# Theoretical investigation of high-energy ions produced from laser-cluster interactions

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#### Abstract

By using an effective dielectric constant to modify the nanoplasma model, the interactions of large Ar clusters with high-intensity femtosecond laser pulses have been studied. It is shown that the resonance absorption mechanism plays a predominant role in the production of highly energetic argon ions, and the calculated mean kinetic energy of Ar ions is in good agreement with our previous experimental results. The scaling of mean kinetic energy and charge states of Ar ions against cluster size and laser intensity has also been analyzed. The results indicate the existence of optimum cluster sizes and optimum laser intensities where the best coupling efficiency of the laser energy can be obtained.

Keywords: Cluster; Femtosecond laser; High-energy ions; Resonance absorption

## 1. INTRODUCTION

Recently, much interest has focused on studying the interaction of high-intensity laser pulses with clusters because they may bridge the gap between a molecular and solid state of matter. In 1993, McPherson et al. first observed anomalous X-ray line emission from highly charged Kr and Xe ions when a high intensity 248-nm laser was focused on Kr and Xe clusters (McPherson et al., 1993). Since then, many other groups, including Lezius et al. (1998), Rose-Petruck et al. (1997), and Ditmire et al. (1995, 1996, 1997a, 1997b, 1998) have studied various aspects of the interaction of clusters with high-intensity femtosecond laser pulses. Many studies have shown that clusters absorb the energy of laser pulses very efficiently (Ditmire *et al.*, 1997*a*). Very bright X-ray emission in the 100-5000 eV range (Ditmire et al., 1995; Zweiback et al., 1999), extremely energetic ions with energy up to 1 MeV (Ditmire et al., 1997b, 1998), and keV electrons (Shao *et al.*, 1996) were observed in these experiments. And it is very exciting that DD nuclear fusion was produced when Ditmire et al. drove explosions in deuterium clusters with a 35-fs laser pulse (Zweiback et al., 2000).

Until now, several different theoretical models (McPherson *et al.*, 1993; Ditmire *et al.*, 1996; Rose-Petruck *et al.*, 1997; Last & Jortner, 1998) have been developed to explain these observations. In these models, the nanoplasma model

(also called the hydrodynamic model) is a better one for large clusters in a high-intensity laser field. In this model, each cluster was treated as a small ball of high-density plasma and the cluster size is large enough to confine the majority of electrons to the cluster region. The cluster was heated by field ionization, collisional ionization, and inverse bremsstrahlung heating. This theory can explain many experimental phenomena, such as the expansion process of the clusters, the production of highly charged and high-energy ions, the observation of highly energetic electrons, and especially the resonance absorption.

However, the nanoplasma model does not give us a detailed description near the resonance point and seems to overestimate the enhancement of the electric field inside the clusters at the resonance point. With some experimental parameters (Liu *et al.*, 2001), the electric field inside the clusters will be enhanced to hundreds of times that in vacuum. If the resonance point occurs exactly at the peak intensity of the laser pulse, for example,  $10^{16}$  W/cm<sup>2</sup>, the intensity of the electric field inside the cluster will increase to  $10^{21}$ W/cm<sup>2</sup>. Such a high electric field can directly produce highly charged ions such as Kr<sup>28+</sup> by optical field ionization (OFI), but none of them has been observed in experiments. Moreover, the average ion energy calculated from this model is much higher than experimental results (Ditmire *et al.*, 1996).

To get more reasonable explanations, a modified nanoplasma model has been proposed by Liu *et al.* (2001), which is reasonable for explaining the generation of highly charged ions and the mean kinetic energy of ions in the interactions

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of large clusters with high-intensity femtosecond laser pulses. In this article, this model has been employed to investigate the scaling of charge states and mean kinetic energy of ions with cluster and laser parameters in laser–cluster interactions. To make it comparable to our experimental works (Li *et al.*, 2000) and give theoretical explanations for our further experiments, our investigations will be aimed at Ar clusters.

### 2. CALCULATION MODEL

A detailed description of the modified nanoplasma model has been given in Liu et al. (2001). Here we will only describe the modified model briefly. In the original nanoplasma model (Ditmire et al., 1996), the cluster is approximately treated as a uniform small ball of plasma that is much smaller than the wavelength of the laser, so the field distribution in the cluster can be also treated as uniform. The electric field in the cluster is given by  $E = 3E_0/|\varepsilon + 2|, E_0$ is the electric field in vacuum. The plasma dielectric constant derived from the Drude model is  $\varepsilon = 1 - \omega_p^2 / \omega (\omega + \omega_p)^2 / \omega (\omega +$  $i\nu$ ), where  $\omega_p = \sqrt{4\pi e^2 n_e/m_e}$  is the plasma frequency,  $\nu$  is the electron-ion collision frequency, and  $\omega$  is the laser frequency. At the resonance point when the electric density decreases to  $3n_{crit}$ , the electric field and the heating rate inside the cluster are evidently enhanced, which leads to a rapid increase in the electron temperature and the expansion velocity of the cluster. Therefore at the resonance point, the quasistatic plasma dielectric constant may not be suitable any longer because the electron density and temperature change so rapidly. In our modified nanoplasma model, by solving the Maxwell equations, we defined an effective plasma dielectric constant  $\varepsilon_{eff} = \varepsilon + i\dot{\varepsilon}/\omega$  to replace the quasistatic one. When the change rate of  $\varepsilon$  is comparable to  $\omega$ ,  $i\dot{\varepsilon}/\omega$  may reach a considerably large value, and therefore weaken the enhancement of the electric field inside the clusters, and a reasonable explanation can be obtained.

The modified nanoplasma model can be described by the following equations:

a. The rate equations

$$\frac{\partial P_k}{\partial t} = -\Gamma_k P_k + \Gamma_{k-1} P_{k-1}, \qquad \frac{\partial n_e}{\partial t} = \sum_K \Gamma_k P_k - W_{FS}, \quad (1)$$

 $\Gamma_k = W_{tun} + W_e$ , where  $W_{FS}$  is the rate of OFI,  $W_{FS}$  is the rate of electron-impact ionization,  $W_{FS}$  is the escape rate of electrons,  $n_e$  is the electron density, and  $P_k$  is the density of the ions of charge state k(k = 0, 1, 2, ...).

b. The kinetic equation

$$\frac{\partial^2 r}{\partial t^2} = 3 \frac{P_e + P_{coul}}{n_i m_i} \frac{1}{r}$$
$$= 10^{-4} \left( 2.9 n_e T_e + 0.166 \frac{Q^2}{r^4} \right) \frac{1}{A n_i r} \quad (nmfs^{-2}), \quad (2)$$

where  $P_{coul} = (Q^2 e^2)/(8\pi r^4)$  is Coulomb pressure,  $P_e = nKT_e$  is the electron thermal pressure, *r* is the radius of the expanding cluster,  $n_i$  is the ion density, and  $m_i$  is the ion mass.

c. The energy equation

$$\frac{3}{2}n_e K \frac{\partial T_e}{\partial t} = \frac{\partial U}{\partial t} - \frac{3}{r}P_e \frac{\partial r}{\partial t} + q_{FS},$$
(3)

where  $q_{FS}$  is the energy loss caused by the hot electrons that escape from the cluster,  $\partial U/\partial t$  is the laser energy deposition rate inside the cluster, and  $(3/r)P_e\partial r/\partial t$  is the work associated with the expanding cluster.

Because a uniform expanding process is assumed in this model, the ion radial velocity increases linearly along with its distance from the center in the cluster; the mean kinetic energy of Ar ions will be calculated as

$$\bar{E} = \frac{m_i v_i^2}{2} \int_0^R \frac{r^2 \cdot 4\pi r^2}{R^2} dr \cdot \frac{3}{4\pi R^3} = 0.3 m_i v_i^2, \qquad (4)$$

where  $m_i = 40m_p$  ( $m_p$  is the mass of a proton) is the mass of Ar ions and  $v_i$  is the cluster expansion velocity.

Employing the model, the dynamics of Ar clusters with high-intensity femtosecond lasers has been simulated.

#### **3. CALCULATIONS**

Figure 1 shows the simulated process of a 5.5-nm (3000 atoms) Ar cluster illuminated by a 780-nm, 150-fs laser pulse at a peak intensity of  $1.5 \times 10^{16}$  W/cm<sup>2</sup>. The ion fraction from Ar<sup>5+</sup> to Ar<sup>10+</sup> and laser pulse envelop as a function of time are shown in Figure 1a; the average charge of Ar ions is about 8.5+. The expanding velocity of the cluster and the mean ion energy calculated from the expanding velocity by Eq. (1) as functions of time are shown in Figure 1b; the calculated mean kinetic energy of ions is about 17 keV, which is very close to our experimental results (Li *et al.*, 2000).

Figure 1 demonstrates a sudden increase of  $Ar^{8+}$  production and a great enhancement of the mean ion energy. These are obviously the results of resonance absorption. In experiments, the resonance point can be controlled through the adjustment of laser and cluster parameters, so we can optimize the cluster explosion to get more energetic and higher charged ions. In the following section, we will present the theoretical investigations of the scaling of the mean kinetic energy and charge states of Ar ions produced from laser-irradiated Ar clusters as functions of cluster size and laser intensity.

#### 3.1 Cluster size dependence

In Figure 1, the resonance point arrives later than the peak intensity of the laser pulse. It may be inferred that for a



Fig. 1. Ar ion fraction from  $Ar^{5+}$  to  $Ar^{10+}$  (a) and laser pulse envelop (b) expanding velocity of cluster and mean kinetic energy of ions as functions of time for a 5.5-nm (3000 atoms) Ar cluster driven by a 780-nm, 150-fs,  $1.5 \times 10^{16}$  W/cm<sup>2</sup> laser pulse.

smaller cluster, it expands rapidly, and this point occurs closer to the peak intensity of the laser pulse; therefore the coupling efficiency of the laser energy will be increased. But for a much smaller cluster, the resonance point comes earlier than the peak intensity of the laser pulse and decreases the energy coupling efficiency. On the other hand, a larger cluster expands slowly, so this point comes much later than the peak intensity of the laser pulse and will also lead to a decrease of energy coupling efficiency. So there should be an optimum cluster size for given laser parameters, where the best absorption efficiency of the laser energy can be obtained.

Figure 2a shows the mean kinetic energy of Ar ions scaling with the cluster sizes for 780-nm, 150-fs laser pulses at different peak intensities. Optimum sizes of cluster can obviously be obtained in the figure: When the peak intensity of the laser is  $1.5 \times 10^{16}$  W/cm<sup>2</sup>, the optimum cluster size is about 7.0 nm in diameter (about 7000 Ar atoms); however, it is 8.0 nm (about 9000 Ar atoms) when the peak intensity is



Fig. 2. Mean kinetic energy (a) and average charge state of Ar ions (b) with varieties of cluster sizes when Ar clusters are irradiated by laser pulses with different intensities  $(1.5, 2.0 \times 10^{16} \text{ W/cm}^2)$ . The laser pulse length is 150 fs and the laser wavelength is 780 nm.

 $2.0 \times 10^{16}$  W/cm<sup>2</sup>. The increase of laser intensity also increases the initial ionization and expansion rates, and the resonance point will occur earlier in the laser pulse; therefore the optimum size will shift toward larger clusters.

The average charge state of Ar ions is also calculated and shown in Figure 2b. We can see that the charge state of Ar ions increases linearly with the cluster size: The larger the cluster size, the higher the charge state of Ar ions. This can be explained by the ionization process where the electronimpact ionization dominates. In the early time of interaction, the electron density increases to a ultrahigh level due to optical field ionization. The electrons are heated by inverse bremsstrahlung and the electron temperature also increases. So, the rate of electron-impact ionization is very large. For a larger size cluster, the heating and electronimpact ionization occur for a longer time, so higher charge states are produced.

#### **3.2.** Scaling with laser intensity

We have already seen that a higher intensity of laser pulse will bring forward the resonance point. Like the scaling with cluster size, an optimum intensity of the laser pulse may exists for a given cluster size, where a best absorption efficiency of the laser energy can be obtained. In Figure 3, the mean kinetic energy and average charge state of ions, together with energy absorption efficiency for several laser intensities and given cluster sizes of 4.0 nm (thin lines) and 5.5 nm (thick lines), are shown. The intensities are from  $10^{15}$  W/cm<sup>2</sup> to  $10^{17}$  W/cm<sup>2</sup>, which are accessible in our experiments. Irradiated by laser pulses with these intensities, the electron density will increase to a much higher value than  $3n_{crit}$  in a short time, due to field ionization, and then fall through  $3n_{crit}$  before the laser pulse vanishes; that is, the resonance absorption occurs within the laser pulse.

In Figure 3, the mean kinetic energy of Ar ions and its average charge state from different-size clusters increase with the laser intensity, and at particular intensities  $(1.1 \times 10^{17} \text{ W/cm}^2 \text{ for 4.0-nm Ar cluster and } 1.2 \times 10^{17} \text{ W/cm}^2 \text{ for 5.5 nm})$ , they rise rapidly then fall down. These lines clearly demonstrate the effect of resonance absorption in laser–cluster interactions.

Because higher intensity will also increase the absolute value of ion energy, the mean kinetic is not suitable for investigating the coupling efficiency of laser–cluster interactions. A simple energy absorption efficiency  $e = \overline{E}/I_{peak}$  ( $\overline{E}$  is the mean energy of ions and  $I_{peak}$  is the peak intensity of laser pulse) is used to solve this problem; its scaling against laser intensity is shown in Figure 3c. Because of the saturation of energy absorption, the energy absorption efficiency is lower for much higher intensities. For a 4.0-nm in diameter cluster, a laser pulse with intensity  $2 \times 10^{15}$  W/cm<sup>2</sup> occurs at the maximum energy absorption efficiency, and for a 5.5-nm cluster, the corresponding intensity is  $3 \times 10^{15}$  W/cm<sup>2</sup>. However, in the vicinity of resonance absorption, the energy absorption will obviously be enhanced because of the resonance.

## 4. CONCLUSION

In our calculations, the mean kinetic ion energy is very close to our observed results; but in Ditmire *et al.* (1996), the calculated kinetic ion energy is close to the maximum ion energy of experimental measurements. The cause might be that the original nanoplasma model overestimates the resonance enhancement. By use of an effective dielectric constant, the modified nanoplasma model is very suitable for investigating the high-energy ions exploded from laser– cluster interactions.

In conclusion, the modified nanoplasma model is used to simulate the interaction between Ar clusters and highintensity femtosecond laser pulses. The calculated mean ion energies are in good agreement with our experimental results. For our further experiments, we are investigating the



**Fig. 3.** Mean kinetic energy of ions (a), average charge state of ions (b), and energy absorption efficiency (c) with varieties of laser intensities. The laser pulse length is 150 fs and the laser wavelength is 780 nm.

scaling of the mean kinetic energy and the charge state of Ar ions with cluster size and laser intensity. An optimum cluster size for a given laser pulse, together with an optimum laser intensity for a given cluster size, are found because of the mechanism of the resonance absorption.

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