Multi-Species Ion Acceleration in Expansion of Finite-Size Plasma Targets

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We investigate ion energy spectra of a droplet target composed of different ion species, which is assumed to be heated by ultrashort laser pulse. The dynamics is studied with three-dimensional particle-in-cell simulation. It is found that the maximum ion energy $E_{\mathrm{i,max}}$ of the ion species with a charge a state Z has proportionality, $E_{\mathrm{i,max}} \propto Z^2$, when multi-species ions exist in large quantities simultaneously. This is a crucial new result different from the scaling $E_{\mathrm{i,max}} \propto Z$, where the fraction of such contaminating ions is small compared with that of the background ions. We discuss this present numerical result by comparing with a self-similar solution, which takes a full account of the charge separation effect.

Keywords: ion acceleration, finite-size plasma, self-similar solution, charge separation effect, 3D PIC simulation

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1. Introduction

Ion acceleration due to plasma expansion into vacuum has been a subject of considerable interest for decades [1–6]. Many theoretical and experimental studies have been carried out on the interaction of an ultrashort laser pulse with finite-size plasma [7–17]. In particular, the energy spectrum and maximum kinetic energy of accelerated ions have been the central issue of controversy. When a finite-size plasma, such as cluster or droplet plasma, is heated by an ultrashort and ultraintense laser pulse, light electrons are rapidly heated to high temperature to burst into vacuum. Compared with electrons, ions are so heavy that in the very early stages they are considered as being at rest. Then the ions are accelerated by the sheath electric field made by charge separation of the ions and electrons. Thus it is crucial to take account of the charge separation effect around the plasma/vacuum interface for evaluation of the maximum ion kinetic energy and energy spectrum. However, most of the theoretical works have assumed quasi charge neutrality. Recently, Murakami and Basko [16] have found a new self-similar solution taking the charge separation effect fully into account. In this paper, we compare our 3D PIC (three-dimensional Particle-In-Cell) simulation results with the self-similar model.

In our system, it is supposed that the electrons of a finite-size plasma are rapidly heated to a temperature $T_{\mathrm{e}0}$ and that subsequent plasma expansion is described by the motion of many particles composed of electrons and ions coupled via a self-consistent electric field. We consider a spatially uniform plasma droplet with a sharp boundary at an initial electron density $n_{\mathrm{e}0}$ and an initial Maxwellian temperature distribution of $T_{\mathrm{e}0}$, and the ions are assumed to be cold and initially at rest with density n_{i0}, where n_{i0} is the ion density for the i-th ion species. As an initial condition, the relation, $n_{\mathrm{e}0} = \sum_i Z_i n_{i0}$, is required for neutral plasma of multi-species ions, where Z_i is the charge state of the i-th ion species. Although the heating process by an ultraintense laser is itself an interesting and important issue, detailed analysis is outside the scope of the present work. We first compare the self-similar solution with 3D PIC simulation results, which are applied to the case of single-species ions. Charge separation is the crucial physical effect in the present study. In particular, the energy spectrum of the ions is expected to be from a Maxwellian distribution. Therefore, it is inappropriate to analyze the ion energy spectrum by using a fluid code, in which the local energy spectrum of ions is merely described by the single parameter, $T_{\mathrm{e}0}(x)$. In contrast, PIC simulation is indispensable for a detailed study of such ion spectrum. Then we investigate the ion energy spectrum for plasma expansion of a droplet plasma target, which is composed of multi-species ions.

It is apparent from elementary electrodynamics that the maximum ion energy, $E_{\mathrm{i,max}}$, of a test particle with charge $+Ze$ (e is elementary charge), which is put on the droplet plasma surface, is proportional to Z. However, for such a droplet target composed of multi-species ions, we have found that $E_{\mathrm{i,max}}$ is not proportional to Z but to Z^2. This is a substantially new and crucial finding that has never been reported elsewhere to the best of our knowledge.

The structure of this paper is as follows: In Sec. 2, we compare the simulation results with the self-similar solution with respect to the maximum ion kinetic energy. Then,

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in Sec. 3, we show that the maximum ion kinetic energy scales as $E_{\mathrm{i,max}} \propto Z^2$ by PIC simulation, and we also provide a physical explanation for this scaling. Section 4 is devoted to a summary.

2. Dynamics of Expansion of Single-Species Ions

We have performed PIC simulations to study the maximum ion kinetic energy and to compare it with the predictions of the self-similar model [16]. In the self-similar solution, an expanding plasma is uniquely characterized by only one external parameter $\Lambda_{\mathrm{s}} = R_0/\lambda_{\mathrm{De0}}$, where R_0 and λ_{De0} are the initial characteristic size and initial Debye length of self-similar plasma, respectively. It should be noted that the ion density profile $n_{\mathrm{i}}(r,t)$ in the self-similar solution is proportional to $\exp(-\xi^2) + 6/\Lambda_{\mathrm{s}}^2$, where $\xi = r/R(t)$, is the self-similar variable, and r and $R(t)$ are position and plasma size, respectively.

Now we consider a case, where a droplet plasma with initial radius R_{u0} has uniform density profiles for both ions and electrons ($Zn_{\mathrm{i0}} = n_{\mathrm{e0}} = n_{\mathrm{u0}}$ for the case of a single ion-species). Note that charge neutrality only holds at $t = 0$, but as time passes, charge separation occurs, in particular, at the plasma surface. In a similar manner to Ref. [16], we can introduce the following dimensionless parameter Λ_{u} to characterize such an initially uniform droplet plasma,

$$\Lambda_{\mathrm{u}} = R_{\mathrm{u0}}\left(\frac{4\pi e^2 n_{\mathrm{u0}}}{T_{\mathrm{e0}}}\right)^{1/2}. \qquad (1)$$

As the plasma expands into vacuum, the initial density profile is expected to asymptotically approach that of the self-similar solution. It turns out from detailed numerical simulation and analytical models that Λ_{s} and Λ_{u} are almost equal to each other, i.e. $\Lambda_{\mathrm{s}} \approx 0.9\Lambda_{\mathrm{u}}$ for $\Lambda_{\mathrm{s}} \gg 1$ [18]. Thus, we can compare the self-similar solution with the results of PIC simulation through equivalent relation of parameters Λ_{s} and Λ_{u}.

For our PIC simulation, the initial plasma droplet configuration can be described as a sphere with radius $R_{\mathrm{u0}} = 0.4\,\mu\mathrm{m}$ located at the center of a computational box with size $36\,\mu\mathrm{m} \times 36\,\mu\mathrm{m} \times 36\,\mu\mathrm{m}$. The boundary conditions are free for the three directions. The initial electron temperature is 30 keV. Supposing that the laser wavelength is 1 μm, this electron temperature approximately corresponds to the laser intensity $I_{\mathrm{L}} \approx 1.6 \times 10^{17}\,\mathrm{W/cm^2}$ [10]. The density of plasma is $n_{\mathrm{e0}} \approx 4 \times 10^{22}\,\mathrm{cm^{-3}}$ (solid density), which is about $36n_{\mathrm{c}}$, where n_{c} is the plasma critical density for a laser with wavelength of $\lambda_{\mathrm{L}} = 1\,\mu\mathrm{m}$. Although the laser can penetrate only the peripheral region of the droplet in the early stages, we postulate in this paper that energetic hot electrons produced by laser absorption on the surface are transported deep into the droplet target. As a result, a uniform initial electron temperature ($T_{\mathrm{e0}} \neq 0$) profile is considered to be established. The ion temperature is assumed to be $T_{\mathrm{i0}} = 0$ at time $t = 0$. The ion mass is the same for each ion species in our simulation, only with different values in the charge state Z, and the ion-to-electron mass ratio is $m_{\mathrm{i}}/m_{\mathrm{e}} = 100$ to save CPU time. Although this value is substantially smaller than the real number, Fig. 1 of Ref. [16] shows that the dependence of maximum ion energy and ion energy spectrum on $m_{\mathrm{i}}/m_{\mathrm{e}}$ is rather weak for $\Lambda_{\mathrm{s}} \gg 1$; note that in our simulation, $10 \le \Lambda_{\mathrm{s}} \le 100$. As a matter of fact, the PIC simulation also shows negligible dependence of plasma expansion on the parameter $m_{\mathrm{i}}/m_{\mathrm{e}}$ at least for the parameter range $100 \le m_{\mathrm{i}}/m_{\mathrm{e}} \le 600$.

Figure 1 shows the spatial distribution of ions and electrons (lower panel) and the temporal evolution of the maximum ion energy normalized by the initial electron temperature, i.e. $E_{\mathrm{i,max}}/T_{\mathrm{e0}}$ (upper panel). In Fig. 1 (upper panel), the horizontal axis denotes time normalized by the initial ion-plasma-frequency f_{pi0} (lower axis) and by the hydrodynamic time scale $R_{\mathrm{u0}}/C_{\mathrm{s0}}$ (upper axis), with C_{s0} being the sound speed given by $C_{\mathrm{s0}} = (ZT_{\mathrm{e0}}/m_{\mathrm{i}})^{1/2}$. It is seen in Fig. 1 (upper panel) that $E_{\mathrm{i,max}}$ monotonically increases with time and almost reaches its maximum at time

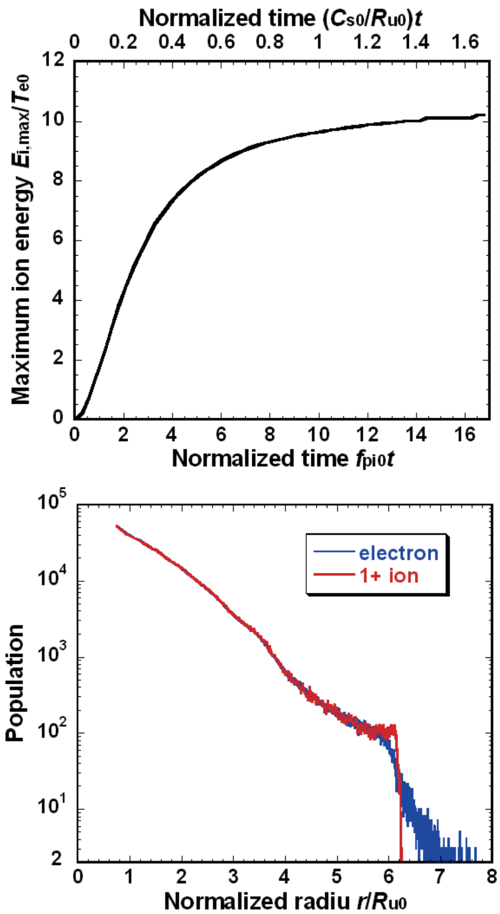

Fig. 1 Temporal evolution of the maximum ion energy (upper panel) and spatial distribution of ions and electrons (lower panel) measured at the normalized time $f_{\mathrm{pi0}}t = 13.8$, where f_{pi0} is the initial ion plasma frequency. Parameters are $T_{\mathrm{e0}} = 30\,\mathrm{keV}$, $R_{\mathrm{u0}} = 0.4\,\mu\mathrm{m}$, and $n_{\mathrm{e0}} \approx 4.0 \times 10^{22}/\mathrm{cm^3}$ ($\Lambda_{\mathrm{s}} \approx 25$).

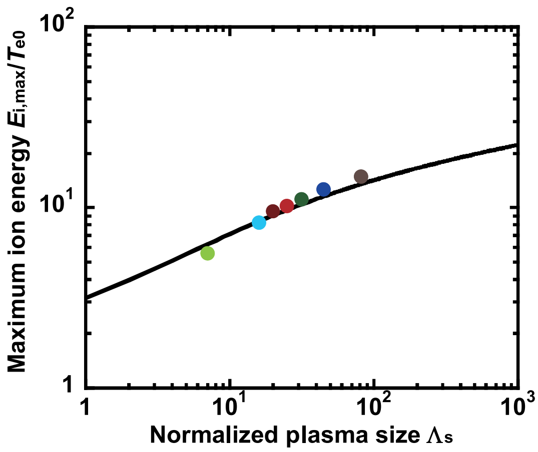

Fig. 2 Dependence of $E_{\mathrm{i,max}}$ on Λ_{s} for single-species ions ($Z = 1$ is fixed). The solid curve is the result of self-similar solution and the circle symbols are the simulation results. In the simulations, Λ_{s} varies in the range, 7∼100, by changing T_{e0}, n_{u0} and R_{u0}.

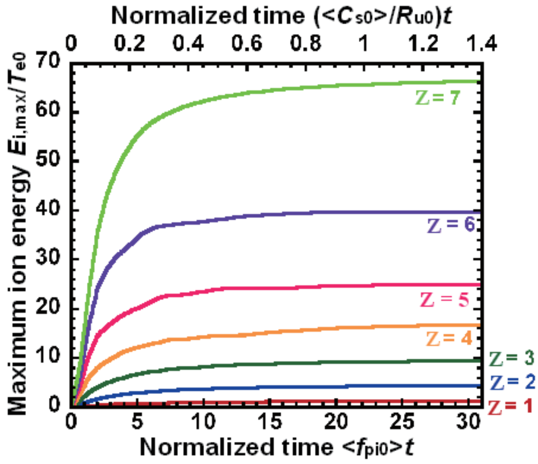

Fig. 3 Temporal evolution of the maximum energy of multi-species ion acceleration. Initial electron temperature and plasma size are $T_{\mathrm{e0}} = 30$ kev and $R_{\mathrm{u0}} = 0.4$ µm, respectively; $\langle C_{\mathrm{s0}}\rangle$ is the average initial ion sound speed. Time is normalized by the average initial ion frequency $\langle f_{\mathrm{pi0}}\rangle$ (lower abscissa) and the ratio of average initial ion sound speed to initial radius of droplet plasma $\langle C_{\mathrm{s0}}\rangle/R_{\mathrm{u0}}$ (upper abscissa).

about $f_{\mathrm{pi0}}\, t \geq 15$, i.e. about $(C_{\mathrm{s0}}/R_{\mathrm{u0}})\, t \geq 1.5$. Figure 1 (lower panel) shows that the peripheral electrons expand into vacuum and the charge separation is formed on the surface. From the parameters used in Fig. 1, the dimensionless plasma size parameter is calculated to be $\Lambda_{\mathrm{s}} \approx 25$.

The self-similar solution provides $E_{\mathrm{i,max}}$ in the form [16],

$$\frac{E_{\mathrm{i,max}}}{T_{\mathrm{e0}}} = 2Z \ln\left(\frac{\Lambda_{\mathrm{s}}^2}{2} \Big/ \ln\frac{\Lambda_{\mathrm{s}}^2}{2}\right). \tag{2}$$

Thus, the maximum kinetic energy of the accelerated ions can be scaled in terms of the initial electron temperature T_{e0}, the initial Debye length λ_{De0} (thus the initial density n_{e0}), and the initial plasma sizeR_0.

Figure 2 shows the comparison between the results of PIC simulation (circle symbols) and the self-similar model (solid curve) for the normalized maximum ion kinetic energy, $E_{\mathrm{i,max}}/T_{\mathrm{e0}}$, as a function of the normalized plasma size Λ_{s}. In the simulations, Λ_{s} varies in the range 7∼100, by changing T_{e0}, n_{u0} and R_{u0}. It is found that the simulation results are well reproduced by the self-similar solution.

3. Dynamics of Expansions of Multi-Species Ions

In this section, we study the expansion of a droplet target plasma, which is composed of multi-species ions. We perform simulations under the same conditions as stated earlier except that the multi-species ions are involved. Ions with charge state from 1+ to 7+ are contained uniformly at an equal density. Each computational mesh contains 5^3 ions for each species. Initial electron temperature and plasma size are $T_{\mathrm{e0}} = 30$ keV and $R_{\mathrm{u0}} = 0.4$ µm, respectively.

Figure 3 shows the temporal evolution of $E_{\mathrm{i,max}}$ for such a simulation. In Fig. 3, we also have two different time-measures as in Fig. 1 (upper panel), i.e. one normalized by the initial ion-plasma-frequency $\langle f_{\mathrm{pi0}}\rangle$ (lower axis), where $\langle x\rangle$ denotes the average of x, and the other normalized by the hydrodynamic time scale $R_{\mathrm{u0}}/\langle C_{\mathrm{s0}}\rangle$, where $\langle C_{\mathrm{s0}}\rangle = \left(\langle Z^2\rangle T_{\mathrm{e0}}/\langle Z\rangle m_{\mathrm{i}}\right)^{1/2}$, is the initial ion sound speed (upper axis). Figure 3 shows that after the normalized time $(\langle C_{\mathrm{s0}}\rangle/R_{\mathrm{u0}})\, t \approx 1$, the maximum ion energy almost reaches its maximum and practical acceleration ceases. The simulations also show that in such plasma expansion, ions of a higher charge state are accelerated more energetically to occupy the outer volume. The ion front with higher Z extends further into the vacuum. Meanwhile, Fig. 4 shows the energy spectrum $\mathrm{d}N/\mathrm{d}E$ at $\langle f_{\mathrm{pi0}}\rangle t = 30.9$. It is clear from Figs. 3 and 4 that the scaling $E_{\mathrm{i,max}} \propto Z$ does not hold, as is expected in a simple case, where a small quantity of high-Z test ions are contained in a bulk of low-Z ions. On the other hand, however, the simulation results obtained in Figs. 3 and 4 present a significantly different physical picture, i.e. $E_{\mathrm{i,max}} \propto Z^2$. We now explain this phenomenon in more detail.

We investigate the dependence of $E_{\mathrm{i,max}}$ on charge state under three different conditions as shown in Fig. 5. Data shown as (a) are the results for the case of single-species ions, and are found to be in good agreement with the self-similar solution in the scaling $E_{\mathrm{i,max}} \propto Z$. Data shown as (b) are the results for two species of ions, i.e. the droplet plasma is composed of background ions with $Z = 1$ and other contaminating ions with high-Z charge state, $Z = 2$∼7. The particle number ratio between 1+ background ions and the other high-Z contaminant ions

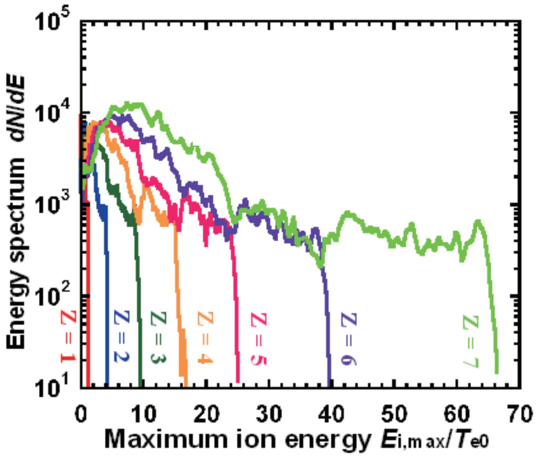

Fig. 4 Energy spectrum of accelerated ions. Initial parameters are the same as in Fig. 3. Normalized observation time is $\langle f_{\mathrm{pi0}} \rangle t = 30.9$.

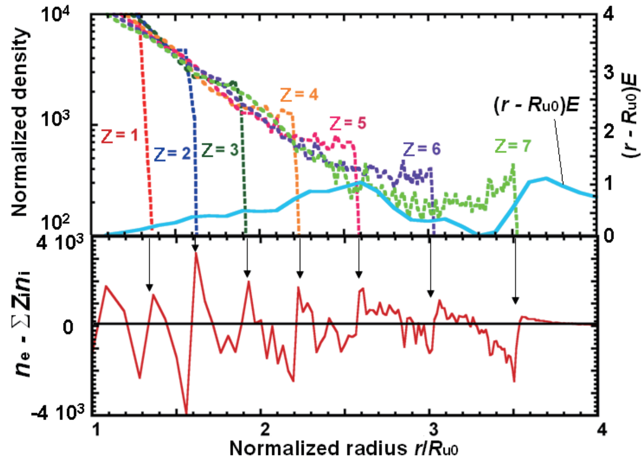

Fig. 6 Spatial distribution of each species of ion and the difference in populations of electrons and ions $n_e - \sum Z_i n_i$. The distance is normalized by R_{u0}. Normalized observation time is $\langle f_{\mathrm{pi0}} \rangle t = 6.71$.

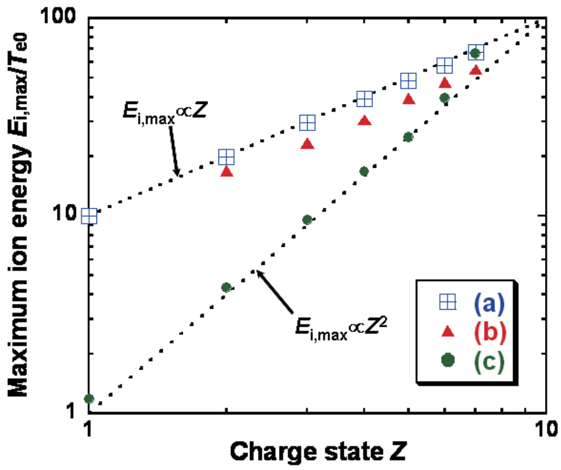

Fig. 5 Dependence of $E_{\mathrm{i,max}}$ on charge state Z. (a) Single-species ions with charge state changing from 1+ to 7+. (b) Two species of ions, 1+ and another contaminating high-Z ion. (c) Multi-species ions with charge states from 1+ to 7+ are placed uniformly at an equal density. The dotted and dashed lines show proportionalities.

is set to be equivalent to 0.8%. In this case, the scaling, $E_{\mathrm{i,max}} \propto Z$, is again observed. On the other hand, data shown as (c), in which the droplet plasma is composed of multi-species ions from $Z = 1$ to $Z = 7$ with equal composition rates, show that $E_{\mathrm{i,max}} \propto Z^2$ but not $E_{\mathrm{i,max}} \propto Z$ as was observed for data shown as (a) and (b).

To understand the underlying physics, we investigate the spatial distribution of the electric field in the expanding plasma. As shown in Fig. 6, we compare it with the density distribution of the multi-species ions (upper half) and the spatial charge, $n_e - \sum Z_i n_i$ (lower half), where the densities are appropriately normalized. Figure 6 also shows the product of $(r - R_{u0}) E$ (solid line in the upper half), where r is the radius and E is the radial component of the induced electric field. The figure shows that electron-rich regions appear ahead of the boundary surface of each ion species that induce the radial electric field E. Moreover, $(r - R_{u0}) E$ linearly increases with respect to Z until $Z = 5$. Therefore the work by the electric field for each species of ion is proportional to the square of the charge states as $ZE(r - R_{u0}) \propto Z^2$. Thus it follows that the maximum ion energy is proportional to the square of the charge, $E_{\mathrm{i,max}} \propto Z^2$.

The above scaling, $E_{\mathrm{i,max}} \propto Z^2$, can also be explained quite easily if we limit our argument to a simple case of a Coulomb explosion [14]. Suppose that a test ion with an electric charge $Z_p e$ is initially put on an ion sphere with radius R and total charge Q. Here we assume that the ion charge of the background is composed of multi-species ions from $Z = 1$ to $Z = Z_p$ at an equal composition rate. Then it is apparent that the total electric charge of the ion sphere is proportional to Z_p, i.e., $Q \propto Z_p$. The test ion is always accelerated ahead of all the other background ions. The maximum kinetic energy of the test ion balances the initial potential energy, i.e., $E_{\mathrm{i,max}} = (1/2)mv^2 = QZ_p e/R \propto Z_p^2$, which explains the Z^2-scaling.

4. Summary

We have investigated the dynamics of finite-size plasma expansion into a vacuum with 3D PIC simulation. We have tested the self-similar solution of single-species ion, which fully takes account of the charge separation effect. The results obtained by the simulation agree well with the self-similar solution. As a result, based on the self-similar solution, such physical quantities of a droplet plasma expansion can be well predicted, where the droplet is characterized by the initial electron temperature T_{e0}, the initial plasma density n_{u0} and the initial plasma size R_{u0}.

We have also investigated ion energy spectra for multi-species-ion expansion by means of 3D PIC simulation. It is found that the maximum ion energy $E_{i,max}$ of each species varies proportionally with the square of the ion charge state, i.e., $E_{i,max} \propto Z^2$, when multi-species ions simultaneously exist in large quantities, which is quite different from the case where only a small quantity of contaminating high-Z ions are doped in low-Z background ions.

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