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A Self-Consistent Study for the Laser-Induced Coulomb Explosion of Large Deuterium Clusters

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Abstract. The laser-induced Coulomb explosion of very large ($\sim 10^6 - 10^7$ atoms) deuterium clusters is studied self-consistently with one-to-one three-dimensional and two-dimensional fully relativistic particle-in-cell simulations. Naturally-occurring small-scale shock shells are observed and a technique to induce the formation of large shock shells inside a single cluster is proposed.

1. INTRODUCTION

Highly-energetic deuterium ions ($E \sim 100$ KeV), capable of driving fusion reactions, can be obtained from the violent Coulomb explosion occurring in deuterium clustered gases irradiated by ultra-short (pulse duration ~ 10-100 fs) and ultra-intense ($I > 10^{16}$ W/cm^2) laser pulses. The resulting ion energy is closely connected with the size of the clusters and, for ideal spherical clusters, the theoretical maximum ion energy attainable scales as the square of the initial radius, being $E_{\max}[\text{KeV}] \approx 6 n_0 [10^{22}\text{cm}^{-3}] R_0^2 [10\text{nm}]$: the explosion of large clusters (radius ~ 10-100 nm) opens the way to the copious production of fusion neutrons in very localized sources [1].

Depending on the clustered gas conditions, the size of the clusters, and laser pulse features, the laser-cluster interaction brings a huge variety of physical scenarios and leads to very rich and nonlinear phenomena, such as the formation of shock shells during the explosion of clusters with smooth (non-step-like) profiles [2], when the laser pulse is short and intense enough to expel all the electrons and leave a sphere of ions at-rest. These conditions are quite stringent, and not easily met by large clusters: description of shocks in this scenario requires a self-consistent treatment of the dynamics of electrons and ions in the laser field, the ionization dynamics, and the full dynamics of the explosion. We show that the electron dynamics plays an important role in the formation of the shocks for these conditions, and the shock shells are small scale, with the corresponding phase-space structure (a multiple-velocity spatial region) very tiny, so that the relative velocities inside the cluster are negligible. We show that the formation of large-scale shock shells is easily obtained using sequential laser pulses (e.g. a weak pulse followed by an ultra-intense one, with a proper time delay Δt).

2. COULOMB EXPLOSION OF VERY LARGE CLUSTERS

Resorting to the OSIRIS framework [3], we investigated the explosion of very large deuterium clusters self-consistently, by performing three-dimensional (3D) and two-dimensional (2D), massively parallel, fully relativistic, electromagnetic particle-in-cell (PIC) simulations. We have carried out simulations both in the nanoplasma approximation [4] (with the initial temperature set to zero for all particles) and including self-consistent field ionization (ADK ionization model [5]). No significant qualitative differences in the physical behavior (explosion dynamics, shock formation) have been observed, as long as the laser intensity is high enough ($I_{peak} > 10^{15}$W/cm^2).

We present results from 3D PIC simulations of the interaction of an ultra-intense laser pulse ($I_{peak} \sim 8 \times 10^{18}$ W/cm^2, pulse duration 35 fs full width at half maximum (FWHM), with an approximately Gaussian envelope and central wavelength $\lambda_0 = 820$ nm) with a spherical cluster of atomic deuterium (radius $R_0 = 32$ nm, uniform step-like radial density profile, $n_0 = 4.5 \times 10^{22}$ cm^{-3}). The simulation box is cubic, with side $L_{box} = \lambda_0$, discretized in a $336 \times 336 \times 336$ uniform spatial grid. We employ 4.75×10^6 particles per species, a value close to the actual number of atoms, for the configuration described.

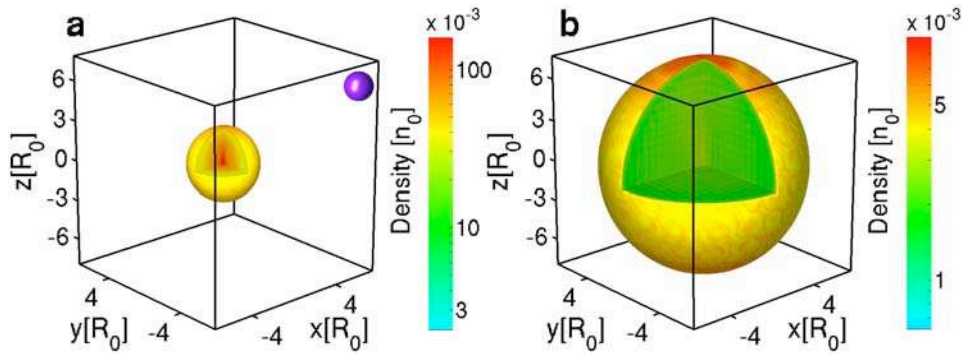

FIG. 1: Ion density distribution in configuration space at time t_a= 37 fs (a), and t_b= 75 fs (b), representing the density variation inside the ion cloud as well as on its outer shell (where the shock front is located). As a reference, a solid sphere having the initial size of the cluster is plotted in (a).

The time history of the ion density distribution (cf. Figs. 1, 2a) reveals the presence of a shock front at the cluster periphery, also showing the anisotropy of the explosion, due to the laser polarization. The electron dynamics in the very initial phase of the interaction has a crucial influence on the subsequent Coulomb explosion, as it is responsible for smoothing out the ion step-like profile, thus leading to the shock formation [2]. The shocks still occur naturally, even when the laser pulse duration is comparable with the time scale of the ion expansion, and the explosion does not start from a purely ion sphere.

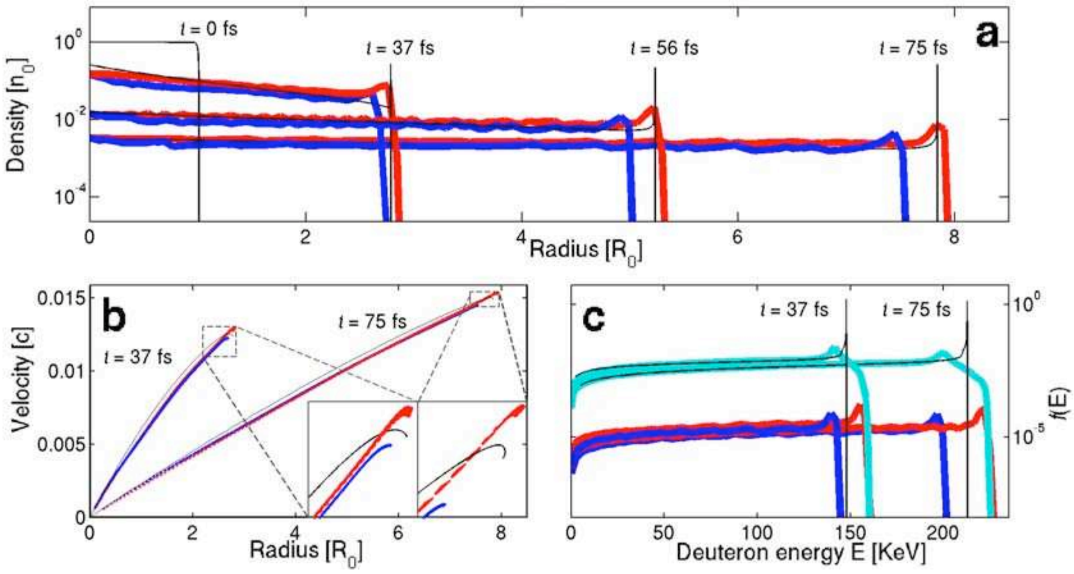

FIG. 2: Evolution of the ion density profile (a), $v_r - r$ phase space (b), and energy spectrum (c): thin black lines refer to the 1D theoretical model. Red and blue thick lines/dots are used for angular dependent quantities from the simulation results (blue for the y direction and red for the z direction, considering the particles contained in a solid angle ΩΩΩ0.035 sr). Cyan lines in (c) represent the total energy spectrum (integrated over the solid angle).

Figure 2b shows the formation and evolution of the shock shell, with the characteristic turning point in the ion $v_r - r$ phase space. The occurrence of a shock also affects the ion kinetic energy spectrum, causing it to peak at the maximum energy value (cf. Fig. 2c). The angular dependence of the energy distribution is a clear signature of the anisotropy induced by the laser field: higher ion energies are reached in the laser polarization direction, z. The numerical results (cf. Fig. 2) have been cross-checked by comparison with a simple 1D radial-symmetric electrostatic model for the Coulomb explosion, which takes into account the neutralizing effect of the electrons within the expanding cluster.

3. GENERATION AND CONTROL OF LARGE SCHOCK SHELLS

The ability to generate shock shells in the clusters opens many different directions [2], but it is also clear from single pulse simulations that only small-scale shells can be produced for realistic clusters, and laser pulses. This difficulty can be overcome, and large-scale shock shells produced, by using sequential laser pulses with different intensities, namely a weak pulse ($I \sim 10^{14} - 10^{16}$ W/cm^2) followed by an ultra-intense pulse ($I \sim 10^{18} - 10^{20}$ W/cm^2), with a proper time delay Δt. The first pulse creates the plasma and heats the electrons, so that a slow expansion, in the hydrodynamic regime, takes place and a smoothly-decreasing plasma density profile is naturally formed. The second laser pulse removes all the electrons from the dense cluster core, causing it to explode violently, with the inner ions overrunning the slowly-expanding outer ions, thus forming a large shock shell, with considerable relative velocities inside the cluster. Our calculations indicate that, with the cluster sizes considered here, collision energies up to 100 KeV are attainable. The main features of explosion dynamics (maximum ion kinetic energy, location of the peak in the ion energy spectrum, radial extension of the shock shell, magnitude of the relative velocities inside the cluster) can be controlled in detail by varying the delay, Δt, between the two pulses, and the intensity of the laser pulses. An experimental confirmation for the occurrence of shocks in clusters can be obtained through the detection of time-resolved fusion-neutron bursts long before the time needed for inter-cluster collisions. Figure 3 shows the ion $v_r - r$ phase space from a 2D simulation, in which a rod-like cluster plasma (with the same particle density and radius as in the 3D case discussed above) is first heated by a weak laser pulse ($I_{peak} \sim 5 \times 10^{15}$ W/cm^2, pulse duration 35 fs, $\lambda_0 = 820$ nm) and then torn apart by a second ultra-intense pulse ($I_{peak} \sim 10^{19}$ W/cm^2, pulse duration 20 fs, $\lambda_0 = 820$ nm), demonstrating the behavior predicted.

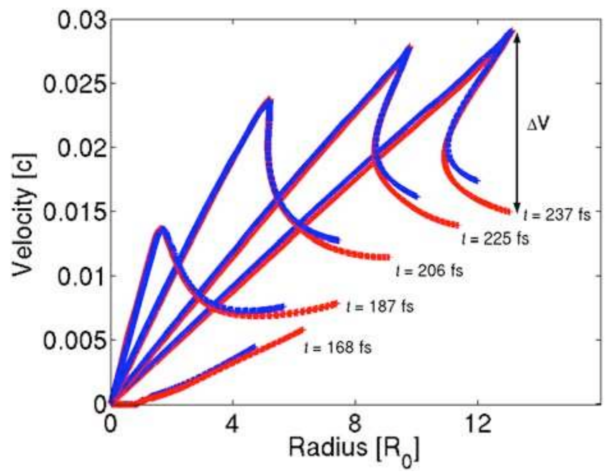

FIG. 3: Evolution of the ion phase-space profile. Blue dots refer to the *x* direction and the red lines to the laser polarization direction, *y*, considering the particles contained in an angle $\approx\approx \approx 0.1$ rad. ΔV corresponds to ~ 200 KeV.

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