greatly. A rough theoretical estimation shows that, when the geometrical size of the calculation domain in the PIC simulation is reduced to \( 1/X \) of the full-scale device, the computing time will be down to \( X^3 \) of that for the case of full-scale size modeling if the number of the macro-particles in each cell and the space interval for the case of small-size simulation are the same as those for the corresponding full-scale size modeling.

Based on the preceding discussions, in order to validate Equation (12), two-dimensional simulations with different scaling ratios are conducted using an open-source PIC code, WARP [6], based on the simulation parameters as listed in table 2. In our modelling, the ion extraction time, \( \tau \), is defined as the time when 90% of the ions are collected. As shown in figure 3, the maximum relative error between the calculated and the measured values [7] of the ion extraction time for different scaling ratios is 16%, which proves that the similarity law [Equation (12)] is reliable.

### Table 2. Simulation parameters for the \( \Pi \)-type electrode configuration [7]

| Case No. | \( L \) (cm) | \( D_s \) (cm) | \( D_p \) (cm) | \( s_0 \) (cm) | \( Q \) (cm) | \( H \) (cm) | \( M \) (cm) | \( m_i \) (amu) | \( T_{c,0} \) (eV) | \( T_{i,0} \) (eV) | \( U \) (kV) | \( n_i (m^{-3}) \) |
|---------|---------------|----------------|---------------|---------------|-------------|-------------|-------------|---------------|----------------|----------------|-------------|-------------|
| 3       | 10            | 9              | 9             | 0.5           | 4.5         | 18          | 1.5         | 137           | 1.06           | 0.1           | 1.0         | 9.0 × 10^{14} |
| 4       | 10            | 9              | 9             | 0.5           | 4.5         | 18          | 1.5         | 137           | 1.06           | 0.1           | 2.0         | 1.0 × 10^{15} |
4. Conclusions

In this paper, based on the analysis of the non-equilibrium transport characteristics of the ion extraction process in a decaying plasma, a similarity law for simulating the full-scale experimental devices is proposed. The major conclusions include:

![Figure 3. Comparison of the ion extraction time between the simulated and the experimentally measured results [7] under different scaling ratios](image)

(1) During the main stage of the ion extraction process, both the sheath expansion and the IRW propagation may influence the non-equilibrium transport process of the charged particles, which would result in different ion density distribution evolutions and the corresponding ion extraction time.

(2) With analysing the ion extraction process theoretically, a similarity law based on the conservation of the Child-Langmuir flux is proposed. Using this similarity law, the ion extraction time in the full-scale experimental devices can be estimated by the PIC simulations with a scaled small size configuration. For typical cases, the simulation results agree well with the experimental data, which verifies the reliability of the similarity law.

Although the preliminary numerical studies show that, with the increase of the value of $X$, the required computing resources can be reduced significantly while simultaneously with enough calculation accuracy on the prediction of the ion extraction time, the value of $X$ should be kept in a reasonable range because a very large $X$ may result in incorrect physical processes in simulations. Consequently, more studies on the optimization of the scaling factor ($X$) is indispensable in future research.

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