

# High Energy Ions Produced by the Interaction of Ultra-Short Laser Pulses with Atomic Clusters

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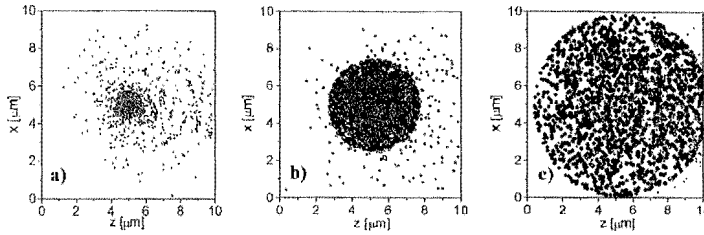
We report on simulations of atomic cluster explosions upon interaction with high-intensity femtosecond laser pulses. By using a 3D fully relativistic PIC code we investigate the dynamics of hydrogen and argon cluster explosions providing information about the time-resolved ion energy spectrum, for different laser intensities. Results indicate that MeV ions are produced through Coulomb explosion of the atomic clusters and the possibility of capturing most of these ions with a specially designed magnetic focusing system is discussed. The results are relevant to the production of high-energy ion collimated sources.

The interaction of laser pulses with atomic and molecular clusters has become a subject of great interest. Recent experiments show that the interaction of short (<ps), intense ( $\sim 10^{17}$  W/cm<sup>2</sup>) laser pulses with rare gas clusters is responsible for the production of highly energetic electrons and ions [1, 2], X-ray emission in the keV range [3], coherent high-harmonic generation [4], plasma waveguide formation [5] and applications to nuclear fusion [6].

The cluster expansion mechanism can be described using either a hydrodynamical model or a Coulombic repulsion model, depending on the laser intensity and pulse duration as well as on the cluster size and charge state. In the hydrodynamic regime, dominant for lower ( $< 10^{17}$  W/cm<sup>2</sup>) intensities and longer pulses, the electrons are held in the cluster via space-charge attraction from neighboring ions and the cluster is heated to very high temperatures [1]. Pressure build-up within the core causes the cluster to expand hydrodynamically. Ion energies up to 1 MeV have been achieved [1]. In the Coulombic regime, dominant for ultra-intense ( $> 10^{17}$  W/cm<sup>2</sup>), ultra-short (<150fs) laser pulses, a sufficient number of electrons are expelled by the laser from the cluster core, leaving behind a positively charged droplet which explodes due to electrostatic repulsion. Also, Coulomb explosions occur preferentially for smaller clusters and produce the most energetic ions (1 MeV) [2].

Numerical models using particle dynamics have been proposed to describe the Coulomb mechanism [7, 8], although requiring substantial computational resources and being unable to account for large number of atoms. A fluid description [9] cannot provide such a detailed insight of the process. To circumvent these limitations we present a novel approach to accurately describe the dynamics of laser-cluster interaction by using a Particle-in-Cell (PIC) code, determining for each time step the position, momentum and energy of the particles under the influence of both the external laser field and the fields generated by the particles themselves, for a very large number of particles and within reasonable computational times.

We use the fully relativistic 3D PIC code KARAT to model the interaction of an ultra-short (30 fs gaussian laser pulse), high-intensity ( $10^{17}$ -  $10^{20}$  W/cm<sup>2</sup>), 800 nm plane wave with

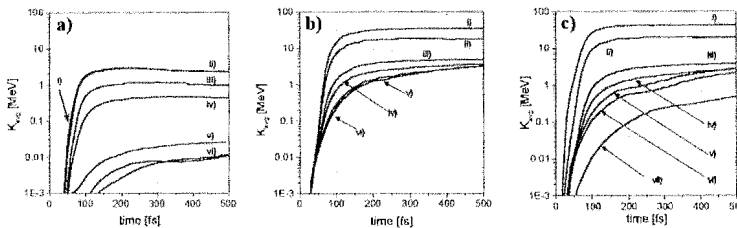


**Figure 1.** Dynamics of cluster expansion for  $I=10^{20}$  W/cm<sup>2</sup> at a)  $t=50$  fs, b)  $t=100$ fs and c)  $t=150$  fs. The ions are depicted in black and the electrons in grey. The laser pulse is plane polarised in the x-axis, propagates along z and is injected from left to right, centred with the simulation box.

a 1  $\mu\text{m}$  diameter plasma sphere of either hydrogen or argon with  $n_i = 5 \times 10^{21}$  cm<sup>-3</sup> and placed in the center of the simulation region. Each cluster is treated as a pre-formed microplasma, the hydrogen cluster being mono-ionized, H<sup>+</sup>, and the argon cluster having either a constant average charge, Ar<sup>9+</sup>, or a different charge according to the laser intensity under study, namely Ar<sup>4+</sup> for  $1 \times 10^{17}$  W/cm<sup>2</sup>, Ar<sup>7+</sup> for  $5 \times 10^{17}$  W/cm<sup>2</sup>, Ar<sup>8+</sup> for  $10^{18}$ - $10^{19}$  W/cm<sup>2</sup>, Ar<sup>10+</sup> for  $5 \times 10^{19}$  W/cm<sup>2</sup> and Ar<sup>13+</sup> for  $1 \times 10^{20}$  W/cm<sup>2</sup>. Different charge states of argon were determined through 2D laser-gas interaction simulations using the ADK optical ionization model [10] and assuming that only the first 25% of the laser pulse are responsible for ionizing the cluster. Our simulation box is  $10\mu\text{m} \times 10\mu\text{m} \times 10\mu\text{m}$  containing  $45 \times 45 \times 90$  cells (x y z).

As the laser reaches the cluster, the electrons begin to oscillate transversally in the E-field of the laser and longitudinally via the  $e[\mathbf{v} \times \mathbf{B}]$  force; ponderomotive blowout in the transverse direction causes electron expulsion from the cluster core. Due to their greater mass, the ions do not respond significantly to the laser field [11]. As the electrons are expelled, a net positive charge builds up inside the cluster, resulting from the ions which were left behind; the cluster undergoes a Coulombic explosion and the ions expand isotropically (figure 1), gaining energies that range from 0.011 to 3 MeV for H<sup>+</sup>, 3 to 33 MeV for Ar<sup>9+</sup> and 0.49 to 42 MeV for Ar<sup>4+</sup> and Ar<sup>13+</sup>, respectively, for laser intensities varying from  $10^{17}$  to  $10^{20}$  W/cm<sup>2</sup> as shown in figures 2a), b) and c). At the initial stages of the explosion, the ions gain a large amount of energy during a short ( $\sim 50$  fs) interval of time, due to Coulomb repulsion, however, as the cluster expands, the separation between neighboring ions will increase and thus the energy gain will not be so dramatic. Eventually, the ions will be so far separated that Coulomb repulsion has little contribution to the energy curve that reaches a saturation value.

We have also looked at the current distribution throughout the explosion. Figure 3 indicates the maximum current observed in our simulations, for the case of the hydrogen cluster irradiated at  $10^{20}$  W/cm<sup>2</sup>. Again, due to isotropy, current yields are similar in all



**Figure 2.** Average ion energy as a function of time for laser intensities of: i)  $1 \times 10^{20}$  W/cm<sup>2</sup>, ii)  $5 \times 10^{19}$  W/cm<sup>2</sup>, iii)  $1 \times 10^{19}$  W/cm<sup>2</sup>, iv)  $5 \times 10^{18}$  W/cm<sup>2</sup>, v)  $1 \times 10^{18}$  W/cm<sup>2</sup>, vi)  $5 \times 10^{17}$  W/cm<sup>2</sup> and vii)  $1 \times 10^{17}$  W/cm<sup>2</sup>. a) for a H<sup>+</sup> cluster b) for an Ar<sup>9+</sup> cluster and c) for an Ar<sup>n+</sup> cluster with charge states of 4<sup>+</sup>, 7<sup>+</sup>, 8<sup>+</sup>, 10<sup>+</sup> and 13<sup>+</sup> for the vii), vi), v) through iii), ii) and i) cases respectively. Difference in energy yields for the simple Ar<sup>9+</sup> case is due to the difference in charge states.

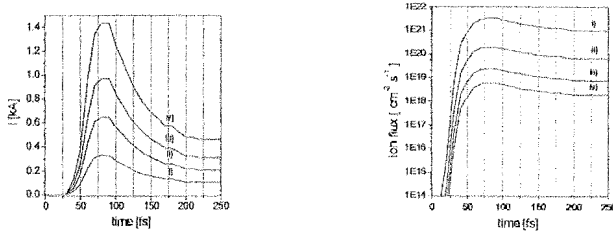


Figure 3. (left) Maximum current observed for the case of a H cluster explosion irradiated at  $10^{20}$  W/cm<sup>2</sup>, corrected for collection angles of i)  $\pm 5^\circ$ , ii)  $\pm 10^\circ$ , iii)  $\pm 15^\circ$  and iv)  $\pm 22.5^\circ$ . Figure 4. (right) Ion flux observed for the case of a H cluster explosion irradiated at  $10^{20}$  W/cm<sup>2</sup>. These values pertain to the collimated ion beam with radius indicated in figure 5 and for collection angles of i)  $\pm 5^\circ$ , ii)  $\pm 10^\circ$ , iii)  $\pm 15^\circ$  and iv)  $\pm 22.5^\circ$ .

directions. At the early times of the explosion we observe a rapid increase of the current due to the acceleration of the ions resulting from Coulomb repulsion, followed by a decrease explained by the fact that although the energy of the ions has reached a saturation value, as stated previously, the cluster is still expanding. Eventually these effects cancel out and a saturation value is reached. Peak current yields varying from 0.31 kA to 1.44 kA are observed. Our simulations also indicate the current pulse duration to be around 100 fs.

To investigate the possibility of producing a high-energy collimated ion source we have designed a point-to-parallel focusing system, composed by a set of three quadrupole magnets, based on the standard thin-lens approximation to calculate the dimensions of the system as well as the magnetic fields required [12]. This magnetic focusing system ensures the production of a circular cross-section collimated ion beam obtained from a point source, such as our cluster. We take the example of a hydrogen cluster irradiated at  $10^{20}$  W/cm<sup>2</sup> and assume the ions to have an energy of 3 MeV, as our simulations indicate. We consider the collection angle of the ions to be  $\pm 5^\circ$ ,  $\pm 10^\circ$ ,  $\pm 15^\circ$  and  $\pm 22.5^\circ$ , thus collecting all particles that emerge from a cone centered with the cluster and with apertures of  $10^\circ$ ,  $20^\circ$ ,  $30^\circ$  and  $45^\circ$  respectively. The design can easily be extrapolated for different collection angles, as well as for the case of the argon cluster explosion, with only a few changes in the parameters. As can be seen from figure 4 and figure 5, collimated ion beams of radius ranging from 6.5 mm to 151.5 mm and fluxes from  $3.0 \times 10^{21}$  cm<sup>-2</sup> s<sup>-1</sup> to  $5.6 \times 10^{18}$  cm<sup>-2</sup> s<sup>-1</sup> for collection angles of  $\pm 5^\circ$  to  $\pm 22.5^\circ$ , respectively, can be obtained with reasonable magnetic fields, so that the whole system can readily be assembled with commercially available components.

Finally, we also present a new concept for using the energetic particles generated via laser-cluster interaction for the study of Inertial Fusion Energy based on our simulation results. We consider a general direct drive scheme. A shell of frozen DT is surrounded by an ablator, solid clusters are held inside the pellet (or on the periphery) and a near vacuum spacing exists

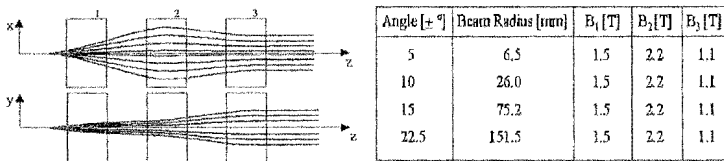


Figure 5. Magnetic focusing system design. The quadrupoles 1, 2 and 3 are placed at a convenient distance from the exploding cluster, depending on the collection angle. Some of the cluster ion trajectories are depicted. A collimated ion beam with a circular cross-section is obtained after the last quadrupole, the overall system length, measured from the cluster position, varying from 13 cm to 64 cm, also depending on the collection angle.

between DT fuel and cluster. In the first step, laser interaction with the ablator produces plasma and the DT fuel is compressed due to high ablation pressure as in the conventional direct drive. In the second step, a second laser beam bores a hole through the expanding coronal plasma. Finally a synchronized Ignition Laser (IL) beam at high intensity channels through the plasma and interacts with the clusters, when the density of the compressing DT fuel is approaching optimum value. Ignition beam can be made to directly interact with the cluster by appropriately modifying the target design. Details of this proposal such as cluster size, density, positioning of the cluster, laser parameters and target designs for optimizing the ignition condition are being worked out and will be presented elsewhere.

In conclusion, we have studied the possibility of manufacturing a high-current, high-energy collimated ion beam source produced via laser-cluster interaction. By using standard off-the-shelf components it is possible to obtain a 3 MeV, 6.5 mm radius parallel ion beam of around 100 fs pulse duration with peak fluxes of  $3.0 \times 10^{21} \text{ cm}^{-2} \text{ s}^{-1}$  and peak currents as high as 1.4 kA. For our parameters, Coulombic explosion is the mechanism responsible for cluster expansion. Moreover, with increasing laser intensity, the expansion approaches the pure electrostatic repulsion case, when all electrons are removed from the cluster core. We have investigated the spatial distributions and energy of the ejected ions and found that the particles have typical energies of 3 MeV for hydrogen, 33 MeV for  $\text{Ar}^{9+}$  and 42 MeV for  $\text{Ar}^{11+}$  at the highest intensities used, and, in the tail of the energy distribution function, for  $10^{20} \text{ W/cm}^2$ , particles with energies up to 7 MeV, 130 MeV and 210 MeV, respectively, are generated.

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