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Coulomb Explosion and Energy Loss of Energetic C_{20} Clusters in Dense Plasmas *

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The molecular dynamics (MD) method is used to simulate the interactions of energetic C_{20} clusters with the dense plasma targets within the framework of the linear Vlasov–Poisson theory. The influences of various clusters (H_2, N_2, C_{20} and C_{60} respectively) on stopping power are discussed. The simulation results show that the vicinage effects in the Coulomb explosion dynamics and the stopping power are strongly affected by the variations in the cluster speed and the plasma parameters. Coulomb explosions are found to proceed faster for higher speeds, lower plasma densities and higher electron temperatures. In addition, the cluster stopping power is strongly enhanced in the early stages of Coulomb explosions due to the vicinage effect, but this enhancement eventually diminishes, after the cluster constituent ions are sufficiently separated. For the large and heavy clusters, the stopping power ratio reaches much higher values in the early stage of Coulomb explosion owing to the constructive interferences in the vicinage effect.

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In recent years, the interaction of energetic cluster-ion beams (CIB) with matter under plasma state has been an active research area. In particular, along with the fast development of accelerator techniques, it is possible to generate the fast heavy clusters.[1] Moreover, owing to their ability to deposit large amounts of energy in very small volumes of targets, fast CIB demonstrate a strong promise for use in materials modification and inertial confinement fusion.[2]

Driven by the experimental advances, the need to understand the complexity of interactions of large clusters with plasma has motivated a number of theoretical studies in recent years. For the energy loss of individual ions, available theoretical models mainly include linear Vlasov–Poisson theory,[3] the binary collision theory,[4] and the nonlinear Vlasov–Poisson theory.[5] Regarding the cluster penetration through plasmas, it has been shown that the total energy loss is strongly influenced by the interferences resulting from the spatial correlation among the cluster constituent particles, this is the so-called vicinage effect. Vicinage effect on the energy loss of ion clusters in plasma targets has been described theoretically[6,7] within the framework of the linear Vlasov–Poisson theory.

Coulomb explosion is an interesting phenomenon for fast clusters travelling in plasmas, especially for larger clusters such as C_{20}. In solids, the coulomb explosions of C_{20} clusters have been reported in an Al target[8] and oxides (Al_2O_3, SiO_2).[9] For molecular ions in plasma targets, we have studied H_2, N_2 and C_{60} clusters,[10–12] the results show that the explosion patterns exhibit strong asymmetries due to the wake effect after long penetration times. In this Letter, we further investigate the Coulomb explosion patterns and the energy losses of C_{20} clusters in a dense plasma target, especially for the effects of variations of the key plasma parameters, such as the plasma temperature and the plasma density.

Consider a fast C_{20} cluster moving with the velocity $\boldsymbol{v}$, which enters a plasma target characterized by the density n and the electron temperature T. Using the linear Vlasov–Poisson equations, the inter-ionic interaction potential $U(\boldsymbol{r}_{jl}, \boldsymbol{v})$ can be obtained, i.e.[12]

$$U(\boldsymbol{r}_{jl}, \boldsymbol{v}) = \frac{1}{2\pi^2} \int \frac{d^3k}{k^2} \frac{\rho_\eta^2(k)}{\varepsilon(k, \boldsymbol{k}\cdot\boldsymbol{v})} e^{i\boldsymbol{k}\cdot\boldsymbol{r}_{jl}}, \quad (1)$$

where $\boldsymbol{r}_{jl} = \boldsymbol{r}_j - \boldsymbol{r}_l$ is the position vector of the jth ion relative to the lth ion, ρ_η is the expression of bound-electron charge densities for a heavy ion in a classical plasma,[13]

$$\rho_\eta(k) = Z_1 e\Big[1 - \frac{\eta}{1 + (k\Lambda)2}\Big], \quad (2)$$

with $\eta = \frac{2}{9}\sqrt{\frac{2}{3\pi}} \frac{\sqrt{Z}}{[1+(v/v_T)^2]^{3/2}}$. The screening length is defined as $\Lambda/\lambda_D = \left(\frac{2\pi}{27}\right)^{1/4} Z^{1/4}$, where $Z = Z_1/N_D$ with $N_D = n\lambda_D^3$ being the number of plasma particles in a typical Debye volume, $\lambda_D = \sqrt{K_B T/4\pi e^2 n}$ and $v_T = \sqrt{K_B T/m_e}$ are the electron Debye screening length and the electron thermal speed, respectively.

In the dielectric formalism, the target is characterized by its dielectric function $\varepsilon(k, \omega)$, which contains relevant information about the response to electronic excitations induced by the charged particle passing through it. In the expression of interaction potential, $\varepsilon(k, \omega)$ is the longitudinal dielectric function of the classical electron plasma, given by

$$\varepsilon(k, \omega) = 1 + (k\lambda_D)^{-2}\Big[X\Big(\frac{\omega}{kv_T}\Big)$$

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$$- (k\lambda_D^2) + iY\left(\frac{\omega}{kv_T}\right)\Big]. \tag{3}$$

In order to simplify the notation, we introduce the dimensionless variables $\tau = k\lambda_D$ and $\varsigma = \omega/kv_T$ and define the auxiliary functions and $X(\varsigma) = \tau^2 + 1 - 2\varsigma e^{-\varsigma^2}\int_0^\varsigma e^{t^2}dt$ and $Y(\varsigma) = \sqrt{\pi}\varsigma e^{-\varsigma^2}$, so that we can write the inverse dielectric function as

$$\frac{1}{\varepsilon(\tau,\varsigma)} = \frac{\tau^2 X(\varsigma)}{X^2(\varsigma)+Y^2(\varsigma)} - i\frac{\tau^2 Y(\varsigma)}{X^2(\varsigma)+Y^2(\varsigma)}. \tag{4}$$

Invoking the assumption of the adiabatic change of the inter-ionic distances during the propagation through the target, we can write the equation of motion for the position of the jth ion in the cluster center of mass (CM) frame of reference as follows:

$$m\frac{d^2\boldsymbol{r}_j}{dt^2} = \boldsymbol{F}_j^s(\boldsymbol{v}) + \sum_{j\neq l=1}^{20}\boldsymbol{F}(\boldsymbol{r}_{jl},\boldsymbol{v}). \tag{5}$$

The self-stopping forces and the interaction forces are obtained from the inter-ionic interaction potential $U(\boldsymbol{r}_{jl},\boldsymbol{v})$, respectively, as follows:

$$\boldsymbol{F}_j^s(\boldsymbol{v}) = -\partial U(\boldsymbol{r}_{jl},\boldsymbol{v})/\partial \boldsymbol{r}_{jl}\big|_{\boldsymbol{r}_{jl}=0}, \tag{6}$$

$$\boldsymbol{F}_j^s(\boldsymbol{r}_{jl},\boldsymbol{v}) = -\partial U(\boldsymbol{r}_{jl},\boldsymbol{v})/\partial \boldsymbol{r}_{jl}, \quad j\neq l. \tag{7}$$

Assuming that the cluster moves in the z direction, the self-stopping force $\boldsymbol{F}_j^s = F_s(v)\boldsymbol{e}_z$ can be written as

$$F_s(v) = \frac{2}{\pi\lambda_D^2}\left(\frac{v_T}{v}\right)^2\int_0^{\tau_{\max}}\tau d\tau\rho_\eta^2(\tau) \cdot\int_0^{v/v_T}\varsigma d\varsigma I_m\left[\frac{1}{\varepsilon(k,\omega)}\right]. \tag{8}$$

Under the assumptions that all ion charges are the same throughout the cluster and are constant during the Coulomb explosion, it is obvious that the self-stopping forces do not influence the evolution of the cluster structure. The equations (5) of motion are solved numerically for all ions in the cluster ($j = 1, 2, \ldots, 20$) subject to the set of the initial conditions $\boldsymbol{r}_j(0) = \boldsymbol{r}_{j0}$ characterizing the equilibrium structure of C_{20}, and with all the initial velocities in the CM frame being set to zero, $\dot{\boldsymbol{r}}_j(0) = 0$, based on the neglect of thermal vibrations of the constituent atoms.

Figure 1 shows several snapshots of the ion positions in the cluster CM frame at the penetration times $t = 0$, 5, 15, 25 fs for a C_{20} cluster entering a plasma target with $T = 2$ eV and $n = 10^{22}\,\mathrm{cm}^{-3}$ at the speed $v = 3v_T$. It is interesting that the C_{20} cluster structure evolves into a basket-like shape, which becomes increasingly elongated in the direction of motion with the increasing time as a direct consequence of the wake-potential asymmetry in the inter-ionic forces.

Figure 2 shows the influence of the cluster speed on the Coulomb explosion patterns after 25 fs in a plasma target with the density $n = 10^{22}\,\mathrm{cm}^{-3}$ and the electron temperature $T = 2$ eV. It can be seen that the Coulomb explosion proceeds faster in the longitudinal direction as the speed increases, whereas the transversal size is roughly insensitive to the increasing cluster speed.

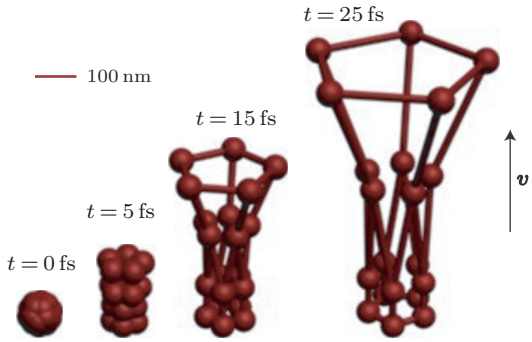


Fig. 1. Three-dimensional Coulomb explosion patterns of C_{20} in a moving frame of reference for penetration time $t = 0$, 5, 15, 25 fs with the cluster speed $v = 3v_T$, the plasma density $n = 10^{22}\,\mathrm{cm}^{-3}$ and the electron temperature $T = 2$ eV.

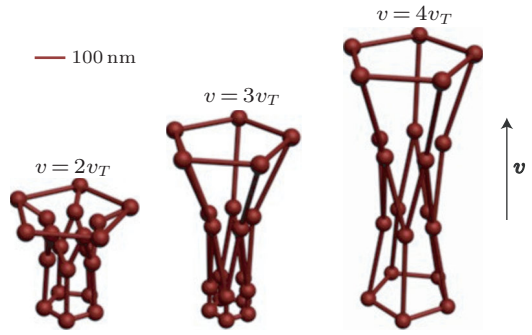


Fig. 2. Influence of various cluster speeds $v = 2v_T$, $3v_T$, $4v_T$, on the C_{20} Coulomb explosion patterns after 25 fs with the plasma density $n = 10^{22}\,\mathrm{cm}^{-3}$ and the electron temperature $T = 2$ eV.

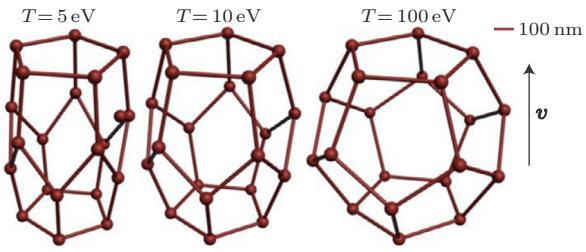


Fig. 3. Influence of plasma electron temperature on the C_{20} Coulomb explosion patterns after 25 fs in plasma with cluster speed $v = 3v_T$, the plasma density $n = 10^{22}\,\mathrm{cm}^{-3}$.

Finally, the effects of changing plasma temperature and plasma density are shown on the Coulomb explosion patterns after 25 fs for C_{20} moving at the speed $v = 3v_T$ through a plasma target with the density $n = 10^{22}\,\mathrm{cm}^{-3}$ in Fig. 3 and electron temperature $T = 2$ eV in Fig. 4. Figure 3 shows that, as the temperature decreases, the transversal expansion is hindered, when the temperature is high enough (see $T = 100$ eV), the C_{20} cluster tends towards a symmet-

ric sphere, whereas the longitudinal expansion of the cluster is roughly insensitive. Figure 4 shows that as the density decreases, the longitudinal and transversal expansion of the cluster are both promoted. Thus it follows that in classical, high-temperature and low-density plasmas, the Coulomb explosion patterns are very close to the spherically-symmetric, or isotropic expansion picture. On the other hand, in the limit of cold and dense plasmas, corresponding to the degenerate electron gas in solid targets, the explosion patterns are very much narrower and elongated in the direction of cluster motion.

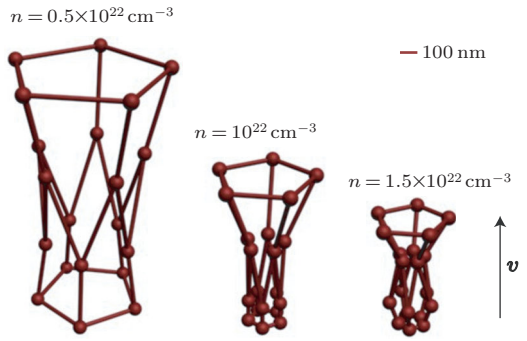


Fig. 4. Influence of various plasma densities on the Coulomb explosion patterns after 25 fs for C_{20} moving through a plasma target with cluster speed $v = 3v_T$, the electron temperature $T = 2\,\mathrm{eV}$.

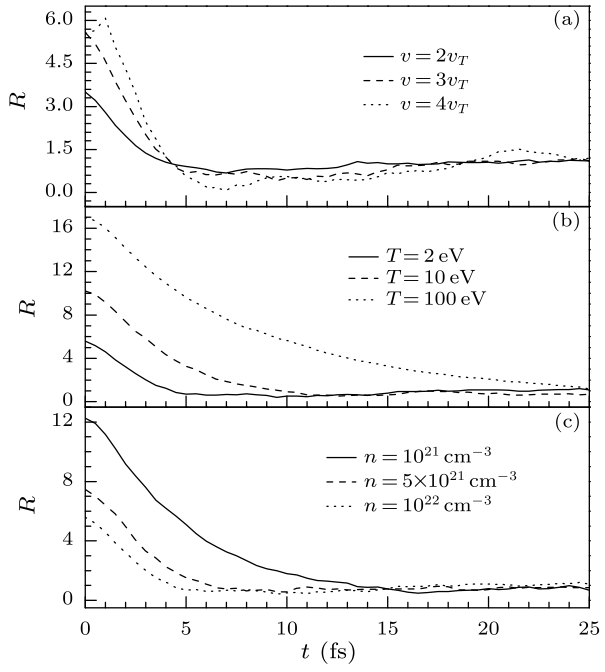


Fig. 5. Stopping power ratio R as a function of the penetration time t during the Coulomb explosion for a C_{20} cluster ion in a plasma target with the cluster speed $v = 3v_T$, the plasma density $n = 10^{22}\,\mathrm{cm}^{-3}$ and the electron temperature $T = 2\,\mathrm{eV}$.

In this work, the stopping power of the cluster ion can be obtained, assuming that the cluster moves in the z direction,

$$S_{cl}(v,t) = S_0(v) + S_v(v,t), \tag{9}$$

where $S_0(v) = -\sum_{j=1}^{20} F_s(v)$ is the contribution from the individual self-stopping forces, while $S_v(v,t) = -\sum_{j=1}^{20}\sum_{j\neq l=1}^{20} (\boldsymbol{F}_{jl})_z(\boldsymbol{r}_{jl},\boldsymbol{v})$ is the vicinage stopping power which describes interferences in the energy losses due to the spatial correlation among the constituent ions. In order to elucidate the magnitude of the interferences in the cluster energy losses due to the vicinage effect, we define the stopping ratio $R = 1 + S_0(v)/S_v(v,t)$.

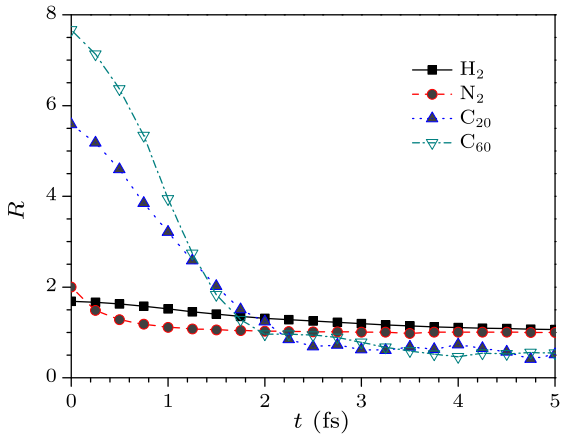


Fig. 6. Influences of different clusters on stopping power ratio R as a function of the penetration time t during the Coulomb explosion for H_2, N_2, C_{20} and C_{60} clusters in a plasma target with the same set of parameters as those used in Fig. 5.

Figure 5 shows the influences of stopping power ratio as a function of the penetration time for a C_{20} cluster moving through plasmas with the variation of (a) the projectile velocity $v = 2v_T$, $3v_T$, $4v_T$, (b) the electron temperature $T = 2\,\mathrm{eV}$, $10\,\mathrm{eV}$, and $100\,\mathrm{eV}$, (c) the plasma density $n = 10^{21}\,\mathrm{cm}^{-3}$, $5\times10^{21}\,\mathrm{cm}^{-3}$, and $10^{22}\,\mathrm{cm}^{-3}$, with a standard set of parameters $v = 3v_T$, $n = 10^{22}\,\mathrm{cm}^{-3}$, and $T = 2\,\mathrm{eV}$. One can see that in the very early stages of Coulomb explosions, the stopping ratio reaches quite high values, indicating that constructive interferences in the vicinage effect can drastically increase the energy losses when the constituent ions are still close to each other. In particular, this enhancement of the energy loss is greater for faster projectiles, lower plasma densities and higher electron temperatures. On the other hand, for prolonged penetration times t, the stopping ratio R approaches 1, indicating that the constituent ions of the cluster have moved so far away from each other in the course of the Coulomb explosion that they essentially behave as independent projectiles. Furthermore, we plot Fig. 6 to show the influences of the different clusters H_2, N_2, C_{20} and C_{60} respectively on the stopping power ratio R with the parameters set as follows: the projectile velocity $v = 3v_T$, the plasma density $n = 10^{22}\,\mathrm{cm}^{-3}$ and the electron temperature $T = 2\,\mathrm{eV}$. Numerical result shows the stopping power ratio reaches much higher values along with the increment of the cluster size in the early stage of the Coulomb explosion. This indicates that the constructive interferences in the vic-

inage effect can drastically increase the energy losses especially for large and heavy clusters.

We have used the MD methods to study the Coulomb explosion dynamics and the vicinage effects on the stopping power of swift C_{20} clusters in a dense plasma target. By solving the equations of motion for individual ions numerically, the Coulomb explosion patterns of fast C_{20} are studied. It shows that the clusters may undergo dramatic distortions in a plasma target. In particular, it is found that the C_{20} cage structure becomes increasingly elongated in the direction of cluster motion, for a range of cluster speeds, when the plasma density increases and its temperature decreases. In the opposite limit of hot and low-density plasmas, the shape of C_{20} tends to retain a spherical symmetry in the course of the Coulomb explosion. Regarding the vicinage effects on the cluster, energy losses exhibit a significant increase in comparison with the case of independent ions at the early stages of Coulomb explosion, when the constituent ions are still quite close to each other. For prolonged penetration times, vicinage effect on the energy loss diminishes and the cluster ions fly apart. In the intermediate penetration times, the stopping power ratio falls faster, showing that the cluster longitudinal elongation due to the wake effects. In comparison of the influences of several clusters (for H_2, N_2, C_{20} and C_{60} cluster respectively) on the stopping power ratio R, one can see that the constructive interferences in the vicinage effect can drastically increase the energy losses especially for large and heavy clusters.

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