Dynamics of Coulomb explosion of hydrogen clusters in a high-intensity femtosecond laser pulse

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Using Bethe model, the dynamics of the ionization and Coulomb explosion of hydrogen clusters (0.5—5 nm) in high-intensity (10^{15}—10^{17} W/cm^2) femtosecond laser pulses have been studied theoretically, and the dependence of energy of protons emitted from exploding clusters on cluster size and laser intensity has been investigated. It is found that the maximum proton energy increases exponentially with the cluster size, and the exponent is mainly determined by the laser intensity. For a given cluster size, the maximum proton energy increases with increasing laser intensity and gets saturation gradually. The calculation results are in agreement with the recent experimental observation.

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In recent years, the interaction of high-intensity laser pulses with atomic or molecular clusters has been a topic of interest. Unlike solid or rarefied gaseous targets where a rapidly created surface plasma prevents the laser from penetrating deeper into target for the former and the density is too low to yield high absorption efficiency for the latter, clusters have been shown to be optimal in the absorption of laser energy[1]. Furthermore, energetic electrons, ions, photons, and neutrons originating from nuclear fusion have been observed in laser-cluster interaction experiments[2−5].

The evolution of laser-cluster interaction in a high intensity laser pulse mainly include two stages. The first is the inner ionization, i.e., the electrons are removed from their parent ion, the second is the rejection of the electrons from the cluster which as a whole is called outer ionization. The buildup of the positive charge due to the outer ionization can result in the Coulomb explosion of the cluster. For rare gas clusters, such as Kr or Xe clusters, higher charge states inside the cluster have been generated compared with that of single atoms of Kr or Xe in the same laser field[3]. Upon which, several mechanisms have been proposed to investigate the increased ionization of clusters in laser field[6,7]. Compared with rare gas clusters, the interaction of hydrogen clusters with laser field is relatively simple because a hydrogen atom has only one electron to be ionized. In spite of that the interaction of hydrogen clusters with laser field has been studied experimentally and theoretically[8−10], the influences of the parameters of cluster and laser pulses on the interaction are still not very clear till now. In this letter, we are aiming at illustrating the ionization and expansion process of hydrogen clusters in high intensity laser pulses by using the above-barrier ionization model, and trying to find the influence of cluster size and laser intensity on the laser-cluster interaction.

According to the above-barrier ionization model presented by Bethe *et al.*[11], the inner ionization of hydrogen cluster occurs when the electric field of the laser pulse $E(t) = \pi\varepsilon_0 I_{\rm p}^2/e^3$. Here, e is the electron charge and $I_{\rm p}$ is the ionization potential of the hydrogen atom. If we assume that the laser pulse has the Gaussian distribution and the time $t = 0$ corresponding to the peak value of the laser pulse, then we can learn when the inner ionization occurs. From the critical time, the outer ionization proceeds sequentially. Similar to the inner ionization, the outer ionization is also derived from the Bethe model. If we mark the number of outer ionized electrons by the laser field as $Q(t)$, the Coulomb potential of the cluster ions at the cluster surface is $eQ(t)/4\pi\varepsilon_0 r_{\rm c}(t)$ where $r_{\rm c}(t)$ is the radius of the cluster. Then, we can obtain $Q(t)$ according to

$$E(t) = eQ(t)/4\pi\varepsilon_0 r_{\rm c}^2(t), \tag{1}$$

where the cluster radius $r_{\rm c}(t)$ is also a function of time. With the commencement of outer ionization and the charge buildup in the cluster, the cluster will expand due to the repulsive force between the protons. According to Newton's law, the variation of the cluster radius $r_{\rm c}(t)$ with time is of the form

$$m\frac{{\rm d}^2 r_{\rm c}(t)}{{\rm d}t^2} = \frac{e^2 Q(t)}{4\pi\varepsilon_0 r_{\rm c}^2(t)}, \tag{2}$$

where m is the mass of a proton. When all the electrons have been rejected from the cluster, $Q(t)$ reaches its maximum N, i.e., the total number of atoms in the cluster. Then the expansion equation of the cluster can be written as

$$m\frac{{\rm d}^2 r_{\rm c}(t)}{{\rm d}t^2} = \frac{e^2 N}{4\pi\varepsilon_0 r_{\rm c}^2(t)}. \tag{3}$$

Combining Eqs. (1) and (3), we can get the dynamics of a hydrogen cluster in intense laser pulses theoretically.

Figure 1 shows the simulation result of the evolution of inner and outer ionizations of a hydrogen cluster (N = 8000) in a femtosecond laser pulse. In the simulation, the peak intensity and duration time (full width at half maximum (FWHM)) of the laser pulse are 10^{16} W/cm^2 and 100 fs, respectively. We employ a hydrogen cluster with atomic density $\rho \approx 5\times10^{22}$ cm^{-3}[12]. From Fig. 1, it can be seen that the inner ionization starts at the time of $t = -125.5$ fs. Since the cluster size is much smaller than the wavelength of the laser, all atoms inside the cluster experience the same laser field, the inner ionization can be taken as finished simultaneously. Compared with

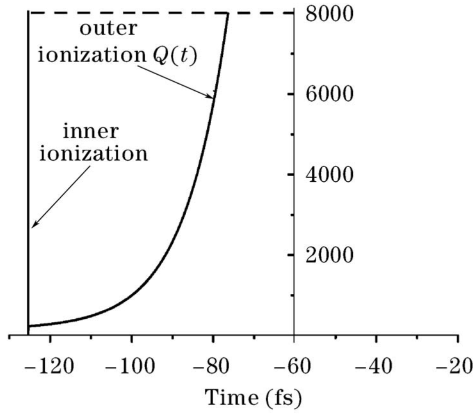

Fig. 1. Inner and outer ionization processes of a hydrogen cluster (8000 atoms) in a high-intensity laser pulse with peak intensity of 10^{16} W/cm^2 and duration of 100 fs.

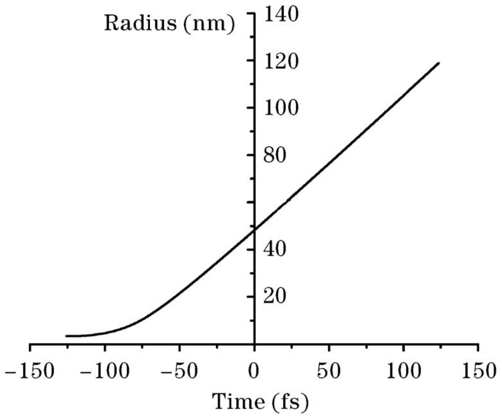

Fig. 2. Radius of the hydrogen cluster as a function of time, the parameters are the same as in Fig. 1.

the inner ionization, the outer ionization of the cluster lasts a comparatively long time, it does not finish until $t = -76.3$ fs. After this time instant, the cluster becomes a positive charge sphere composed of protons. In Fig. 2, the variation of the cluster radius with time is given. We can see that with the beginning of the outer ionization, the cluster starts to expand. At the beginning stage of the outer ionization, the radius increases slowly as the charge buildup in the cluster is very limited and the expansion velocity of the cluster increases slowly. But with the continuation of outer ionization, especially in the time period near the fulfillment of the outer ionization, the velocity increases sharply, and the radius increases rapidly. Finally, the radius of the cluster exhibits linear increase with time, indicating that with the expansion of the cluster, the Coulomb repulsion force between the protons decreases gradually, and the expansion velocity of the cluster reaches a steady value.

To inquire into the influence of cluster size on the laser-cluster interaction and the final proton energy, the simulations of ionization and expansion processes of different cluster sizes has also been performed. Figure 3 shows the expansion velocities of different cluster sizes as functions of time in a laser field with peak intensity of 10^{15} W/cm^2 and duration of 100 fs. It indicates that the expansion velocities of the clusters increase with the increase of cluster size, though the time needed for the outer ionization

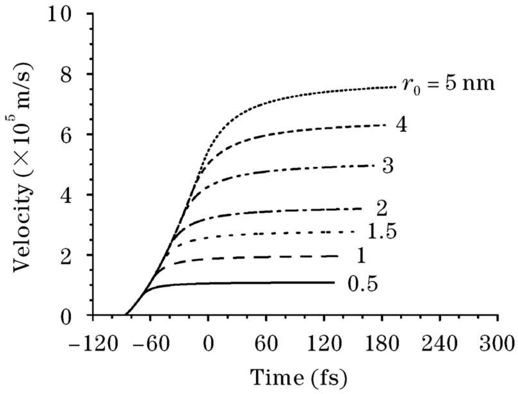

Fig. 3. Expansion velocities of different size hydrogen clusters as functions of time in a high-intensity laser pulse with peak intensity of 10^{15} W/cm^2 and duration of 100 fs.

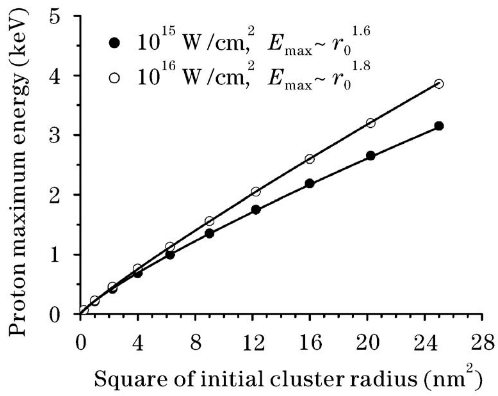

Fig. 4. Relation between maximum proton energy and the square of initial cluster radius at different laser intensities.

increases accordingly. This means that large cluster size benefits the production of energetic protons. Figure 4 shows the relationship between the maximum energy of protons emitted from exploding hydrogen clusters and the square of the initial cluster radius r_0. For the laser intensity of 10^{15} W/cm^2 and duration of 100 fs, the maximum energy increases from 0.06 to 3.2 keV when the cluster radius r_0 increases from 0.5 to 5 nm. This result is in agreement with the experimental results[8]. The relationship between the maximum energy of proton and the cluster size is given by $E_{\max} \propto r_0^{1.6}$, which is similar to our recent experimental result of argon clusters[13], but slightly different from the simulation result of Ref. [10]. In Ref. [10], the interaction of small hydrogen clusters (less than 309 atoms per cluster) with high intensity laser pulses has been studied using classical dynamic method, and the results show that the exponent is 2 rather than 1.6 of our result. For comparison, we also calculated the maximum proton energy of different cluster sizes at the laser intensity of 10^{16} W/cm^2 (the pulse duration time is constant). As shown in Fig. 4, for the same cluster size, the maximum energy of protons is larger for higher laser intensity, and the exponent of the maximum proton energy to the cluster size is increased from 1.6 to 1.8.

For typical Coulomb explosion of clusters, the maximum energy $E_{\max}$ of ions emitted from a cluster and the initial radius r_0 of the cluster should satisfy $E_{\max} \propto r_0^2$. For the validity of the relation, a prerequisite is that the outer ionization process should be fulfilled in very short time, for example, it should be much shorter than the time needed for the cluster to expand to double of its initial radius[12]. Parks *et al.*[14] thought that for a given laser intensity, the initial cluster radius should be less than a certain maximum value, r_0 (nm)$< r_{\max} = 1.653 \times 10^{-8} I^{1/2}$ (W/cm^2), in order to have Coulomb explosions in deuterium clusters. For laser intensities of 10^{15} and 10^{16} W/cm^2, the maximum values are approximately 0.5 and 1.6 nm, respectively. In fact, if we divide the cluster size in Fig. 4 into two ranges, i.e., $r_0 \approx 0.5$—1.5 nm and $r_0 \approx 1.5$—5 nm, we can find that the maximum proton energy is basically proportional to the square of the initial cluster radius for radius less than 1.5 nm at the laser intensity of 10^{16} W/cm^2, consistent with above criterion. As for the clusters with radius larger than 1.5 nm, as well as the clusters in the laser field with intensity of 10^{15} W/cm^2, the outer ionization process prolongs accordingly with increasing the cluster size, which results in the further increase of the cluster size. For these clusters, comparatively longer outer ionization process weakens the effect of Coulomb explosion, as a result, the maximum proton energy is not proportional to the square of cluster radius. But because the electrons in these clusters can be fully outer ionized by the laser field, the explosion of the clusters is still driven by the repulsive force between the protons. For the given laser intensity, too large cluster even results in that only a part of the electrons can be outer ionized and a fraction of electrons remains in the cluster due to the attraction of the protons, this can further worsen the situation. For this case, the mechanism of expansion of the clusters cannot be simply defined as Coulomb explosion and other mechanisms should be taken into account. Obviously, for a given cluster, higher laser intensity can speed up the outer ionization process, so the Coulomb explosion is much more violent, and the final proton energy is larger than that of lower laser intensity, just as shown in Fig. 4.

It is worth noting that although high laser intensity is beneficial to the production of energetic protons, it is not meant that the maximum energy of protons could be enhanced unrestricted by increasing the laser intensity. Figure 5 shows the evolution of the expansion velocity of the same size cluster as in Fig. 2 at three different laser intensities (the pulse duration time is constant). It reveals that due to the difference of the laser intensity, the time moments of the starting point of ionization are also different. With the increase of laser intensity, the time needed for the outer ionization decreases, and the final expansion velocity increases accordingly. This is just the situation mentioned above. But we should also note that when the laser intensity increases from 10^{16} to 10^{17} W/cm^2, the final expansion velocity of the protons increases only a little, much less than that when the laser intensity increases from 10^{15} to 10^{16} W/cm^2. Simulation also shows that further increasing laser intensity can make very limited contribution to the increase of proton energy, and the proton energy gets saturated gradually with laser intensity.

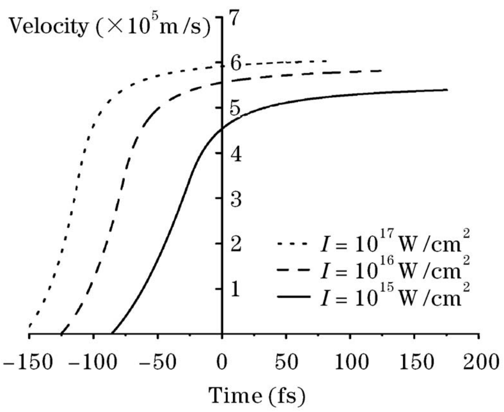

Fig. 5. Expansion velocities of a hydrogen cluster as a function of time at different laser intensities.

In conclusion, using Bethe model, we have simulated the ionization and explosion processes of hydrogen clusters in a high-intensity laser pulse. The result shows that the maximum proton energy increases exponentially with the cluster size, with the exponent determined by the laser intensity. For a given cluster size, the maximum proton energy increases with laser intensity and gets saturated gradually.

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