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Overrun phenomenon and neutron yield in Coulomb explosion of deuterated alkane clusters driven by intense laser field*

Hong-Yu Li(李洪玉)†, Mei-Dong Huang(黄美东), Ming Kang(康明), and De-Jun Li(李德军)

College of Physics and Materials Science, Tianjin Normal University, Tianjin 300387, *China*

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By using a simplified Coulomb explosion model, the laser-driven Coulomb explosion processes of three deuterated alkane clusters, i.e., deuterated methane $(CD_4)_N$, ethane $(C_2D_6)_N$ and propane $(C_3D_8)_N$ clusters are simulated numerically. The overrun phenomenon that the deuterons overtake the carbon ions inside the expanding clusters, as well as the dependence of the energetic deuterons and fusion neutron yield on cluster size, is discussed in detail. Researches show that the average kinetic energy of deuterons and neutron yield generated in the Coulomb explosion of $(C_2D_6)_N$ cluster are higher than those of $(CD_4)_N$ cluster with the same size, in qualitative agreement with the reported conclusions from the experiments of $(C_2H_6)_N$ and $(CH_4)_N$ clusters. It is indicated that $(C_2D_6)_N$ clusters are superior to $(CD_4)_N$ clusters as a target for the laser-induced nuclear fusion reaction to achieve a higher neutron yield. In addition, by comparing the relevant data of $(C_3D_8)_N$ cluster with those of $(C_2D_6)_N$ cluster with the same size, it is theoretically concluded that $(C_3D_8)_N$ clusters with a larger competitive parameter might be a potential candidate for improving neutron generation. This will provide a theoretical basis for target selection in developing experimental schemes on laser-driven nuclear fusion in the future.

Keywords: deuterated alkane cluster, Coulomb explosion, deuteron kinetic energy, neutron yield

PACS: 36.40.Wa, 52.50.Jm, 52.38.Kd, 25.45.–z **DOI:** 10.1088/1674-1056/27/6/063602

1. Introduction

Gas clusters irradiated by intense laser pulses can generate MeV ions and intense x-rays.[1,2] Especially, the laser-driven explosions of clusters containing deuterium can produce energetic deuterons and trigger nuclear fusion, thus opening up a new way for making a table-top neutron source.[3,4] In 1999, an efficiency of about 10^5 neutrons per joule of incident laser energy was achieved from the interaction of laser with deuterium clusters in the experiment designed by Ditmire *et al.*,[5] but in order to meet the requirements for practical applications the output efficiency must reach $10^7 \sim 10^8$ neutrons/J.[6,7] Therefore, many researchers constantly search for all kinds of excellent targets to enhance the neutron yield, including some targets composed of different materials.[8,9] It is found that the deuterated heteronuclear clusters (i.e., deuterated methane $(CD_4)_N$ clusters and deuteroxide $(D_2O)_N$ clusters)[10–12] are more suitable for serving as the targets for the laser-induced fusion than pure deuterium $(D_2)_N$ clusters.[13,14] Liu's group has obtained a conversion efficiency of 1.9×10^7 neutrons/J from the Coulomb explosions (CE) of large-size $(CD_4)_N$ cluster jets under the irradiation of intense femtosecond laser pulses.[15–18] This conversion efficiency is dramatically increased as compared with that using the similar sized homonuclear $(D_2)_N$ clusters. The researchers also measured that the final average kinetic energy of protons from the CE of ethane $(C_2H_6)_N$ clusters is higher than that from the same sized methane $(CH_4)_N$ clusters.[19] Therefore they inferred that large-size deuterated ethane clusters $(C_2D_6)_N$ will be more favorable for higherefficiency neutron generation than $(CD_4)_N$ clusters. However, the relevant experiment that can confirm their inference has not been carried out yet. Even the theoretical research relating to the nuclear fusion from the laser-heated $(C_2D_6)_N$ clusters has rarely been reported. In the experiments of laser-cluster interaction, clusters are generally produced by an adiabatic expansion of gases through a conical nozzle into vacuum.[5,12–19] At normal temperature, only methane CH_4, ethane C_2H_6 and propane C_3H_8 are in gaseous state.[20] However, there is no investigation on the interaction of propane $(C_3H_8)_N$ clusters with intense laser pulses, which is attributed to the fact that the physical properties of propane gas are unstable and the corresponding clusters are not easy to form.

In this work, we will use a simplified Coulomb explosion model to investigate laser-irradiated expansions of $(CD_4)_N$, $(C_2D_6)_N$, and $(C_3D_8)_N$ clusters generated by deuterated gaseous alkanes. Besides the overrun effect determined by the accelerations of deuterons and carbon ions, the deuteron energy spectrum and D–D fusion neutron yield are calculated, and the calculations are compared with the results of reported experimental inference.[19] It is confirmed that the deuteron energy and neutron yield produced in $(C_2D_6)_N$ clusters are greater than those of $(CD_4)_N$ clusters. Another deduction is that the $(C_3D_8)_N$ clusters might be a potential target for laser-driven nuclear fusion.

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†Corresponding author. E-mail: wlxylhy@mail.tjnu.edu.cn

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2. Models for pure Coulomb explosion of heteronuclear clusters

The evolution of a cluster under the irradiation of an ultrashort intense laser field mainly consists of three subprocesses: inter ionization, outer ionization and cluster expansion.[10,21] Firstly, the atoms or molecules in the cluster will be ionized by the optical field. According to the one-dimensional barrier-suppression model,[22] the threshold laser intensity necessary to permit the bound electrons to be free without tunneling, is given as

$$I_{\rm th}\left(\mathrm{W\cdot cm^{-2}}\right) = 4.00\times 10^{9}\frac{E_{\rm ion}^{4}\,(\mathrm{eV})}{Z^{2}}. \tag{1}$$

According to the empirical formula, the threshold intensity for ionizing carbon atoms into carbon ions with charge state $Z=+4$ is 4.33×10^{15} W/cm^2, while the intensity for ionizing deuterium atoms into deuterons with charge state $Z=+1$ is 1.37×10^{14} W/cm^2. Secondly, the electrons generated in the first-step ionization process may obtain high energy from the laser field to escape out of the cluster ball, so that the cluster acquires a positive charge. Thirdly, the ions residing in the cluster repulse each other by the Coulomb forces and the cluster expands outward accompanied with some hydrodynamic processes. If a laser field has no enough high intensity or enough short rising time, part of electrons still stay inside the cluster, slowing down the cluster expansion. This is called non-pure Coulomb explosion which is anisotropic due to the oscillation of electrons dragged by the laser field.[23–25] On the contrary, if the total electrons with high energy obtained from an ultra-intense laser field can be stripped out of the cluster immediately, the removal of electrons prior to cluster expansion leads to a powerful Coulomb potential energy stored in the cluster and makes the expansion more violently. In this way, the cluster expansion can be simplified into a pure Coulomb explosion (PCE)[10,26] and the required critical laser intensity is[21]

$$\begin{aligned} & I_{\rm crit}\left(10^{14}\mathrm{W\cdot cm^{-2}}\right) \\ &= \frac{8\pi^{2}c^{3}m_{\rm e}\rho_{\rm e}R_{0}^{2}}{3\lambda^{2}} \\ &\approx 6.46\times\left(\rho_{\rm e}/10^{22}\ \mathrm{cm^{-3}}\right)\cdot\left(\frac{R_0/\mathrm{nm}}{\lambda/\mu\mathrm{m}}\right)^{2}, \end{aligned} \tag{2}$$

where λ is the central wavelength of a laser filed, R_0 is the initial radius of a cluster, and $\rho_{\rm e}$ is the number density of electrons inside the cluster. For a fully ionized heteronuclear cluster ball $(A_{n_A}^{q_A+}B_{n_B}^{q_B+})_N$, $\rho_{\rm e}$ can be calculated from $\rho_{\rm e}=\rho_0(n_{\rm A}q_{\rm A}+n_Bq_B)$ where ρ_0 is the number density of molecules $A_{n_A}B_{n_B}$ in the heteronuclear cluster at a state of electrical neutrality before the inner-ionization. The wavelength λ is chosen to be 800 nm, which is equal to that used in the experiment.[19] It is assumed that in the deuterated alkane clusters, all deuterium atoms are completely ionized to charge state of $+1$, and carbon atoms are ionized to $+4$. The molecular number densities of $(CD_4)_N$, $(C_2D_6)_N$, and $(C_3D_8)_N$ clusters are chosen to be 1.6×10^{22}/cm^3,[12,20,27] 1.1×10^{22}/cm^3,[19,20,27] and 8.5×10^{21}/cm^3[20] respectively. Based on Eq. (2), it is calculated that the critical laser intensities for PCE of the three clusters with radius $R_0=5$ nm are 3.2×10^{17} W/cm^2, 3.9×10^{17} W/cm^2, and 4.3×10^{17} W/cm^2, respectively. This magnitude of laser intensity has already been achieved in the reported experiments.[12,28–30] Therefore, it is reasonable to simplify the Coulomb expansion of the three alkane clusters irradiated by a strong laser field into a PCE process. When the cluster size increases, the PCE can also be realized by enhancing the laser intensity experimentally.

Considering the complexity of using molecular dynamic model or particle in cell (PIC) model,[10,11] we use a simplified CE model to study the explosion process of the deuterated clusters. In this model, the expansion of a $(A_{n_A}^{q_A+}B_{n_B}^{q_B+})_N$ cluster is nearly isotropic in space, the repulsion force pushing the light ions A and the heavy ions B outward resources from the Coulomb force between these positively charged ions. The movements of the two types of ions abide by the Newton's second law of motion[31]

$$m_A\frac{\mathrm{d}^2r_A}{\mathrm{d}t^2} = F_{AA}+F_{AB}, \tag{3}$$

$$m_B\frac{\mathrm{d}^2r_B}{\mathrm{d}t^2} = F_{BA}+F_{BB}, \tag{4}$$

where F_{AA} represents the Coulomb rejection force from all A ions contained in a sphere with radius r_A acting on one A ion with mass of m_A at the radial position r_A. F_{AB}, F_{BA}, and F_{BB} have the similar definitions to the above. Because the mass, charge and density of light and heavy ions differ from each other in a heteronuclear cluster, the ions at the same position may have different accelerations, which results in the so-called overrun phenomenon. The first overrun phenomenon is that the light ions can attain a higher acceleration than the heavy ones at the same initial position if the kinematic parameter $\eta=q_Am_B/q_Bm_A$ of the cluster is larger than 1.[11] The light ions will move out from the configuration framework of the heavy ions as the cluster expands, and obtain higher and higher kinetic energy. For the deuterated clusters, the energetic deuterons flying away from different clusters will collide with each other, leading to the intercluster fusion. These hot deuterons are also likely to collide with the cold deuterons in the surrounding gas, initiating the beam–target fusion.[12] The second overrun phenomenon occurs for the competitive parameter of the cluster $\zeta=n_Bq_B/n_Aq_A>2$.[31,32] Under this condition, the fast light ions in inner layers can catch up with and even overtake their peers having slower expansion velocities in outer layers, thus forming a thin shock shell.[33] The

nuclear reaction might occur in pace with collisions among deuterons inside the shock shell, which is termed the intra-cluster fusion.

3. Calculation results and discussion

Table 1 shows the values of kinematic parameter and competitive parameter of the fully ionized clusters, i.e., $(C^{4+}D_4^+)_N$, $(C_2^{4+}D_6^+)_N$, and $(C_3^{4+}D_8^+)_N$. The kinematic parameters of the three clusters are all equal to 1.5, and the values of competitive parameters are less than 2 and increase in turn. Accordingly, the deuterons (light ions) in inner layers will surpass the carbon ions (heavy ions) even if they are initially distributed at the same positions, but will not catch up with the deuterons in outer layers. However, a larger competition parameter means that if a deuteron at a certain radial position is selected as the research object, the Coulomb force sourced from carbon ions (heterogenous force), acting on this deuteron, has more intense repulsion effect than the force from other deuterons (homogenous force).[31] Although the deuterons in inner layer cannot catch up with their peers in outer layer, the trend to catch-up is more obvious if the cluster has a larger competitive parameter. As a result, more inner deuterons are pushed to the outer space and assemble together. The detailed differences in ion movement and energy spectrum among the three clusters led by the competition parameter are shown in Figs. 1 and 2.

Table 1. Values of kinematic parameter η and competitive parameter ζ of three deuterated alkane clusters.

Cluster	η	ζ
$(C^{4+}D_4^+)_N$	3/2	1
$(C_2^{4+}D_6^+)_N$	3/2	4/3
$(C_3^{4+}D_8^+)_N$	3/2	3/2

It can be seen from Fig. 1 that the motion patterns of light and heavy ions are qualitatively consistent with each other for the three expanding clusters. For example, the carbon ions of the $(C^{4+}D_4^+)_N$ cluster are uniformly distributed in the ball space with the radial coordinate $r = 21$ nm or so, where only a small number of deuterons are uniformly distributed (i.e., the density is constant). The expansion velocity of an ion is defined as the derivative of its radial coordinate r with respect to time t. The expansion velocities of the two kinds of ions are both directly proportional to the radial coordinate. However, a large number of deuterons, due to having greater acceleration than the carbon ions, eventually leave the space frame formed by the carbon ions and accumulate in outer space of $r = 24$ nm–29 nm. The increasing trend of deuteron velocity with radial coordinate slows down, and the deuteron density along radial direction rises sharply. This is because, as long as a deuteron can overtake the carbon ions at the same initial location, the Coulomb repulsive force from the inner ions becomes nonlinear along the radial direction, and then drives deuterons with different velocities to accumulate in some space. As the expansion process is carried on, more and more deuterons overrun the carbon ions. When the cluster expansion ends at infinity (the terminal time instant is set to be 500 fs in our simulations), the group of carbon ions is surrounded by a thin layer of deuterons with huge quantity and maximal velocity. The radially inhomogeneous expansion is also in accordance with that of methane cluster $(C^{4+}H_4^+)_N$ obtained by the particle dynamics simulation method.[34] It can be seen from the comparison among Figs. 1(a)–1(c) that due to the largest ion density, the expansion scale of $(C_3^{4+}D_8^+)_N$ cluster is greatest. The velocity and density of deuterons for $(C_2^{4+}D_6^+)_N$ and $(C^{4+}D_4^+)_N$ clusters decrease in turn.

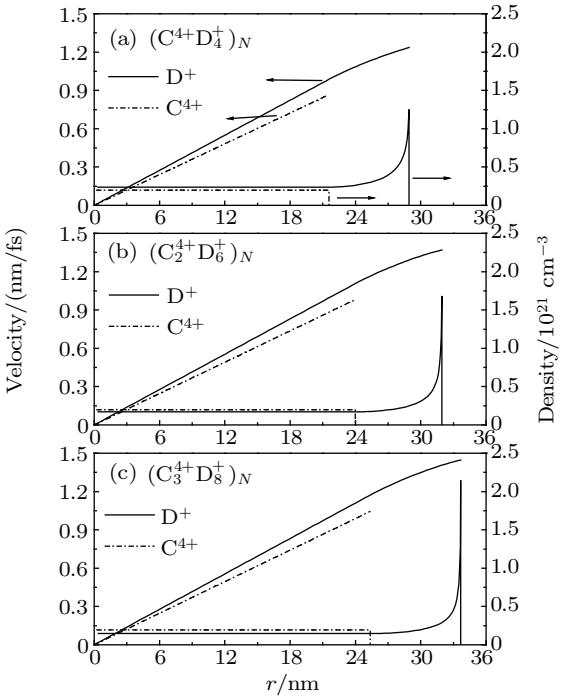


Fig. 1. Plots of expansion velocity and the number density of ions in (a) $(C^{4+}D_4^+)_N$, (b) $(C_2^{4+}D_6^+)_N$, and (c) $(C_3^{4+}D_8^+)_N$ clusters with $R_0 = 5$ nm versus radial coordinates r at the time instant of 20 fs after PCE.

Figure 2 shows that for any of the three clusters, most of the deuterons are distributed in a narrow region of high energy, and the power of the distribution reaches a peak value at the maximum energy. The maximum kinetic energy E_M of deuterons in the $(C_3^{4+}D_8^+)_N$ cluster is larger than in the $(C_2^{4+}D_6^+)_N$ cluster, and the value of E_M in the $(C^{4+}D_4^+)_N$ cluster is smallest. In the vicinity of maximum energy, the energy distribution curve of $(C_3^{4+}D_8^+)_N$ rises fastest while the rising trend of $(C^{4+}D_4^+)_N$ is slowest. As shown in Table 1, the competition parameter of $(C_3^{4+}D_8^+)_N$ is largest, which means that the advantage of the heterogenous force over the homogenous force is most distinct: more deuterons are pushed to the

outer space. The closer to the outer layer the deuteron, the higher its kinetic energy is. Hence the $(C_3^{4+}D_8^+)_N$ cluster has the largest distribution in the high energy region. The proportion of deuterons in the high energy region for $(C^{4+}D_4^+)_N$ and $(C_2^{4+}D_6^+)_N$ clusters decreases in turn since the two clusters have the smaller competition parameters.

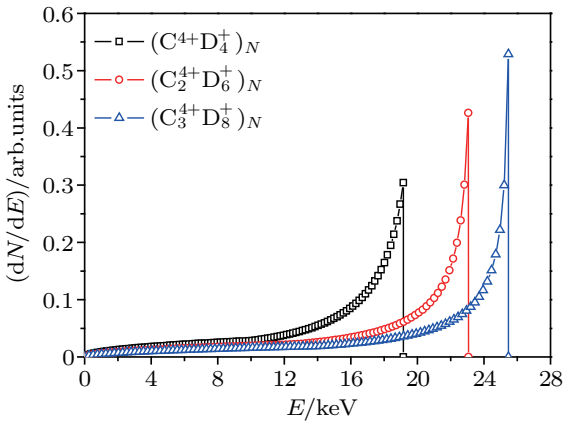


Fig. 2. (color online) Energy spectra of deuterons generated from $(C^{4+}D_4^+)_N$, $(C_2^{4+}D_6^+)_N$, and $(C_3^{4+}D_8^+)_N$ clusters with radius $R_0 = 5$ nm at the time instant of 500 fs after PCE.

It is indicated in Fig. 2 that the maximal values of deuteron kinetic energy of $(C^{4+}D_4^+)_N$, $(C_2^{4+}D_6^+)_N$ and $(C_3^{4+}D_8^+)_N$ clusters are 19.16 keV, 23.06 keV, and 25.47 keV respectively. In our previous work,[31] an extreme case for the expansion of a $(A_{n_A}^{q_A+}B_{n_B}^{q_B+})_N$ cluster was considered. On the precondition that the heavy ions B are approximately static and no overrun occurs between the homogenous ions A, the final kinetic energy of an ion A initially located at r_0 is expressed as

$$\begin{aligned} E_{\rm k}(r_0) &= \int_{r_0}^{\infty}(F_{AA}+F_{AB})\,{\rm d}r \\ &= \int_{r_0}^{\infty}\frac{1}{4\pi\varepsilon_0}\frac{4\pi}{3}\frac{r_0^3\rho_0 n_A q_A^2 e^2}{r^2}\,{\rm d}r \\ &\quad+\int_{r_0}^{R_0}\frac{1}{4\pi\varepsilon_0}\frac{4\pi}{3}\frac{r^3\rho_0 n_B q_B q_A e^2}{r^2}\,{\rm d}r \\ &\quad+\int_{R_0}^{\infty}\frac{1}{4\pi\varepsilon_0}\frac{4\pi}{3}\frac{R_0^3\rho_0 n_B q_{\rm B} q_A e^2}{r^2}\,{\rm d}r \\ &= \frac{\rho_0 q_A e^2}{3\varepsilon_0}\left(n_A q_A r_0^2+n_B q_B\frac{3R_0^2-r_0^2}{2}\right). \end{aligned} \tag{5}$$

Although the theoretical derivation of formula (5) is based on the aforementioned approximate condition, it is obvious that the formula is useful in calculating the final kinetic energy of deuterons initially located at the outermost shell of a deuterated cluster and in this case the formula evolves into a very similar representation to Eq. (7) in Ref. [19]. According to this formula, the maximum deuteron energy $E_{\rm M}$ in the three clusters can be estimated at 19.30 keV, 23.22 keV, and 25.63 keV, almost the same as the results obtained by numerical simulation in this work. Furthermore, with the aid of the formula $\overline{E} = \int_0^{E_{\rm M}} E f(E)\,{\rm d}E / \int_0^{E_{\rm M}} f(E)\,{\rm d}E$ and the energy spectrum shown in Fig. 2, the average deuteron energies $\bar{E}$ of the three clusters are calculated to be 14.43 keV, 17.94 keV, and 20.14 keV respectively, and the ratios of $\bar{E}$ to $E_{\rm M}$ are 0.75, 0.77, and 0.79. These ratios only depend on the cluster species, and do not change with cluster size.

Table 2. Maximum kinetic energies of deuterons in three deuterated alkane clusters with different sizes.

Cluster	R_0/nm	Numbers of C^{4+}	$E_{\rm M}$/keV
$(C^{4+}D_4^+)_N$	5.05	8.63×10^{30}	19.35
$(C_2^{4+}D_6^+)_N$	5.00	1.15×10^{31}	23.06
$(C_3^{4+}D_8^+)_N$	4.95	1.30×10^{31}	24.96

In order to further explain the rejection effect of carbon ions on the deuterons, we choose different radii for $(C^{4+}D_4^+)_N$, $(C_2^{4+}D_6^+)_N$, and $(C_3^{4+}D_8^+)_N$ clusters to make a comparison, and the relevant data are listed in Table 2. The selection of various sizes makes the three clusters have the same number of deuterons. In this case, the cluster with more carbon ions will produce deuterons with higher kinetic energy. When the number of deuterons is set to be equal, the $(C_3^{4+}D_8^+)_N$ cluster has the minimal initial radius and the most carbon ions in number, and the maximum electrostatic potential energy is stored inside the cluster, which will be converted into the highest kinetic energy of deuterons during the subsequent cluster expansion. In contrast to $(C_3^{4+}D_8^+)_N$ cluster, the deuteron energy produced by PCE of the $(C_2^{4+}D_6^+)_N$ cluster becomes lower and the deuteron energy of the $(C^{4+}D_4^+)_N$ cluster decreases to a minimum value.

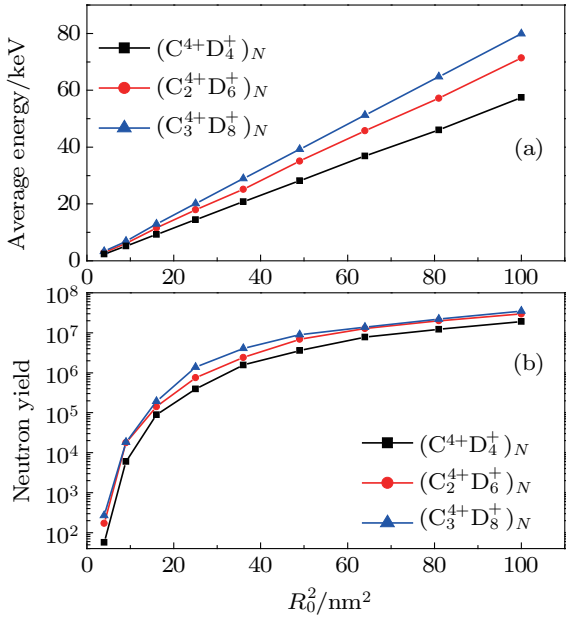


Fig. 3. (color online) Plots of (a) average kinetic energy of deuterons and (b) fusion neutron yields from $(C^{4+}D_4^+)_N$, $(C_2^{4+}D_6^+)_N$, and $(C_3^{4+}D_8^+)_N$ clusters versus the square of initial cluster radius R_0^2.

As is well known, the two prerequisites for nuclear fusion are the high density and high temperature in the reaction

region. For the compact table-top deuteron–deuteron fusion driven by laser pulses,[5,9,12–18] the high density refers to the number density of deuterons in the laser-heated plasma filaments while the high temperature depends on the kinetic energy of deuterons. In a series of experiments,[15–19] Liu *et al.* studied the Coulomb explosion processes of $(CH_4)_N$, $(CD_4)_N$, and $(C_2H_6)_N$ clusters irradiated by intense laser pulses, but they have not carried out the research on $(C_2D_6)_N$ clusters yet. By analyzing the experimental data and theoretical simulations, they concluded that due to the significant increase of deuteron kinetic energy, the $(C_2D_6)_N$ cluster is more suitable for the nuclear fusion to attain higher neutron yield than $(CD_4)_N$ cluster. However, there has been no literature on experimental verification of their conclusion to date.

To test and verify their hypothesis, the variations of average kinetic energy of deuterons and the neutron yield generated in PCE of the three clusters with cluster size are plotted in Fig. 3. It is shown that the average kinetic energy of deuterons grows linearly with increasing the square of cluster radius, which is independent of the cluster species. The $(C_3^{4+}D_8^+)_N$ cluster has the most obvious growth trend of the deuteron average energy. These hot deuterons collide with each other, so that the fusion reaction of $D^+ + D^+ \rightarrow {}^3He^{2+}\,(0.82\ \text{MeV}) + n\,(2.45\ \text{MeV})$ is triggered with the generation of neutrons. As described above, the neutron yield is the sum of contributions from the inter-cluster nuclear fusion and the beam-target fusion. When the cluster is small, the Coulomb potential energy accumulated within clusters is also limited, and then the low deuteron energy transferring from the potential results in a low probability with which a nuclear fusion reaction produces a small number of neutrons. As the cluster size increases, the deuteron energy and accordingly the neutron yield grows gradually. For example, if the mean radius of clusters is estimated at 10 nm, the neutron yields corresponding to $(C^{4+}D_4^+)_N$, $(C_2^{4+}D_6^+)_N$, and $(C_3^{4+}D_8^+)_N$ clusters are 1.9×10^7, 2.9×10^7, and 3.5×10^7 respectively. The neutron yield produced by $(C_2^{4+}D_6^+)_N$ clusters is much higher than that of $(C^{4+}D_4^+)_N$ clusters at the same size, which is in agreement with the results obtained from the experiments of $(C_2H_6)_N$ and $(CH_4)_N$ clusters.[19] It is also deducted that the neutron yield of $(C_3^{4+}D_8^+)_N$ cluster is even higher than that of $(C_2^{4+}D_6^+)_N$ cluster. In theory, $(C_3D_8)_N$ cluster will be favorable for higher- efficiency neutron generation. Its advantage can be attributed to energetic boosting effects in the overrun processes due to the large competitive parameter. Therefore if deuterated propane $(C_3D_8)_N$ clusters with large sizes can be generated in the future experiments, this kind of cluster with a higher energy region as well as a higher proportion of deuterons distributed in the energy region, seems to be a likely candidate for enhancing total neutron yield compared to $(C_2D_6)_N$ or $(CD_4)_N$ clusters.

4. Conclusions and perspectives

In this work, the Coulomb explosions of $(CD_4)_N$, $(C_2D_6)_N$, and $(C_3D_8)_N$ clusters have been investigated theoretically by use of a simplified electrostatic model. It is validated that apart from the kinetic parameter, the competitive parameter fixed by the ratio of charge density of the carbon ions to that of deuterons also plays a significant role in the process of deuterons overtaking carbon ions. As a result, a deuterated propane cluster $(C_3D_8)_N$ with a large competitive parameter has a high deuteron distribution in the high-energy region due to the heterogeneous overrun effect. The fusion neutrons generated from PCE of the three clusters depending on cluster size are estimated, confirming the reported conclusions based on the experiments of $(C_2H_6)_N$ and $(CH_4)_N$ clusters. It is inferred that $(C_3D_8)_N$ cluster with large size can be chosen as a laser-heated target to obtain higher neutron yield.

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