Coulomb explosion of nanosize cylindrical target

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Abstract. We considered the Coulomb explosion of single-component cylindrical nano-clusters. The analytical expression for the energy spectra of ions is obtained, as well as the spectral dependence on the cluster geometrical size is investigated. The laser ionization efficiency for cylindrical and spherical clusters is compared. It is shown that cylindrical targets are preferable in comparison with spherical ones, allowing obtain accelerated ions with higher energy at the same target radius.

1. Introduction

The laser technology development has led to the appearance high-power lasers that generate TW femtosecond pulses, allowing accelerate ions to energies of several MeV \cite{1}. The unique characteristics of ion beams, generated by the ultrashort laser pulses are of great interest due to the possible applications when creating neutron sources, for isotope production and in solving other problems, including technologies of radiation impact on solids and different secondary nuclear reactions. It should be noted that the pulse technology for production micro-beams of protons and neutrons can be used for various medical applications \cite{2}.

In interaction laser radiation of ultra-high intensity with nano-clusters and micro-targets the large relativistic gamma factor \( \gamma = \sqrt{1 + I \lambda^2 / 2.75 \times 10^{18}} \) \( ([\lambda] - \mu m, [I] - W/cm^2) \) provides great ponderomotive potential \( U_p = m_e^2 (\gamma - 1) \). The ponderomotive force action results in spatial separation electrons and ions, depending on target's composition, shape and size, as well as the laser field parameters. Electrons, leaving the target, have characteristic energy distribution, caused by the action of the electromagnetic wave field. These electrons, moving in a strong field, can participate in the nonlinear Thomson scattering \cite{3}, and in the secondary electro-stimulated nuclear reactions \cite{4}.

After the laser pulse, nano-target takes uncompensated positive charge, and ions further fly away under the action the Coulomb repulsion. Such expansion of the nanosize clusters is called the Coulomb explosion. Already the experiments with relatively moderate laser field intensity \( I \geq 10^{16} W/cm^2 \), ionizing the clusters of Xe, have demonstrated the formation of multiply charged ions up to the charge 40\(^+\) and ion acceleration in the subsequent Coulomb explosion to the energy \( \sim 1\text{MeV} \) \cite{5}. These experiments stimulated theoretical description the Coulomb explosion and searching its optimal parameters. In particular, impact nonsphericity of clusters on the Coulomb explosion was discussed earlier \cite{6}. It was found that geometry of target significantly influences on the...
parameters of the Coulomb explosion [7]. An opportunity to reach the maximum ion energy provides formation the ion spot by irradiation thin films using high-power ultrashort laser pulses. On the other hand, investigation of micro sources for various types of nuclear radiation shows that jets of spherical clusters can be very promising for these purposes. At the same time, the cylindrical clusters have an advantage of slow field decrease with distance compared with the spherical targets, and one can expect large final ion energy at the same target diameters. As a consequence of this, we focused on the study of accelerating ions in the Coulomb explosion of the cylindrical targets.

2. Ionization of cylindrical nano-targets

Let us consider cluster ionization within a strong laser field during atomic times, i.e., almost immediately, proceeding from the fact that the degree of ionization is determined by the field strength $F$. We assume that ionization occurs basically in instants of time when laser field reaches the maximum values. According to this approach [8], we assume that the ionization process follows to Bethe's mechanism of the above-threshold ionization [9], that allows to determine the ionization degree of nano-target. For a spherical target, taking the charge distribution inside of it uniform, one can write an expression for the potential energy of an electron in the cluster field with a charge $Q$ in the form

$$ U(r) = \begin{cases} \frac{Q}{2R} \left( 3 - \frac{r^2}{R^2} \right), & r \leq R, \\ -\frac{Q}{r}, & r \geq R. \end{cases} \quad (1) $$

Here $R$ is the radius of the target, $r$ is the distance from the center ($e = 1$). The ionization energy we take equal the modulus of the electron potential energy $|U(R)| = Q / R$ on the cluster periphery.

In the presence of a laser field polarized in the radial direction, the total potential energy of the system target + field is determined by the expression $U_i(r) = U(r) - Fr$, and the derivative in the maximum is

$$ \frac{dU_i(r)}{dr} \bigg|_{r=r_0} = 0. \quad (2) $$

Scenario the above-threshold cluster ionization is determined by the equality the binding electron energy and the maximum value of the potential energy. Hence, one can define the ionization threshold as

$$ U(r_0) - Fr_0 = U(R). \quad (3) $$

Equation (3) gives us the maximum charge $Q$ of the cluster at which the above-threshold ionization is possible and the relevant value for the degree of the cluster ionization $\alpha = Q / ZN$, where $Z$ is the charge of cluster atoms, and $N$ is the total number of atoms. Thus, for spherical cluster ($Q = 4FR^2$) with concentration of atoms $n$ the ionization degree is defined by the expression

$$ \alpha_s = \frac{3F}{\pi Z n}. \quad (4) $$

In the same way, we can estimate the ionization degree for cylindrical cluster. The monotonically increasing potential of electron in such a system has the form

$$ U(r) = \begin{cases} -\pi \rho \left( R^2 - r^2 \right), & r \leq R, \\ \frac{2\pi R^2 \rho \ln(r / R)}{r^2}, & r \geq R. \end{cases} \quad (5) $$
where \( \rho = Q / N \) is the bulk charge density. The condition of unstable equilibrium on the top of the potential barrier (2) is now written as

\[
\frac{2\tau}{r_0} = F,
\]

where \( \tau = \pi R^2 \rho \) is linear charge density, i.e., \( r_0 = 2\tau / F \).

The potential energy of an electron on the boundary of uniformly charged cylindrical target is taken as zero, so that equation (3) for the above-barrier ionization of cluster is written down as

\[
2\tau \ln \left( \frac{2\tau}{FR} \right) - \frac{2\tau}{F} = 0.
\]

By solving equation (7), we obtain the value of the linear charge density of the cylindrical cluster, formed as a result of the above-threshold ionization, and

\[
\tau = FR / 2.
\]

The expression for the ionization degree of the target is

\[
\alpha_c = \frac{\tau}{Zn\pi R^2} = \frac{F}{2Zn\pi R}.
\]

From the comparison of equations (4) and (9), we can conclude that for spherical and cylindrical targets the ionization degree is described by the same function of the field and the target radius, differing only by a numerical factor, so that

\[
\frac{\alpha_s}{\alpha_c} = \frac{3F}{\pi Zn R} = 6.
\]

Table 1 shows the results of calculation the ionization degree of spherical and cylindrical nano-targets with different composition and radius for various laser intensities.

| Ion  | D   | Li  | C   | Kr  | Xe  | Pt  |
|------|-----|-----|-----|-----|-----|-----|
| \( Z \) | 1  | 3   | 6   | 36  | 54  | 78  |
| \( I, \text{W/cm}^2 \) | \( R, \text{nm} \) | 10\(^{17} \) | 10\(^{19} \) | 10\(^{21} \) |
| 1    | 1.00 / 1.00 | 1.00 / 0.72 | 1.00 / 1.00 | 0.74 / 0.12 | 0.67 / 0.11 | 0.13 / 0.02 |
| 10   | 1.00 / 0.32 | 0.43 / 0.07 | 1.00 / 0.17 | 0.07 / 0.01 | 0.07 / 0.01 | 0.01 / 0.00 |
| 20   | 0.96 / 0.16 | 0.22 / 0.04 | 0.52 / 0.09 | 0.04 / 0.01 | 0.03 / 0.01 | 0.01 / 0.00 |
| 30   | 0.64 / 0.11 | 0.14 / 0.02 | 0.35 / 0.06 | 0.02 / 0.00 | 0.02 / 0.00 | 0.00 / 0.00 |
| 40   | 0.48 / 0.08 | 0.11 / 0.02 | 0.26 / 0.04 | 0.02 / 0.00 | 0.02 / 0.00 | 0.00 / 0.00 |
| 1    | 1.00 / 1.00 | 1.00 / 1.00 | 1.00 / 1.00 | 1.00 / 1.00 | 1.00 / 1.00 | 1.00 / 1.00 |
| 10   | 1.00 / 0.32 | 0.43 / 0.07 | 1.00 / 0.17 | 0.07 / 0.01 | 0.07 / 0.01 | 0.01 / 0.00 |
| 20   | 0.96 / 0.16 | 0.22 / 0.04 | 0.52 / 0.09 | 0.04 / 0.01 | 0.03 / 0.01 | 0.01 / 0.00 |
| 30   | 0.64 / 0.11 | 0.14 / 0.02 | 0.35 / 0.06 | 0.02 / 0.00 | 0.02 / 0.00 | 0.00 / 0.00 |
| 40   | 0.48 / 0.08 | 0.11 / 0.02 | 0.26 / 0.04 | 0.02 / 0.00 | 0.02 / 0.00 | 0.00 / 0.00 |
The data presented in the table correspond to the lower boundary degree of the cluster ionization, because strong laser field provide also other ionization mechanisms, that are comparable in efficiency with the above-threshold ionization, such as the tunneling ionization and the electron impact ionization stimulated by the laser field. Following these estimates, we conclude that the technically accessible laser fields can ionize completely relatively large clusters. In particular, when the laser field intensity is $10^{19}$ W/cm$^2$, clusters consisting of light atom elements with a radius up to 10 nm, are ionized completely regardless of their form. It is worth noting that maximum of experimentally accessible intensity greatly exceed this value. Thus lower cylindrical target ionization efficiency is compensated by a significant gain in energy of ions produced in the Coulomb explosion as compared with the spherical target. Therefore, the use of cylindrical clusters is justified when they have sufficiently large length.

3. Coulomb explosion of a uniform cylinder

For further comparison, we will reproduce, at the beginning, the results of the calculation the Coulomb explosion of fully ionized clusters of cold ions, neglecting initial ion velocities. Let's start with a spherical target with a uniform initial density distribution. Since the field strength inside the uniformly charged ball monotonically increases from the center to the periphery, the acceleration of the ions in the outer layers is always greater, and they get the maximum energy at the end of expansion according to the energy conservation law. Thus, the shock waves are not formed in the homogeneous targets. For a spherical layer of thickness $dr$ the number of particles is

$$dN = n4\pi r^2 dr.$$  

Energy of ion emitted from such a layer is defined by its potential energy, i.e.,

$$\varepsilon = -ZU(r) = Z^2 n \frac{4\pi^3}{3} \frac{1}{r} = \frac{\varepsilon_{\text{max}}}{R^2} r^2,$$

where $\varepsilon_{\text{max}} = 4\pi Z^2 n R^2 / 3$ is the maximum ion energy equal to the potential energy at the cluster boundary. Consequently, the distribution of the emitted ions over the energy is of the form [8]

$$\frac{dN}{d\varepsilon} = \frac{dN}{d\varepsilon / dr} = \frac{3R}{2Z^2} \sqrt{\frac{\varepsilon}{\varepsilon_{\text{max}}}}, \, \varepsilon < \varepsilon_{\text{max}},$$

and the average value of the energy is

$$\varepsilon_{\text{av}} = \frac{3}{5} \varepsilon_{\text{max}}.$$  

We turn to the description of the Coulomb explosion of a fully ionized homogeneous cylindrical cluster. Inside it, the electric field increases monotonically in a radial direction as in the spherical cluster which means the absence of shock waves at the expansion. However, the direct use the model of infinite cylinder to obtain the final distribution of the ion energy, after the expansion cylindrical target of finite length, is impossible, because to get the finite energy, one need to take into account the asymptotic behavior of potential at the infinity like the field of a point Coulomb source. Thus, we should propose a model for expanding the target of finite size. To determine the energy of the expanding ions, we replace the finite cylinder by the elongate ellipsoid with a major semi-axis $a$ and small semi-axes $R$ ($a > R$). The volume of the ellipsoid is

$$V = \frac{4\pi}{3} a R^2,$$

and the total charge for a uniform density of ions is
\[ Q(R) = \frac{4\pi}{3} nZ\alpha R^2. \] (16)

The number of particles in cylindrical layer thickness \( db \) is equal to
\[ dN = n \frac{8\pi}{3} ab db. \] (17)

The potential energy (the kinetic energy at infinity) of the charge \( Z \) that is located on the surface of the ellipsoid with the current maximum radius \( b \), a constant potential along the surface and the total charge \( Q \) is given by the equation [10]
\[ U_i(b) = \varepsilon(b) = \frac{ZQ(b)}{2\sqrt{a^2 - b^2}} \ln \frac{a + \sqrt{a^2 - b^2}}{a - \sqrt{a^2 - b^2}}. \] (18)

When \( b = a \), the equation (18) becomes exactly the same as for the charged sphere. The differential variation of ion energy \( d\varepsilon \) with a change \( db \) of the distance from the target axis is given by the expression
\[ d\varepsilon = \frac{2\pi}{3} ab n Z^2 \left( 2a^2 - b^2 \right) \ln \left( \frac{a + \sqrt{a^2 - b^2}}{a - \sqrt{a^2 - b^2}} \right) - 2a \sqrt{a^2 - b^2} \right)^{3/2} db. \] (19)

The energy distribution for ions after the Coulomb explosion, in the final state can be written as
\[ \frac{dN}{d\varepsilon} = \frac{dN/db}{d\varepsilon/db} = \frac{4(a^2 - b^2)^{3/2}}{Z^2} \left( 2a^2 - b^2 \right) \ln \left( \frac{a + \sqrt{a^2 - b^2}}{a - \sqrt{a^2 - b^2}} \right) - 2a \sqrt{a^2 - b^2} \right)^{-1}. \] (20)

It is not possible to obtain an analytic expression for the function \( b(\varepsilon) \) from (18), since equations (18) and (20) give us the spectrum of ions at infinity in parametric form, however, the numerical calculations of the function are simple. The numerical dependences \( b(\varepsilon) \) obtained for different values of the parameter \( a \) are shown in figure 1.

**Figure 1.** The functional dependence of the initial ion coordinate \( b \) and final kinetic energy \( \varepsilon \)

The dashed line shows the dependence \( b(\varepsilon) \) for the spherical cluster. The energy distributions for ions after the Coulomb explosion of fully ionized deuterium clusters with a radius \( R = 5 \text{nm} \) are shown in figure 2. The ratios between the longitudinal and transverse target sizes are indicated under the curves.
With increasing $a$, as was expected, we see growth the maximum energy of ions, and for $a/R = 30$ the fourfold gain of energy is achieved compared with the spherical clusters. The ion energy is completely determined by the Coulomb energy of the target and, therefore, depends on the initial cluster charge. With increasing the target radius one can obtain ions with greater energy, but sized effect is restricted by the concomitant reduction in the ionization degree. More effective, in this regard, are the complex targets comprising ions that differ significantly in mass and charge.

4. Conclusions
The quasi-static theoretical model of the Coulomb explosion the cylindrical clusters has allowed us to calculate the energy spectra of ions. The results of numerical simulation showed that for homogeneous cylindrical cluster maximum achievable energy of the ions is much greater than for a spherical cluster of the same radius. The spectrum of expanding target containing deuterium, substantiated the possibility acceleration deuteron to 18 keV if one obtained a uniformly charged cylindrical target with the radius 5 nm and the length 150 nm. In a collision of deuterons having such energies, we should expect the initiation of nuclear fusion reactions with a significant output of monoenergetic neutrons. Control the laser field intensity and the length of the cylindrical target, clearly, provides the possibility to obtain the required energy deuterons.

As promising for obtaining high-energy ion flows in the Coulomb explosion, the carbon nanotube targets can be considered. Their sizes are optimal for location in the focal spot of the laser field, and the ratio of the length to the radius can reach several hundred units. In addition, the development of nanotechnology opens up broad opportunities for their synthesis. For example, long cylindrical clusters with diameters a few nanometers can be synthesized as carbon nanotubes filled by different compositions [11, 12]. A numerical simulation of the Coulomb explosion of the nanometer-sized carbon-gold nanotubes, containing gold atoms and filled by hydrogen, was carried out [13] showing the formation of highly collimated and almost monoenergetic protons with energies of few MeV.

Further studies suggest simulation the yield of nuclear fusion reactions at counterpropagating expansion of cylindrical targets with different compositions.

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