Modified hydrodynamic model and its application in the investigation of laser-cluster interactions

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By solving the Maxwell equations, an effective plasma dielectric constant is obtained to replace the quasistatic plasma dielectric constant derived from the Drude model. In the vicinity of resonance absorption, the electron density and temperature undergo such a rapid change that the quasistatic dielectric constant is no longer appropriate to describe the behavior of resonance absorption. Using this effective dielectric constant to modify the hydrodynamic model developed by Ditmire and co-workers, we studied the interaction between different-sized atomic clusters and high-intensity laser pulses of different wavelengths. Reasonable agreement between the calculated results and published experimental results was found.

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I. INTRODUCTION

In recent years the interaction of clusters with high-intensity laser pulses has been studied by a number of groups. McPherson *et al.* [1–3] observed anomalous x-ray line emission from high Kr and Xe charge states when a high-intensity $[(0.5\text{–}80)\times10^{17}\ \mathrm{W\,cm^{-2}}]$ 248 nm laser was focused on Kr and Xe clusters. Zweiback *et al.* [4] reported the observation of nuclear fusion from the explosion of deuterium clusters driven with a compact high-repetition-rate table-top laser. Many studies on the interaction of a cluster target with laser pulses have shown that these interactions can be very energetic. Very bright x-ray emission in the 100–5000 eV range, extremely energetic ions with energy up to 1 MeV, and keV electrons have been observed in these interactions; these are the signatures of the efficient coupling of the laser light with the cluster medium. To explain the observed anomalous x-ray line emission from highly charged states of Kr and Xe, McPherson *et al.* suggested that it was the result of inner-shell vacancies produced by collisions of laser driven electrons with atoms in small clusters. If enough of these inner-shell vacancies can be produced in the interactions, the cluster will become a promising lasing medium to achieve a short-wavelength x-ray laser (<2 nm) [5]. However, this interaction picture is far from being understood in either theory or experiments.

Until now, three models have been developed to explain the interaction of clusters with ultrashort pulse high-intensity lasers. First, McPherson *et al.* proposed a coherently driven multielectron model in which the coherently driven multielectron motions can greatly increase the ionization strength of the inner-shell electrons. The group of coherently energized electrons acts like a quasiparticle with a charge Ze and a mass Zm_e where Z denotes the number of field ionized electrons [3], hence presenting a sharply augmented coupling resembling that associated with energetic ion-atom collisions. However, the model is not able to give a quantitative description of the interaction. Second is the "ionization ignition model" which was proposed by Rose-Petruck *et al.* [6] to describe the ultrafast electron dynamics and inner-shell ionization in laser driven clusters. The ionization ignition model indicated that the ionization enhancement is driven by a combination of the laser field and the strong field originating from the ionized cluster atoms (this is to some extent similar to the hydrodynamic model to be mentioned below). However, this model employed classical trajectory Monte Carlo simulation and can only simulate the dynamics of small clusters; it cannot describe the collective behavior of electrons. Third, Ditmire and co-workers proposed a hydrodynamic model that treats the expanding cluster as a spherical nanoplasma. Although the hydrodynamic model cannot explain the energy spectrum of the highly energetic ions released from the driven clusters, recent experiments [7–10] have shown that the model can explain the expansion process of the clusters, the resonance absorption, and the production of highly charged ions and highly energetic ions. In this model, each cluster was considered as a small ball of high-density plasma; the cluster size should therefore be so large that the majority of electrons will stay in the cluster during the expansion. From this point of view, the hydrodynamic model is a better model for large-size clusters . However, near resonance where the electron density is near $3n_{crit}$ (n_{crit} is the critical electron density of the corresponding driving laser wavelength), the electric field in the cluster will be enhanced to become much larger than the laser field if the quasistatic plasma dielectric constant is employed. This model seems to overestimate the enhancement of electric field in clusters. In this paper, an effective plasma dielectric constant is proposed to replace the quasistatic plasma dielectric constant. The resonance enhancement is found to be weakened when the proposed plasma dielectric constant is employed in the hydrodynamic model. Using this modified hydrodynamic model, we investigate the interaction between clusters of different sizes and laser pulses of different wavelengths.

This paper is organized as follows. In the second section we describe the modified hydrodynamic model developed in this work. In Sec. III we describe the simulation model and present simulation results of the interaction between clusters

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of different sizes and laser pulses of different wavelengths. In Sec. IV we discuss the unresolved problems of the hydrodynamic model, and we summarize this work in the final section.

II. HYDRODYNAMIC MODEL

The hydrodynamic model treats the cluster as a dielectric sphere which becomes a microplasma sphere after being illuminated by an ultrashort high-intensity laser pulse. The electric field in the cluster is a combination of the laser field and the polarization field originating from the free electrons inside the cluster. The main processes involved in the interaction of the clusters with the laser field are optical field ionization (OFI), collisional ionization by thermal and laser driven electrons, heating through inverse bremsstrahlung, and expansion of the cluster. Enhancement of the electric field in the cluster occurs when the electron density in the cluster drops to three times the critical electron density, at which point the electric field in the cluster becomes larger than the laser field in vacuum. Here in this paper the heating mechanism of the cluster is discussed only briefly in order to introduce an effective plasma dielectric constant. A more detailed description of the dynamics in laser-cluster interactions was given in Ref. [11].

A. Heating mechanism

The cluster is approximately treated as a uniform microplasma. For laser pulses at intensities less than 10^{18} W/cm^2, it is reasonable to assume that the laser primarily deposits its energy into the free electrons in the cluster and that this energy deposition is through collisional inverse bremsstrahlung. The heating rate is the same as the laser deposition rate in a dielectric sphere and can be given as

$$\frac{\partial U}{\partial t}=\frac{\omega}{8\pi}\mathrm{Im}(\varepsilon)|E|^2=7312.5\omega\ \mathrm{Im}(\varepsilon)|E|^2 \quad \mathrm{eV\,nm^{-3}\,fs^{-1}}, \tag{1}$$

where the electric field E is given in atomic units and the laser frequency ω is given in fs^{-1}. Since the diameter of the cluster considered here is much smaller than the wavelength of the laser, the field distribution in the cluster can be treated as uniform. The electric field in the cluster is given by $E=3E_0/|\varepsilon+2|$, E_0 being the amplitude of the laser field in vacuum. The plasma dielectric constant derived from a simple Drude model is $\varepsilon=1-\omega_p^2/\omega(\omega+i\nu)$, where $\omega_p=\sqrt{4\pi e^2 n_e/m_e}$ is the plasma frequency and ν is the electron-ion collision frequency which is described by the following formalism [11,12]:

$$\nu=\frac{4}{9}\left(\frac{2\pi}{3}\right)^{1/2}\frac{Zn_e e^4}{m_e(T_e+U_p)^{3/2}}\ln\Lambda$$

$$=0.563\frac{Zn_e}{(T_e+U_p)^{3/2}}\ln\Lambda \quad \mathrm{fs^{-1}}. \tag{2}$$

Here the electron density n_e is given in nm^{-3}, the ponderomotive energy U_p and electron temperature T_e are given in eV, and $\ln\Lambda$ is the standard Coulomb logarithm which generally varies between 5 and 20. $\ln\Lambda$ can be calculated by the following formulation [12]:

$$\Lambda=\frac{3}{2Ze^3}\left(\frac{K^3T^3}{\pi n_e}\right)^{1/2}=1.55\times10^{10}\frac{T_e^{3/2}}{Zn_e^{1/2}}. \tag{3}$$

At the early stage of the interaction when the electron density in the cluster is much higher than $3n_{crit}$, the field inside the cluster is weaker than the laser field in vacuum, and this shielding results in a slow heating rate. However, when the electron density decreases to $3n_{crit}$ owing to the expansion of the cluster, the 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. A simple estimation may be made of the degree of this enhancement. At the resonance point, the electron density is set as $n_e=3n_{crit}=4.8\times10^{21}$ cm^{-3} (the wavelength of the laser is 800 nm), the electron temperature is assumed as 1000 eV, the average charge state of the ions is Kr^{8+}, and the Coulomb logarithm is set as 10; the electron-ion collision frequency is thus calculated as $\nu\approx0.007$ fs^{-1}. The field inside the cluster is therefore $E=3E_0/|\varepsilon+2|\approx300E_0$. If the resonance point occurs exactly at the peak intensity of the laser (it can be controlled by adjusting the cluster size or the laser pulse duration), the intensity of the electric field inside the cluster will be increased to 10^{21} W cm^{-2} for an illuminating laser at the intensity of 10^{16} W cm^{-2}. Such a high electric field can directly produce highly charged ions such as Kr^{28+} by OFI. However, ions with such high charge numbers have not been observed in experiments. Moreover, such enhancement of the electric field in the cluster will unavoidably make the laser deposition much larger than the laser flux. This absorption model is obviously unreasonable and should be improved.

B. Effective plasma dielectric constant

In fact, the enhancement of the electric field inside the cluster at the resonance point was significantly overestimated. Owning to the resonance heating and expansion of the cluster in the vicinity of resonance absorption, the electron density and temperature undergo such a rapid change that the quasistatic plasma dielectric constant derived from the Drude model is not suitable to describe the absorption. We can solve the Maxwell equations in the plasma to understand the absorption process [13]:

$$\nabla\times\boldsymbol{H}-\frac{\varepsilon_0}{c}\dot{\boldsymbol{E}}=\frac{4\pi}{c}\sigma\boldsymbol{E}, \tag{4}$$

$$\nabla\times\boldsymbol{E}-\frac{\mu}{c}\dot{\boldsymbol{H}}=\boldsymbol{0}, \tag{5}$$

$$\nabla\cdot\boldsymbol{E}=\frac{4\pi}{c}\rho \quad \text{and} \quad \nabla\cdot\boldsymbol{H}=\boldsymbol{0}, \tag{6}$$

where ε_0 is the vacuum dielectric constant. From the above equations (4) and (5), E satisfies the following equation on the elimination of H:

$$\nabla\times(\nabla\times\boldsymbol{E})=\frac{\mu}{c^2}[(\dot{\varepsilon}_0\dot{\boldsymbol{E}}+\varepsilon_0\ddot{\boldsymbol{E}})+4\pi(\dot{\sigma}\boldsymbol{E}+\sigma\dot{\boldsymbol{E}})]. \quad (7)$$

If $E=E_0e^{-i\omega t}$ is used to simplify the above equation, it may be transformed to

$$\begin{aligned}\nabla\times(\nabla\times\boldsymbol{E})&=\frac{\mu}{c^2}[(-\omega^2\varepsilon_0-i\omega\dot{\varepsilon}_0)+4\pi(\dot{\sigma}-i\omega\sigma)]\boldsymbol{E}\\&=-\frac{\mu\omega^2}{c^2}\left[\left(\varepsilon_0+i4\pi\frac{\sigma}{\omega}\right)+i\left(\dot{\varepsilon}_0+i4\pi\frac{\dot{\sigma}}{\omega}\right)/\omega\right]\\&=-\frac{\mu\omega^2}{c^2}\left(\varepsilon+i\frac{\dot{\varepsilon}}{\omega}\right), \quad (8)\end{aligned}$$

where we have used the usual plasma dielectric constant $\varepsilon=\varepsilon_0+i4\pi\sigma/\omega=1-\omega_p^2/\omega(\omega+i\nu)$. From the above wave equation, we can define an effective plasma dielectric constant for a rapidly expanding plasma as $\varepsilon_{\rm eff}=\varepsilon+i\dot{\varepsilon}/\omega$. When the change rate of the dielectric constant is comparable to the laser frequency, $i\dot{\varepsilon}/\omega$ has a considerably large value and cannot be ignored. At the resonance point, the rapid change of electron density and temperature results in the rapid change of the plasma current density associated with the free electrons. This plasma current density will produce an electric field that to some extent weakens the resonance enhancement of the electric field inside the cluster. Figure 1(a) shows the development of the plasma dielectric constant and the effective dielectric constant as a function of time in the vicinity of resonance absorption during the interaction of a 7.5 nm Kr cluster with a high-intensity laser pulse (800 nm, 140 fs, 2×10^{16} W cm^{-2}). It can be seen that the imaginary part of the effective dielectric constant Im($\varepsilon_{\rm eff}$) has a very large value in the vicinity of resonance absorption. In contrast to this, the quasistatic dielectric constant Im(ε) has a minimum value. Figure 1(b) shows the time-varying electric field inside the cluster in the vicinity of resonance. The electric field is given in atomic units. It can be seen that, if the effective dielectric constant is employed, the enhanced electric field (solid line) inside the cluster is less than $10E_0$ (E_0 is the laser field in vacuum). However, the electric field (dashed line) is much higher if the quasistatic dielectric constant is used. Therefore the introduction of the effective dielectric constant will weaken the resonance enhancement of the electric field inside the cluster. Figure 1(c) shows the ion fraction resulting from the interaction of a 7.5 nm Kr cluster with the same laser pulse as a function of time where the quasistatic dielectric constant is used. It can be seen that for a short time in the vicinity of resonance very highly charged ions such as Kr^{20+} would be produced owing to the OFI of the enhanced electric field inside the cluster. This result is obviously unreasonable.

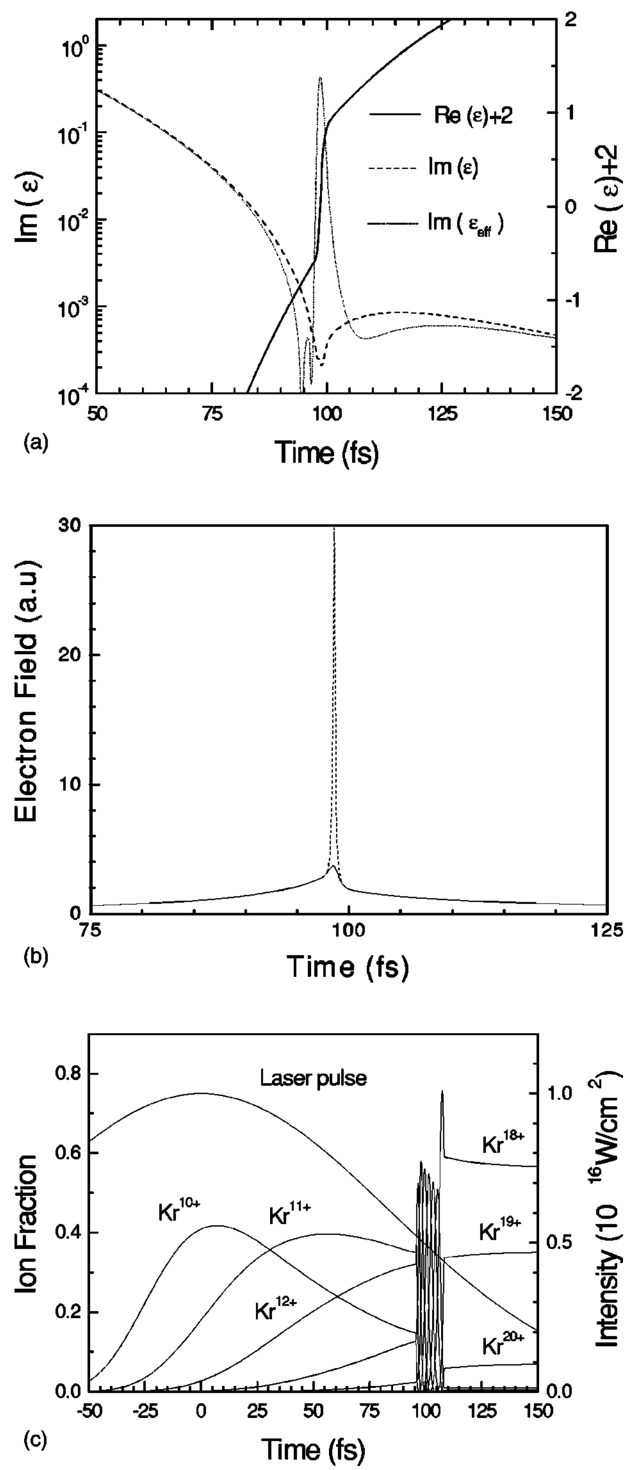

FIG. 1. (a) The plasma dielectric constant and the effective dielectric constant as functions of time in the vicinity of the resonance absorption in the interaction of 7.5 nm Kr clusters with a high-intensity laser pulse (800 nm, 140 fs, 2×10^{16} W cm^{-2}). (b) The time-varying electric field inside the cluster in the vicinity of resonance with (solid line) and without (dashed line) the effective dielectric constant included. (c) Kr ion fraction resulting from the interaction of 7.5 nm Kr clusters with the same laser pulse as a function of time where the quasistatic dielectric constant is used.

III. SIMULATION RESULTS

After introducing the effective dielectric constant for the rapidly expanding plasma to calculate the laser deposition rate, the modified hydrodynamic model is employed to investigate the dynamics of Kr clusters of different sizes driven by ultrashort high-intensity laser pulses of different wavelengths.

A. Simulation model

1. The rate equations

$$\frac{\partial P_k}{\partial t} = -\Gamma_k P_k + \Gamma_{k-1} P_{k-1},$$

$$\frac{\partial n_e}{\partial t} = \sum_k \Gamma_k P_k - W_{FS}. \tag{9}$$

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

2. The kinetic equation

$$\frac{\partial^2 r}{\partial t^2} = 3\frac{P_e + P_{Coul}}{n_i m_i}\frac{1}{r}, \tag{10}$$

where $P_{Coul} = Q^2 e^2/8\pi r^4$ is the Coulomb pressure caused by the net positive charges Q inside the cluster. $P_e = n_e k T_e$ is the electron thermal pressure. r is the radius of the expanding cluster, and n_i and m_i are the ion density and ion mass, respectively.

3. The energy equation

$$\frac{3}{2} n_e K \frac{\partial T_e}{\partial t} = \frac{\partial U}{\partial t} - \frac{3}{r} P_e \frac{\partial r}{\partial t} - q_{out}, \tag{11}$$

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

B. Cluster-size effect in the interaction

Many studies have shown that the cluster size can greatly influence the coupling efficiency of laser energy during the interaction of clusters with lasers. A small-sized cluster in a laser field behaves like a molecule; it expands and dissasembles rapidly, and thus the absorption efficiency decreases rapidly. On the other hand, a cluster that is large expands slowly in a laser field and the electron density is higher than $3n_{crit}$ until the end of the laser pulse, so the absorption efficiency is also low. In order to study the cluster-size effect in the interactions, the dynamics (such as the expansion of the cluster, the electron temperature, and the ionization of atoms) of different-sized Kr clusters illuminated by a laser pulse

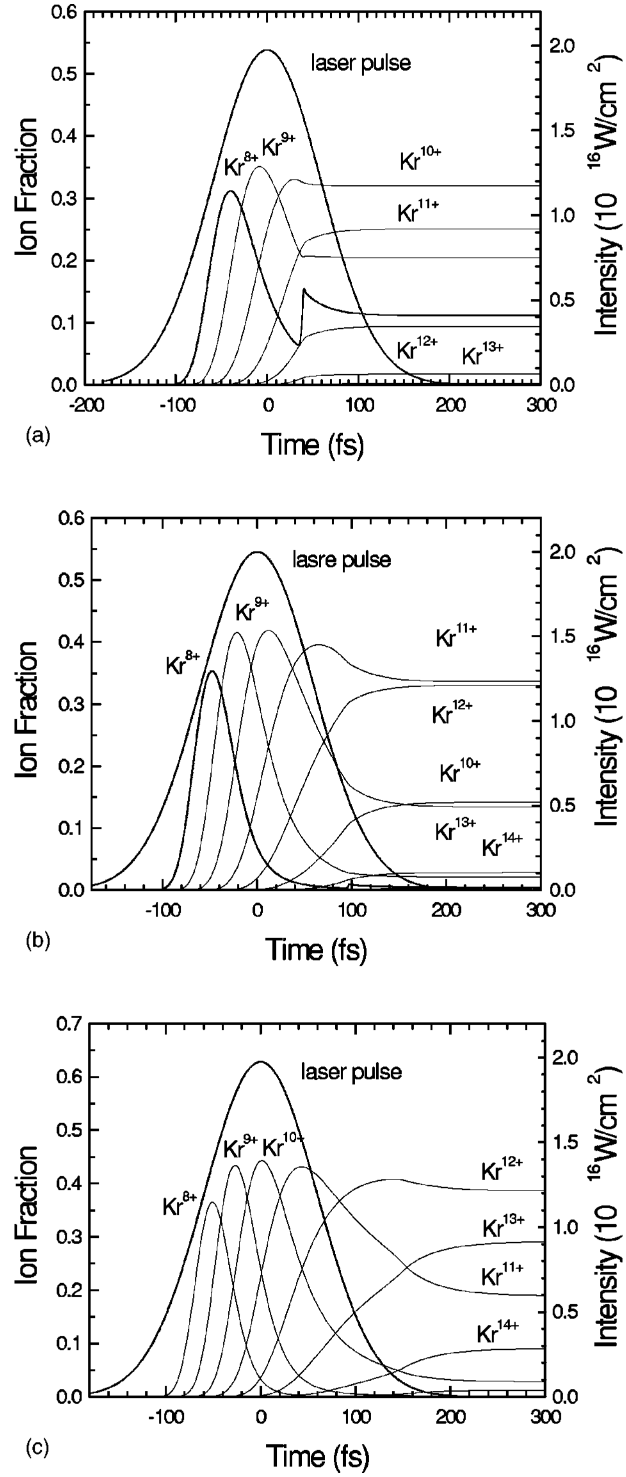

FIG. 2. Kr ion fraction from Kr^{8+} to Kr^{15+} as a function of time for different cluster sizes. The cluster radius is (a) 5.0, (b) 7.5, and (c) 10 nm.

(800 nm, 140 fs, 2×10^{16} W/cm^2) have been calculated. The results are shown in Figs. 2, 3, 4, and 5. Figure 2 shows the ion fraction from Kr^{8+} to Kr^{15+} as a function of time for different cluster sizes; the cluster radius is (a) 5.0, (b) 7.5, and (c) 10 nm. Figure 3 shows the ion velocity as a function of time for different cluster sizes. Figure 4 shows the elec-

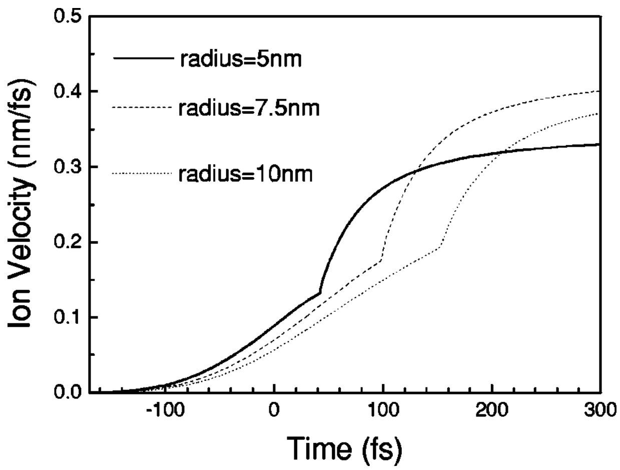

FIG. 3. Ion velocity as a function of time for different cluster sizes.

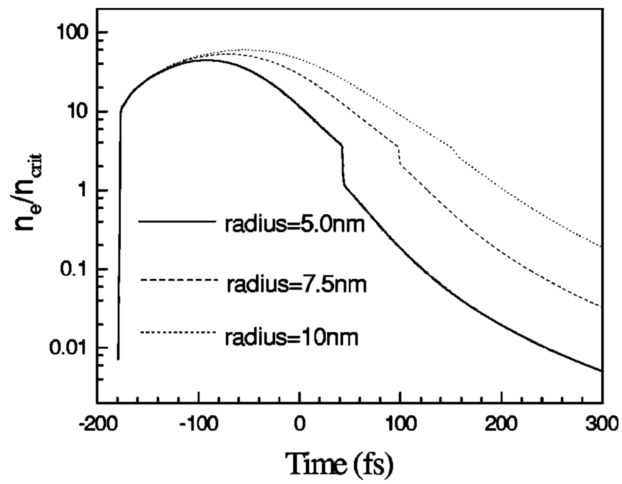

FIG. 4. Electron density as a function of time for different cluster sizes.

tron density as a function of time for different cluster sizes and Fig. 5 shows the electron temperature as a function of time for different cluster sizes.

The following conclusions can be drawn from Fig. 2, 3, 4, and 5. (1) The larger the cluster size, the higher the ionization degree of the ions becomes. The average charge states are Kr^{10+}, Kr^{11+}, and Kr^{12+} for cluster sizes of 5.0, 7.5, and 10 nm, respectively. This result can be explained by the ionization process where the electron-impact ionization dominates. The optical field ionization makes a major contribution in the early stage of the interaction and plays the role of ionization ignition. The electron density increases to become higher than $3n_{crit}$ in a short time; the electric field inside the cluster is then smaller than the laser field in vacuum. The electrons are heated by inverse bremsstrahlung and the electron temperature increases. Since there is a high electron density, the rate of electron-impact ionization is also high. For a larger-sized cluster, the heating and electron-impact ionization occur for a longer time, so that higher-charge ions can be produced in the interaction. (2) The calculated expanding velocities for Kr clusters with radii of 5.0, 7.5, and 10 nm are 0.33, 0.4, and 0.36 nm/fs, respectively. Since a uniform expansion of the cluster is assumed, the ion radial velocity linearly increases from zero as the radial position increases in the cluster, so the average kinetic energy of the ions is calculated as $E_{ion}=0.3m_i v^2$, where m_i is the ion mass. The average kinetic energy of the ions for Kr clusters with radii of 5.0, 7.5, and 10 nm is 24, 36, and 27 keV, respectively. Consequently, for a given laser pulse, there exists an optimum cluster size to achieve the maximum ion energy.

In [7], Ditmire *et al.* studied experimentally and theoretically the high-intensity femtosecond photoionization of inertially confined noble-gas clusters. Figure 9 in that reference examined the scaling of the ion energy distribution in Xe clusters. The experimental results showed that the average energy of ions increased slowly with increasing cluster size. The average kinetic energy of ions resulting from the interaction of a 2500-atom Xe cluster (~ 4 nm in radius) is about 41 keV and the maximum energy E_{max} (defined as the energy at which the signal drops to 10^{-5} of its maximum) is 1 MeV. Figure 10 in the same reference also examined the scaling of the ion energy distribution in Kr clusters. It can be seen that the average energy of Kr ions is a little lower than that of Xe ions for the same cluster size. Therefore it is to be expected that the average ion energy of Kr ions for a cluster size of 5 nm will be close to or maybe lower than 40 keV. That is close to our calculated results. In Refs. [14,15], Springate *et al.* compared their calculated results with the measured maximum energy of ions instead of with the average kinetic energy of ions.

C. The dynamics of clusters in driving laser fields of different wavelengths

The modified hydrodynamic model for the laser-cluster interaction has also been adopted to simulate the dynamics of Kr clusters in laser fields with different frequencies (the laser wavelength corresponding to the fundamental frequency referred to in this work is 800 nm). The radius of the Kr cluster is set as 14 nm, but for a laser with a wavelength of 800 nm it is set as 10 nm (otherwise the radius of 14 nm is so large

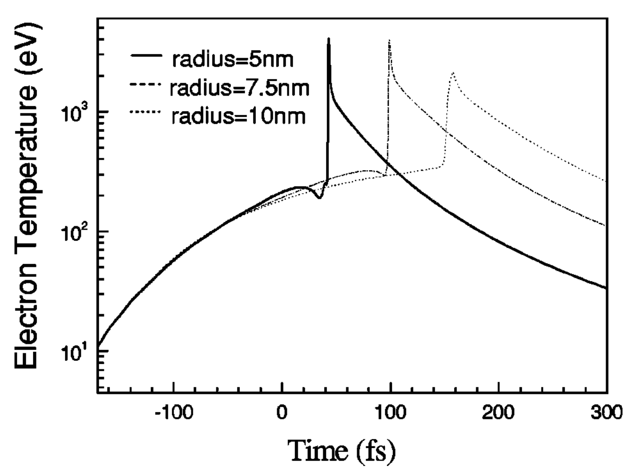

FIG. 5. Electron temperature as a function of time for different cluster sizes.

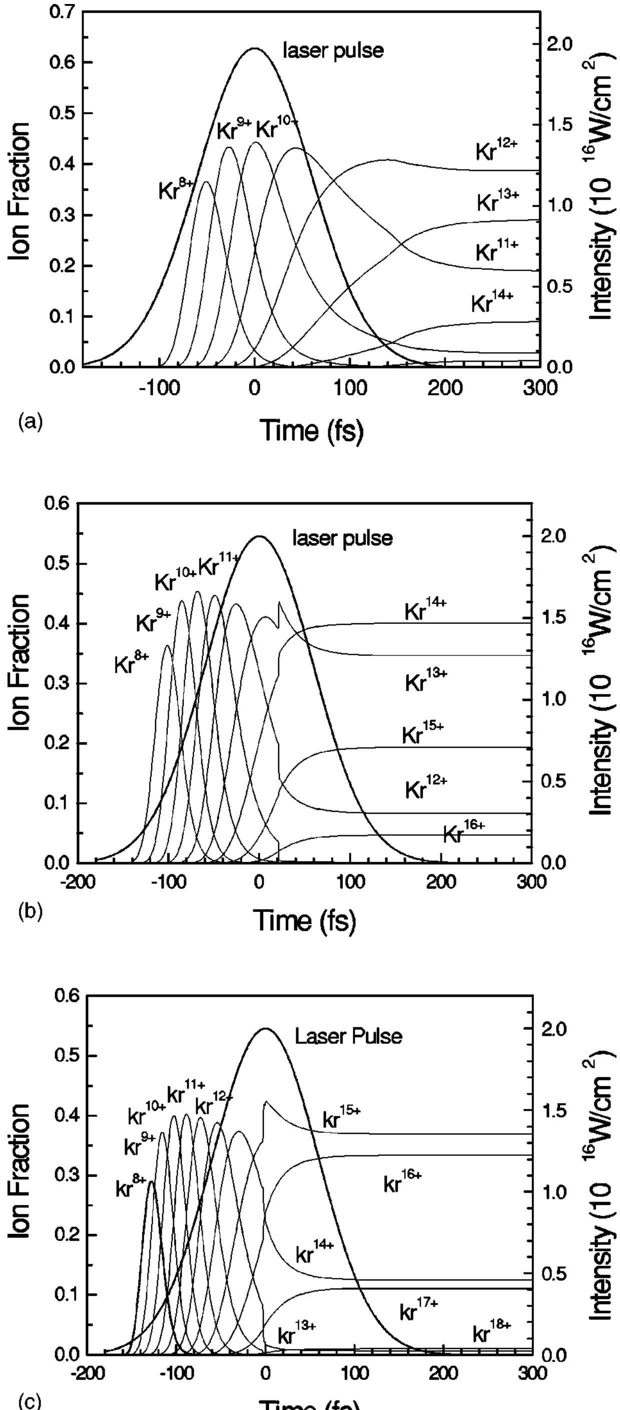

FIG. 6. Kr ion fraction from Kr^{8+} to Kr^{17+} as a function of time for different laser frequencies. The laser frequency is (a) ω_0, (b) $2\omega_0$, and (c) $3\omega_0$.

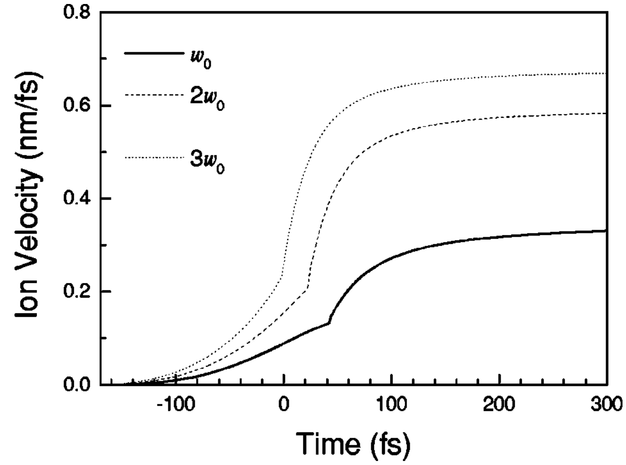

FIG. 7. Ion velocity as a function of time for different laser frequencies.

that the resonance occurs after the end of the laser pulse). The dynamics of the ionization and the expansion of the cluster are shown in Figs. 6 and 7 respectively. It can be seen that as the laser wavelength decreases from IR to UV, the ionization rate of ions and the expanding velocity increase. The corresponding average charge states are Kr^{12+}, Kr^{15+} and Kr^{16+}, and the calculated average kinetic energy of the ions is 27, 74, and 96 keV. The simulation results show that the absorption efficiency is higher for a laser pulse with shorter wavelength. This can be explained by the heating mechanism [Eq. (1)] mentioned above. The laser energy deposition rate in the cluster is proportional to the laser frequency. Moreover, for a laser pulse with shorter wavelength, the critical electron density is higher and the shielding that reduces the electric field in the cluster is weaker; therefore the laser and cluster coupling efficiency becomes higher. However, owing to the more rapid expansion of the cluster in a laser field with shorter wavelength, the cluster size should be increased to enhance the absorption efficiency. In Ref. [16] where a large size (2.9×10^6) of Xe clusters was obtained, the measured x-ray emission from the high charge states of Xe ions for UV KrF laser irradiation was much stronger than those for Ti:sapphire laser irradiation. It is clear that the charge states of ions for short wavelength laser irradiation were higher than those for long wavelength laser irradiation.

IV. DISCUSSION

Since a uniform expansion of the cluster is assumed in the hydrodynamic model and the expansion velocity of ions with different charge states is also treated as the same, the energy spectrum of ions cannot be derived. For a uniform expansion, the number of ions is proportional to their kinetic energy (v^2), which means that the number of ions with higher energy is larger than that of ions with lower energy, but this is in contradiction with experiments. In our future work, the ion energy spectrum will be obtained by using particle simulation. However, from the viewpoint of energy conservation, the average kinetic energy (instead of the maximum energy) can be obtained by calculating the expanding velocity of the cluster. In our simulations, the calculated average kinetic energy of ions is near to the observed results, but in Refs. [14,15] the calculated kinetic energy was close to the measured maximum energy of the ions. This discrepancy may be explained by assuming that the hydrodynamic model without including the effective dielectric constant overestimates the resonance enhancement. This implies that the modified hydrodynamic model is in better agreement with experiments.

The model is reasonable for explaining the production of highly charged ions. If only the optical field ionization is considered, a laser field at the intensity of 2×10^{16} W cm^{-2} can produce only Kr^{8+}. The generation of Kr^{12+}, Kr^{13+}, Kr^{14+}, Kr^{15+}, Kr^{16+}, and Kr^{17+} ions requires a laser field at the intensity of 4.6×10^{17}, 6.2×10^{17}, 8.4×10^{17}, 1.1×10^{18}, 1.4×10^{18}, and 1.7×10^{18} W cm^{-2}, respectively. Therefore the production of highly charged ions is mainly caused by electron-impact ionization or tunnel ionization by the enhanced electric field. The model has also been employed to simulate the dynamics of Ar and Xe clusters in a laser field. The simulations have shown that a considerable fraction of neonlike Ar^{8+} and nickel-like Xe^{26+} can be achieved if appropriate cluster size and laser intensity are selected. These results imply that these clusters may become a promising lasing medium for keV x-ray lasers.

V. CONCLUSIONS

An effective dielectric constant is derived to modify the hydrodynamic model for the interaction between clusters and a short-pulse high-intensity laser. The cluster-size effect and driving laser wavelength dependence of the interaction dynamics were investigated by using the modified hydrodynamic model. The calculated results are in reasonable agreement with the experimental results. In particular, our model can explain more reasonably the average kinetic energy of ions and the generation of highly charged ions.

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