§13. Molecular Dynamics Simulations of Proton Nanotube Accelerators by Au Guard Cells

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The proton accelerator is an interesting problem by principle, and it becomes quite crucial in non-neutral applications of high-energy intense lasers[1,2].

We are following an exact simulation of N bodies because of rapid expanding protons and also electrons, not like standard particle-in-cell simulations. However, its cost becomes huge as the N^2 terms are pairwise. Previously, it was only few thousand particles used in a nanocluster, but we should devise a clever method to deal with 500,000 molecular dynamics simulation.

Methodology

One does the exact N-body molecular dynamics simulation, on the RHS with the Coulomb and 12-6 Lennard-Jones potentials and the laser electric field,

$$m_i \frac{d\mathbf{v}_i}{dt} = -\nabla \sum_j \left[\frac{q_j q_i}{r_{ij}} + 4\varepsilon_{LJ} \left\{ \left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right\} \right] + \mathbf{E}_p(\omega).$$

We have protons, C (carbon) and Au (gold) ions and electrons in a nanotube; the gold ions are used to protect carbon atoms. The charge states are H(+1), C(+6), and Au(+Z) where the gold ion depends on the state Z= 5, 10, 20, 40 or 60. Electrons are single states, but the pseudo $-Z_e$ electrons are used for a computational time. All units are all realistic expect for the proton mass ratio $m_p / m_e = 100$.

We have to impose a cutoff radius that is 10 Angstrom in three dimensions[3]; the cutoff on the average is 15 Angstrom in $3\times3\times3$ cutoff meshes. Beyond each of the $300\times300\times500$ Angstrom distance from the origin (nanotube), a particle is free to expand in infinity.

Three-Dimensional Molecular Dynamics

The Au ionization state is a semi-logarithmic law versus the laser intensity in Fig.1; it is assumed to be the 5th and 60th states at 10^{15}W/cm^2 and 10^{21}W/cm^2, respectively.

For the 800 nm laser field (ruby-sapphire laser), we specify the electric field with the sinusoidal form, where the electric field points the **x**-direction; the short pulse field has the Gaussian shape. This means that the wave pulse takes 7.8fs before it reaches the origin, and the same time to decay. We are dedicated to have any form – x, z, or 2D (ellipsoid) shape, but we have known that the degree of acceleration is optimum in the *z* (axial) direction; for this reason we will show details below.

Figure 2 depicts the energy maximum of proton acceleration $E_{\max}$, which occurs mainly along the *z* direction. It turns out to be a logarithmic scaling, $E_{\max} \propto \log(\mathrm{W/cm^2})$; the maximum intensity of the proton E_{max} is 200 times, or their velocity V_{max} is 14 times, for the laser intensity of 10^6 increase.

The pulse is changed as sinusoidal $\sin(kz - \omega t)$, but the increase of protons is only 10% in magnitude because most of electrons diffuse away from the nanotube. Contrarily, because of the mass of 197m_p, the gold ions are expanding slowly at the origin.

However, the velocity of protons is better estimated at real mass (m_p/m_e=1836). It is whether the proton acceleration can be intensified at different geometries, or the magnetic field may be limited at a high intense case.

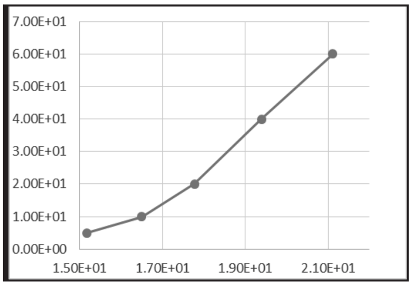

Fig.1 The ionization state of Au (from 5 to 60 states) versus field intensity from 10^{15} to 10^{21}W/cm^2.

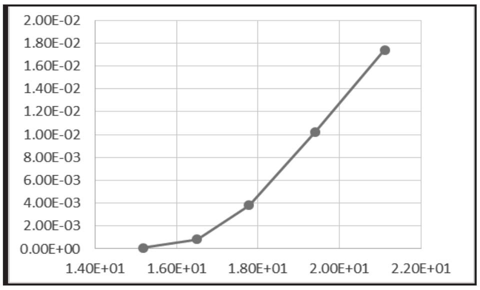

Fig.2 Energy maxima of accelerated protons in v^2/c^2 where the gold ions are still staying around the origin.

1. M.Murakami and M.Tanaka, Appl. Phy. Lett., **102**, 163101 (2013).
2. Proton beams from a nanotube accelerator, Physics Today (AIP, 2013). *http://www.physicstoday.org/*
3. M.Tanaka and M.Sato, J. Chem. Phys. **126**, 034509 (2007).