§19. Molecular Dynamics Simulation of Proton Beam Acceleration by Ultra-Intense Laser from Carbon Nanotubes

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Ultra intense laser of 10^{18} W/cm^2 at 800 nm wavelength (Ti sapphire laser) can produce well collimated and mono-energetic proton beams of several MeV in energy. This is realized when it is radiated to hydrogen pellets embedded inside of a nanometer-size cylindrical cage called carbon nanotube [1,2]. Such high energy protons can be applied to medical therapy including cancer treatment and high resolution engineering measurements.

Basic properties of such accelerated proton beam are predicted using analytical theory if the carbon cage remains intact. However, in reality any nano-scale molecular structures are subject to destruction under ultra-intense laser. In order to establish quantitatively the possibility of proton acceleration under such conditions, we have performed molecular dynamics simulations.

Since electrostatic interactions by Coulomb forces need to be calculated as accurately as possible, usual PIC (particle-in-cell) numerical technique which smears out forces in space grids cannot be utilized. Instead, we use the molecular dynamics technique [3,4] in which the Newton equations of motion are solved exactly for many number of charged particles for i= 1,.., N, typically with N= 500,000.

Here, on the righthand side of Eq.(1), the first term is the Coulobmic forces and the second term is the Lennard-Jones force, with

$$m_i \frac{d\mathbf{v}_i}{dt} = -\nabla \left[\sum_j \left\{ \frac{q_i q_j}{\left|\mathbf{r}_i - \mathbf{r}_j\right|} + \Phi_{LJ}(\mathbf{r}_{ij}) \right\} \right] + \mathbf{E}(t)$$

$$\frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i, \ \Phi_{LJ}(\mathbf{r}_{ij}) = \varepsilon_{ij} \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right]$$

$r_{ij} = \left|\mathbf{r}_i - \mathbf{r}_j\right|$ is the distance between i-th and j-th particles. The Lennard-Jones force provides the binding force between carbon atoms of the carbon nanotube. The third term is the laser electric field, which has the form of either sinusoidal $\mathbf{E} = \mathbf{E}_0 \sin \omega t$, or a Gaussian pulse with $\mathbf{E} = \mathbf{E}_0 \exp[-\{(t-t_0)/\tau\}^2] \sin \omega t$.The period of 800 nm electromagnetic waves is 2.7 fs. The spatial variation of the wave field is not taken into account since the wavelength is much longer than the system size.

In the simulation light electrons are blown off in a couple of wave periods by the intense laser field, and the cage carbon atoms and pellet hydrogen get positively charged. Strong repulsion between positive ions provides extremely large acceleration forces, and protons are squeezed out of the carbon nanotube. At the same time, carbon ions with (+6e) are affected by the strong repulsion and the cage itself falls apart. Thus, the time race between diffusion of protons and carbon nanotube set the maximum to the proton beam speed. Figure 1 shows the generation of proton beam for the case where the polarization of the applied laser electric field is parallel to the carbon nanotube axis.

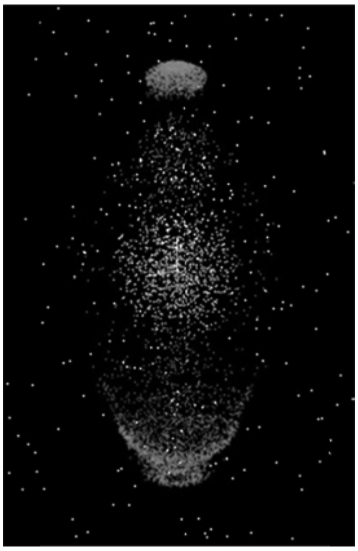

Fig1.Accelerated protons (two caps) above and below the carbon nanotube in 15 fs after the application of ultra-intense laser electric field.

1. M. Murakami and M. Tanaka, Applied Phys. Letters, 102, 163101 (2013).
2. Editorial article in Physics Today (American Physical Society, 2013).
3. M. Tanaka and M. Sato, J. Chem. Phys. vol.126, 034509 (2007).
4. M.Murakami and M.Tanaka, Phys.Plasmas, 15, 082702 (2008).